

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040122\
 Data File : VN071780.D
 Acq On : 02 Apr 2022 02:58
 Operator : JC\MD
 Sample : N2222-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-19

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_N\methods\82N033022W.M
 Title : SW846 8260

Signal : TIC: VN071780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	36	45	60	rBV3	130793	511501	15.00%	2.286%
2	2.440	70	77	85	rVB	105386	172034	5.05%	0.769%
3	3.134	188	195	204	rVB	90860	206188	6.05%	0.921%
4	3.522	250	261	273	rVB5	13656	43223	1.27%	0.193%
5	4.581	433	441	449	rBV2	14269	40222	1.18%	0.180%
6	5.081	514	526	532	rBV5	10013	34724	1.02%	0.155%
7	5.363	563	574	590	rBV2	32882	121628	3.57%	0.544%
8	5.616	603	617	636	rBV	115315	399198	11.71%	1.784%
9	7.151	868	878	886	rVB2	25148	71211	2.09%	0.318%
10	7.686	960	969	981	rBV2	43608	119440	3.50%	0.534%
11	8.022	1014	1026	1031	rBV	410391	997234	29.25%	4.456%
12	8.086	1031	1037	1048	rVV	779655	1812999	53.18%	8.102%
13	8.439	1088	1097	1109	rBV2	479417	1325540	38.88%	5.924%
14	8.963	1177	1186	1200	rBV	1151222	2414484	70.82%	10.790%
15	9.457	1258	1270	1278	rBV4	37621	101004	2.96%	0.451%
16	10.439	1428	1437	1445	rBV	1850929	3409207	100.00%	15.235%
17	10.639	1463	1471	1477	rVB7	17102	42598	1.25%	0.190%
18	11.127	1548	1554	1560	rVB3	20417	40744	1.20%	0.182%
19	11.745	1650	1659	1670	rBV	1725549	3153205	92.49%	14.091%
20	11.839	1670	1675	1682	rVV	80298	137762	4.04%	0.616%
21	11.957	1686	1695	1711	rVB	59170	125065	3.67%	0.559%
22	12.580	1794	1801	1805	rBV2	25364	42940	1.26%	0.192%
23	12.727	1819	1826	1838	rBV	1257366	2173018	63.74%	9.711%
24	12.916	1852	1858	1865	rBV	53633	90872	2.67%	0.406%
25	13.016	1865	1875	1879	rVV	42703	79814	2.34%	0.357%
26	13.216	1903	1909	1916	rBV	112498	186897	5.48%	0.835%
27	13.363	1928	1934	1944	rVB	196411	326166	9.57%	1.458%
28	13.674	1979	1987	1999	rBV	1378047	2547732	74.73%	11.385%
29	13.833	2009	2014	2017	rBV	50976	82481	2.42%	0.369%
30	13.874	2017	2021	2026	rVV	109686	181089	5.31%	0.809%
31	13.910	2026	2027	2037	rVB3	25082	41862	1.23%	0.187%
32	14.063	2047	2053	2058	rBV	34585	55553	1.63%	0.248%
33	14.127	2059	2064	2067	rBV	44675	72164	2.12%	0.322%
34	14.215	2073	2079	2084	rVB	86354	136927	4.02%	0.612%
35	14.321	2092	2097	2104	rVB2	105731	184627	5.42%	0.825%
36	14.457	2114	2120	2125	rVB	35689	54842	1.61%	0.245%

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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

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Title : SW846 8260

37	14.539	2128	2134	2137	rBV	74984	132906	3.90%	0.594%
38	14.574	2137	2140	2146	rVB	99989	145441	4.27%	0.650%
39	14.810	2174	2180	2185	rBV	46559	80724	2.37%	0.361%
40	14.927	2192	2200	2207	rBV2	141226	299474	8.78%	1.338%
41	15.192	2237	2245	2249	rBV3	26090	57403	1.68%	0.257%
42	15.310	2256	2265	2272	rVB5	31981	76867	2.25%	0.344%
43	15.504	2292	2298	2305	rBV	26180	48434	1.42%	0.216%

