

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
 Data File : VN083825.D
 Acq On : 12 Sep 2024 12:08
 Operator : JC\MD
 Sample : P3913-08
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 9424-D-F-82924-D

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\82N091024W.M
 Title : SW846 8260

Signal : TIC: VN083825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.077	17	21	40	rVB	75984	163956	9.45%	0.856%
2	2.289	51	57	72	rVB3	41327	115789	6.68%	0.604%
3	2.659	114	120	137	rVB	132614	251055	14.47%	1.310%
4	2.812	141	146	149	rBV5	11478	23831	1.37%	0.124%
5	3.189	206	210	220	rVB6	6754	17556	1.01%	0.092%
6	3.512	257	265	274	rVV3	8469	21214	1.22%	0.111%
7	3.824	311	318	329	rVB3	7583	21261	1.23%	0.111%
8	4.283	383	396	411	rBV	120845	381004	21.97%	1.988%
9	4.424	412	420	443	rVB	135311	420353	24.24%	2.193%
10	4.730	461	472	486	rBV2	30664	117640	6.78%	0.614%
11	6.136	700	711	727	rBV2	20093	69159	3.99%	0.361%
12	6.736	806	813	825	rVB4	26863	86490	4.99%	0.451%
13	7.224	885	896	906	rBV2	95789	280912	16.20%	1.466%
14	7.488	928	941	956	rBV	99034	263975	15.22%	1.377%
15	7.788	980	992	1003	rBV	127980	340101	19.61%	1.775%
16	8.165	1046	1056	1060	rBV	112799	261844	15.10%	1.366%
17	8.224	1060	1066	1078	rVB	179779	423029	24.39%	2.207%
18	8.535	1108	1119	1132	rBV2	607751	1734416	100.00%	9.051%
19	8.653	1132	1139	1150	rVB2	26397	122733	7.08%	0.640%
20	9.100	1207	1215	1224	rVB	312931	642859	37.06%	3.355%
21	9.271	1236	1244	1254	rBV	72386	159380	9.19%	0.832%
22	9.529	1281	1288	1295	rBV	71615	138248	7.97%	0.721%
23	9.600	1295	1300	1302	rVV4	11093	18675	1.08%	0.097%
24	9.653	1302	1309	1326	rVB	153414	313787	18.09%	1.637%
25	10.341	1416	1426	1427	rBV8	6976	17957	1.04%	0.094%
26	10.565	1456	1464	1471	rBV	461696	853543	49.21%	4.454%
27	10.629	1471	1475	1482	rVB	42287	77813	4.49%	0.406%
28	10.959	1525	1531	1536	rBV2	12752	21651	1.25%	0.113%
29	11.123	1545	1559	1567	rBV	45744	131397	7.58%	0.686%
30	11.259	1577	1582	1583	rBV2	18015	23535	1.36%	0.123%
31	11.300	1583	1589	1594	rVV	150250	266930	15.39%	1.393%
32	11.347	1594	1597	1603	rVB2	31021	48873	2.82%	0.255%
33	11.412	1603	1608	1615	rVB3	11610	24418	1.41%	0.127%
34	11.512	1615	1625	1643	rBV	246982	601922	34.70%	3.141%
35	11.865	1675	1685	1690	rBV	549670	1016902	58.63%	5.306%
36	11.906	1690	1692	1698	rVV	108699	163495	9.43%	0.853%