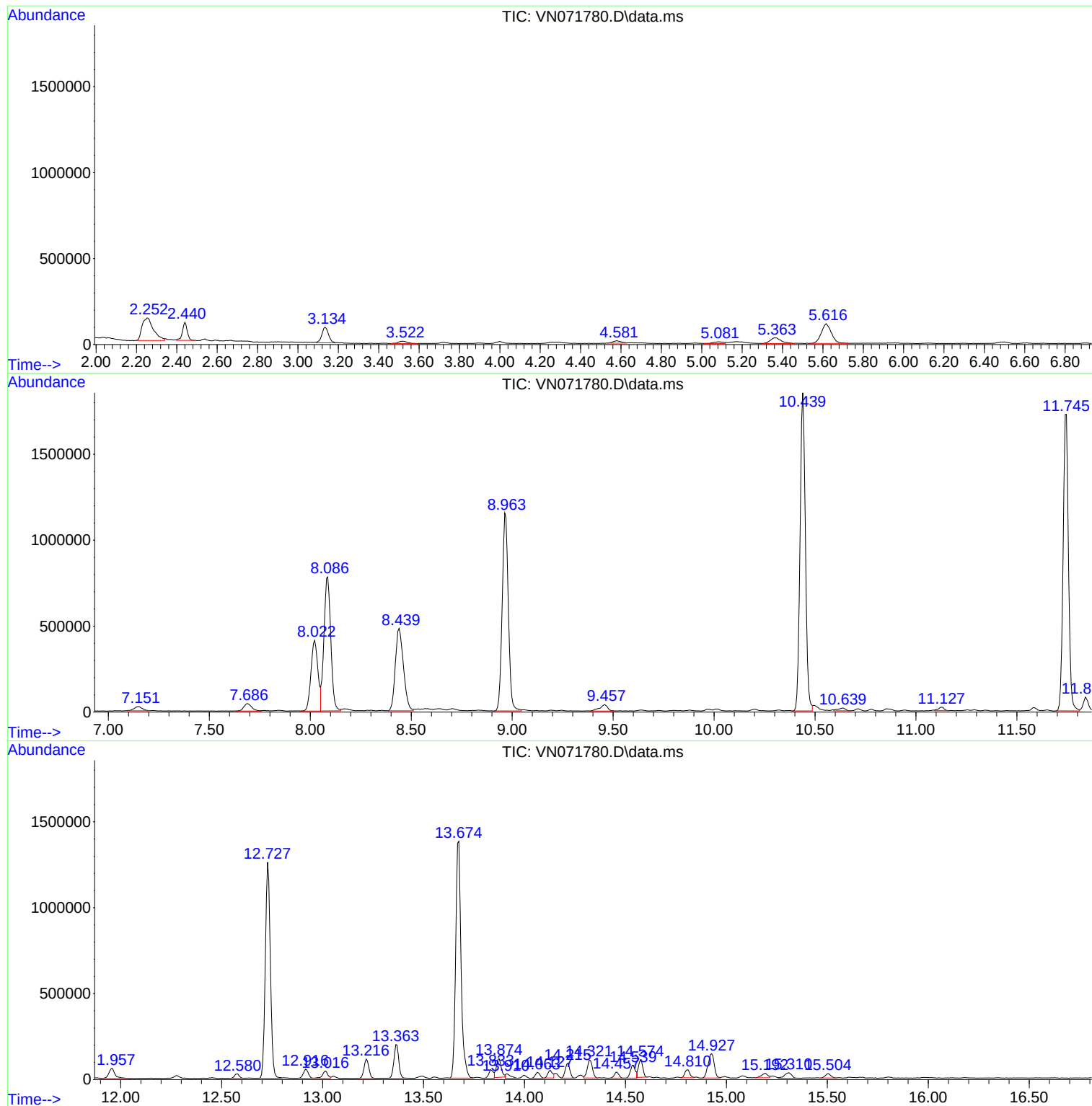
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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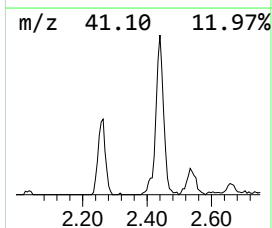
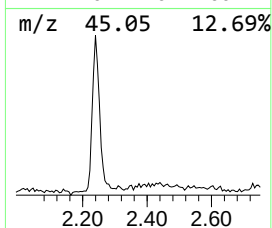
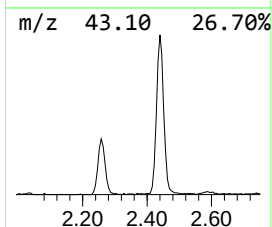
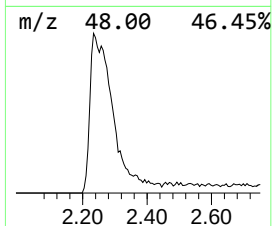
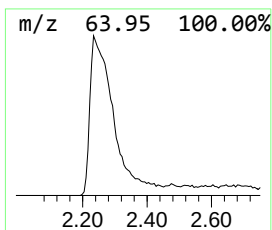
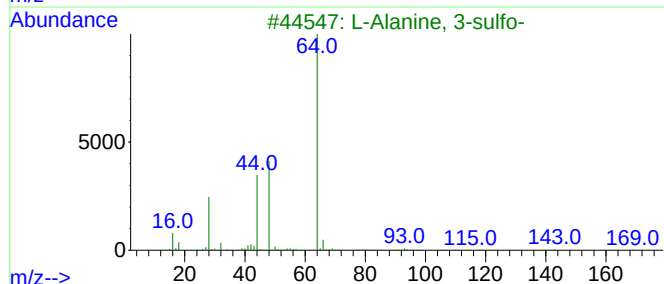
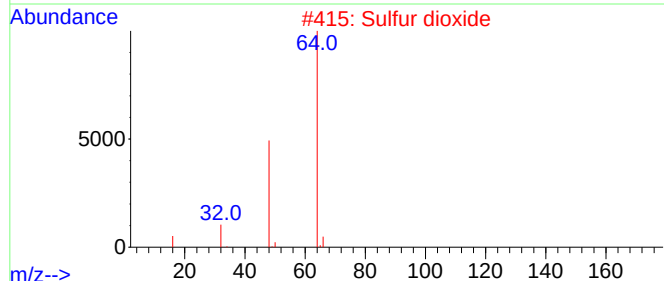
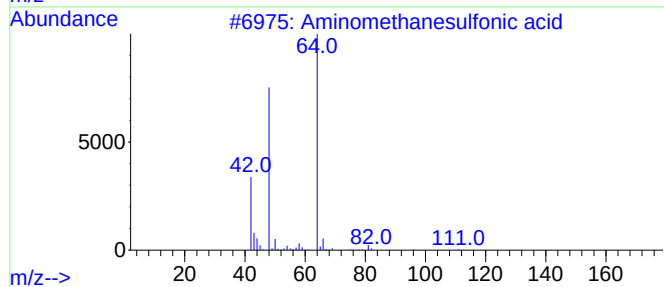
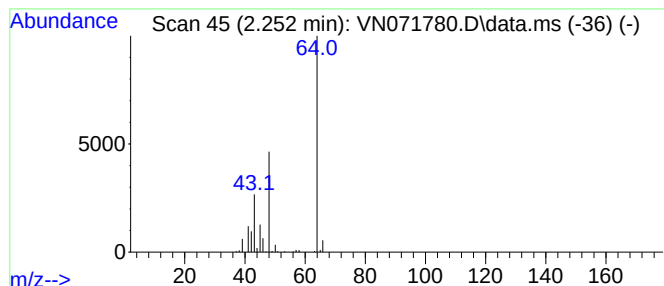
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	14.11 ug/l	511501	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	78
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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ALS Vial : 41 Sample Multiplier: 1