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

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37	11.970	1698	1703	1708	rVV2	17374	33133	1.91%	0.173%
38	12.029	1708	1713	1714	rVV4	15146	25541	1.47%	0.133%
39	12.065	1714	1719	1728	rVB2	82030	157676	9.09%	0.823%
40	12.165	1729	1736	1739	rBV2	33593	61898	3.57%	0.323%
41	12.235	1739	1748	1757	rVB2	100566	250460	14.44%	1.307%
42	12.353	1764	1768	1771	rBV2	16067	25760	1.49%	0.134%
43	12.412	1771	1778	1783	rVV5	53058	142801	8.23%	0.745%
44	12.459	1783	1786	1798	rVB3	26888	53348	3.08%	0.278%
45	12.565	1798	1804	1812	rBV5	108197	220366	12.71%	1.150%
46	12.635	1812	1816	1820	rVV4	32355	59629	3.44%	0.311%
47	12.688	1820	1825	1832	rVB2	64215	118331	6.82%	0.617%
48	12.794	1834	1843	1844	rBV5	9831	23319	1.34%	0.122%
49	12.847	1845	1852	1858	rVV	446470	789055	45.49%	4.117%
50	12.888	1858	1859	1864	rVB3	32781	41048	2.37%	0.214%
51	13.035	1879	1884	1887	rBV2	19604	32089	1.85%	0.167%
52	13.076	1887	1891	1894	rVV3	29209	53204	3.07%	0.278%
53	13.123	1894	1899	1912	rVB	224485	449110	25.89%	2.344%
54	13.235	1912	1918	1921	rBV6	15950	35891	2.07%	0.187%
55	13.300	1925	1929	1931	rVV2	30328	46799	2.70%	0.244%
56	13.335	1931	1935	1944	rVB3	169326	354070	20.41%	1.848%
57	13.423	1944	1950	1952	rBV2	29146	47858	2.76%	0.250%
58	13.464	1952	1957	1967	rVV4	140490	478372	27.58%	2.496%
59	13.541	1967	1970	1978	rVV	76263	137708	7.94%	0.719%
60	13.623	1979	1984	1989	rVV	56843	91768	5.29%	0.479%
61	13.682	1989	1994	2000	rVV	49015	96012	5.54%	0.501%
62	13.788	2003	2012	2020	rVV	659033	1207473	69.62%	6.301%
63	13.870	2021	2026	2036	rVB	456202	770947	44.45%	4.023%
64	13.994	2042	2047	2051	rBV5	19751	44242	2.55%	0.231%
65	14.106	2062	2066	2073	rVB3	88260	163655	9.44%	0.854%
66	14.182	2073	2079	2084	rBV2	58847	129108	7.44%	0.674%
67	14.241	2084	2089	2101	rVB	819643	1282320	73.93%	6.691%
68	14.547	2134	2141	2146	rBV3	74928	151985	8.76%	0.793%
69	14.706	2164	2168	2171	rBV6	24658	43686	2.52%	0.228%
70	14.953	2203	2210	2216	rVB	111268	173899	10.03%	0.907%
71	15.035	2218	2224	2227	rVV6	27641	57130	3.29%	0.298%
72	15.088	2228	2233	2247	rVB8	81828	252039	14.53%	1.315%
73	15.317	2268	2272	2278	rVB7	14645	31343	1.81%	0.164%
74	15.470	2293	2298	2299	rBV4	17375	25900	1.49%	0.135%
75	15.506	2300	2304	2312	rVB6	36179	83406	4.81%	0.435%
76	15.594	2312	2319	2324	rBV3	140179	317957	18.33%	1.659%

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Integration Parameters: RTEINT.P

Integrator: RTE

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77	15.641	2324	2327	2335	rVB	86018	154172	8.89%	0.805%
78	15.829	2348	2359	2369	rVB	189059	478800	27.61%	2.498%
79	16.011	2387	2390	2402	rVB8	22161	51213	2.95%	0.267%
80	16.405	2451	2457	2461	rBV5	15399	31663	1.83%	0.165%
81	16.458	2461	2466	2475	rVV7	31390	77840	4.49%	0.406%
82	16.541	2477	2480	2486	rVV5	21525	40604	2.34%	0.212%
83	16.611	2486	2492	2501	rVB7	32742	71256	4.11%	0.372%
84	16.782	2513	2521	2522	rBV2	32628	60074	3.46%	0.313%