Instrument :
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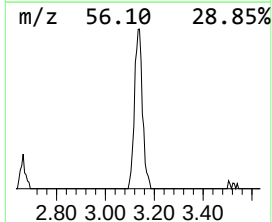
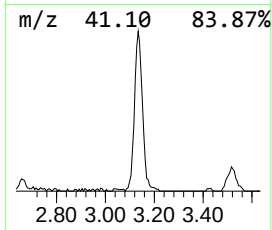
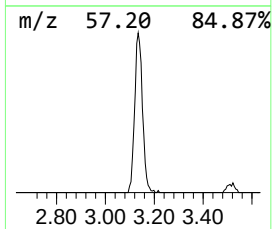
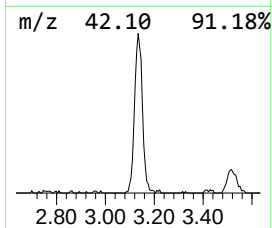
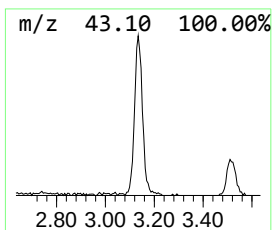
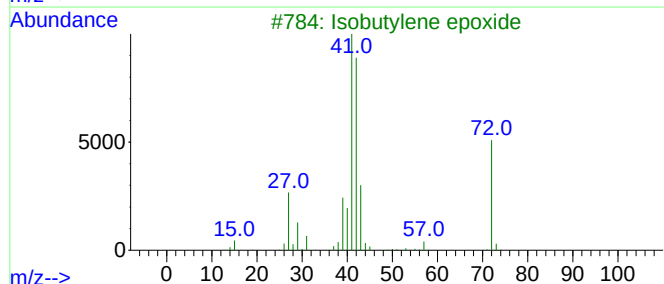
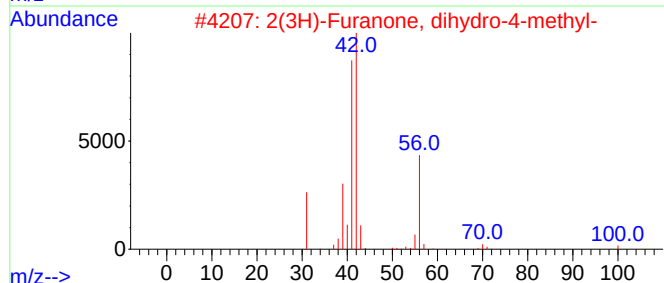
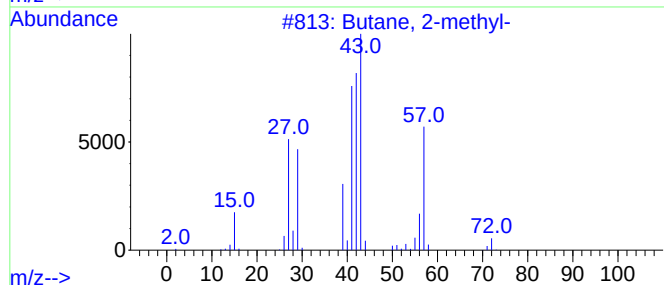
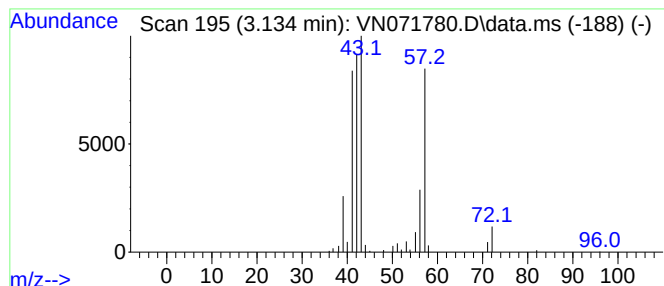
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Peak Number 2 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	5.69 ug/l	206188	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	80
2			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	40
3			Isobutylene epoxide	72	C4H8O	000558-30-5	38
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
5			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33