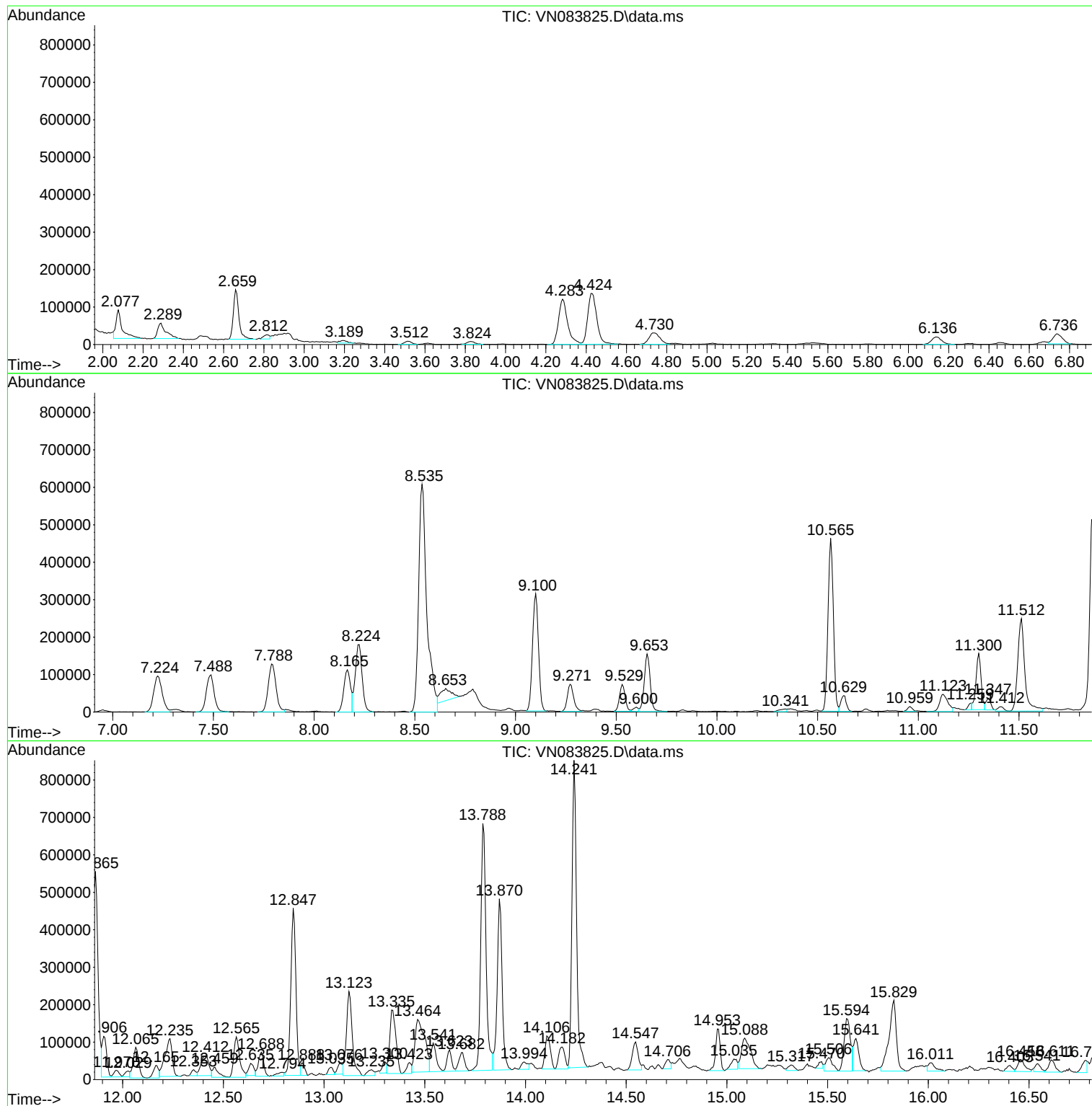
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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