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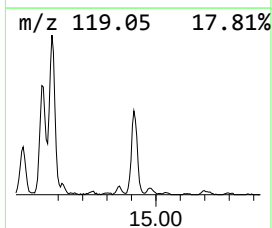
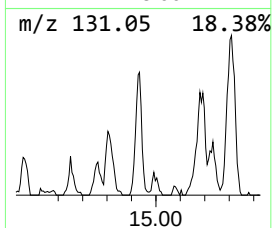
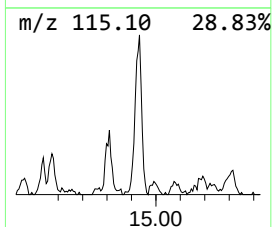
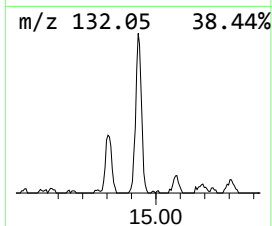
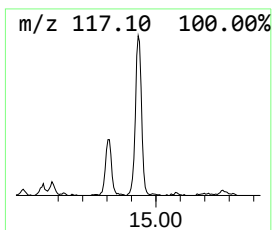
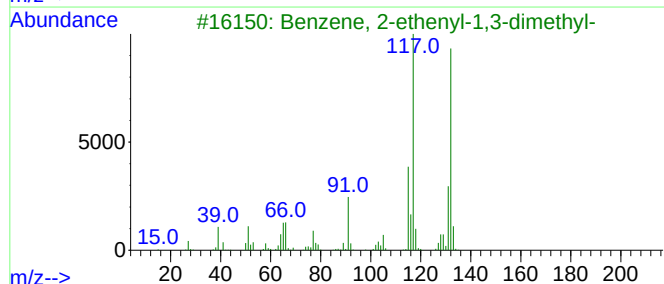
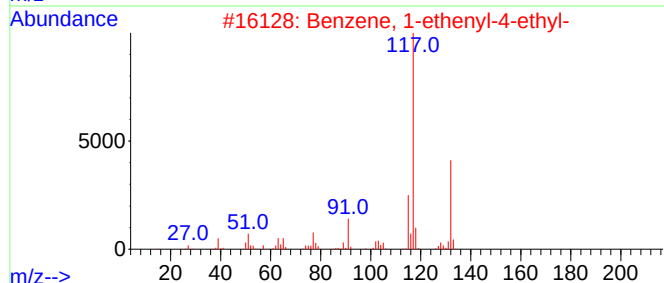
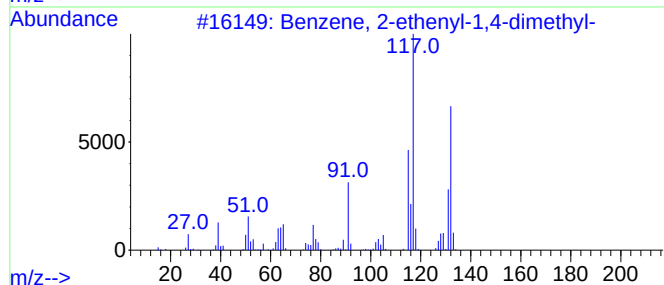
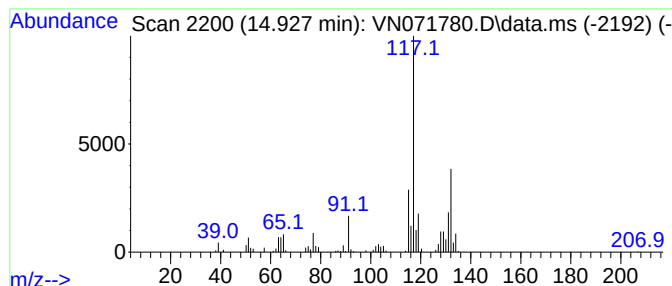
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.927	5.88 ug/l	299474	1,4-Dichlorobenzene-d4			13.674
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-		132	C10H12	002039-89-6	93
2	Benzene, 1-ethenyl-4-ethyl-		132	C10H12	003454-07-7	90
3	Benzene, 2-ethenyl-1,3-dimethyl-		132	C10H12	002039-90-9	87
4	Benzene, (2-methyl-2-propenyl)-		132	C10H12	003290-53-7	87
5	Benzene, 1-methyl-2-(2-propenyl)-		132	C10H12	001587-04-8	83



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	2.252	14.1	ug/l	511501	1	8.086	1813000	50.0
Butane, 2-methyl-	3.134	5.7	ug/l	206188	1	8.086	1813000	50.0
Benzene, 2-ethe...	14.927	5.9	ug/l	299474	4	13.674	2547730	50.0