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Sample : P3913-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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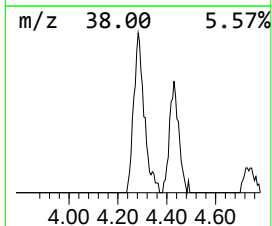
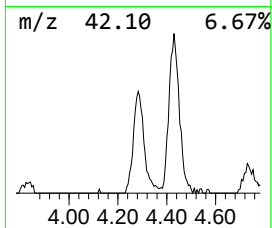
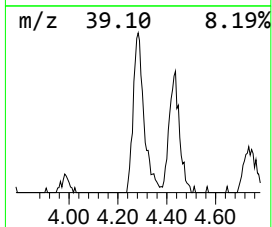
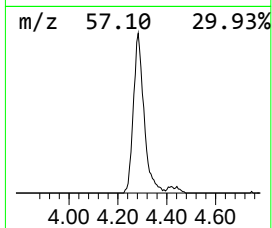
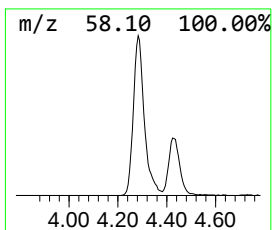
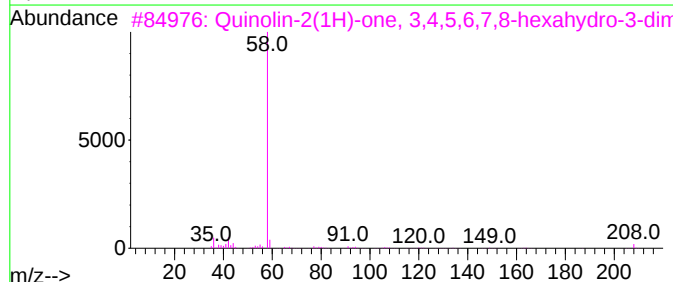
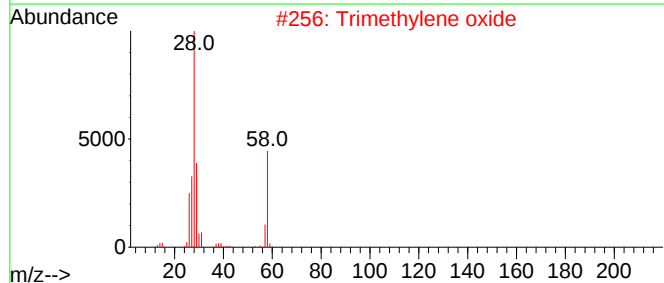
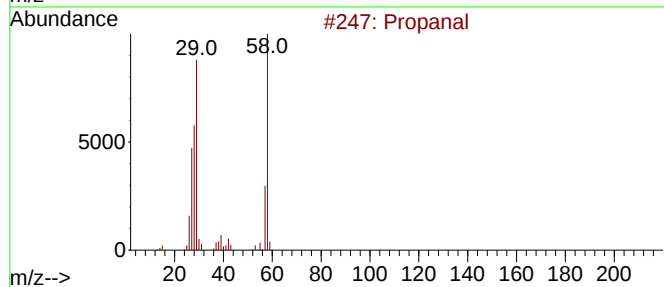
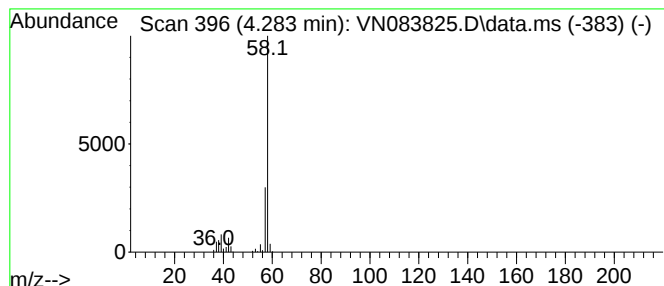
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 2 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.283	45.03 ug/l	381004	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	72
2			Trimethylene oxide	58	C3H6O	000503-30-0	56
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5			Propylene oxide	58	C3H6O	000075-56-9	5



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Sample : P3913-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-D-F-82924-D

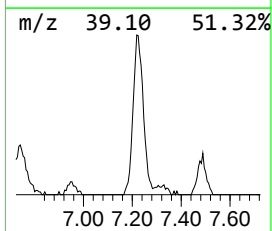
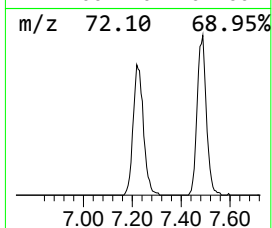
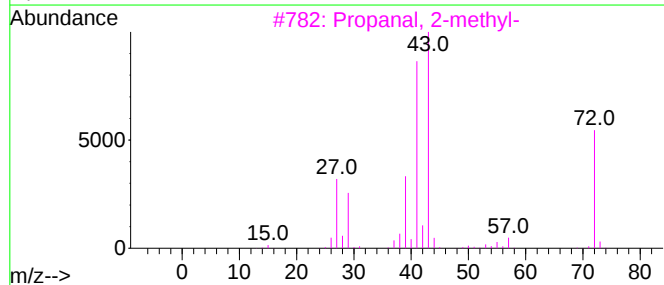
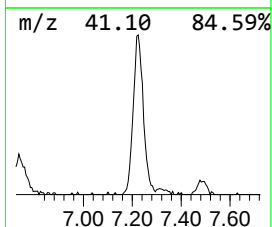
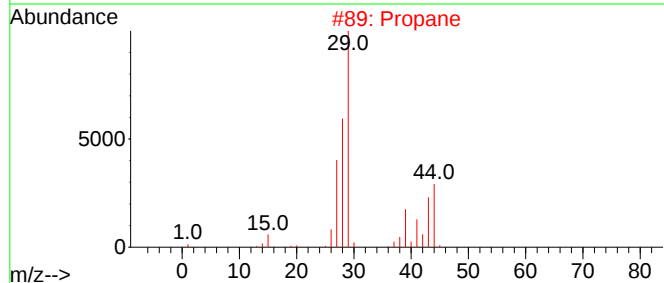
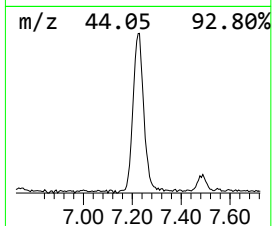
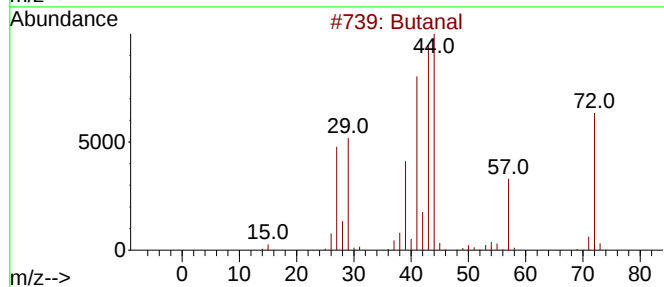
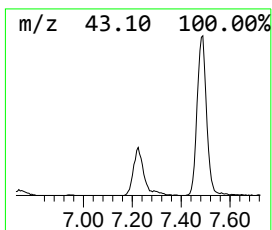
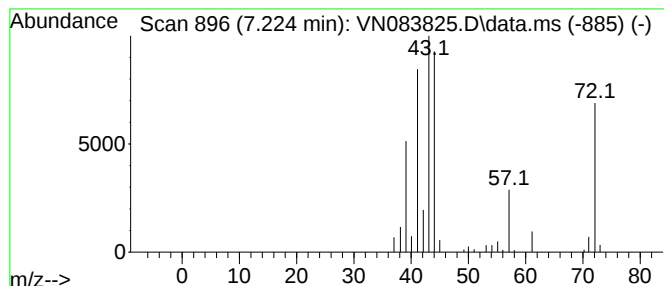
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	33.20 ug/l	280912	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propane	44	C3H8	000074-98-6	43
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4			Ethene, ethoxy-	72	C4H8O	000109-92-2	37
5			Methacrolein	70	C4H6O	000078-85-3	27



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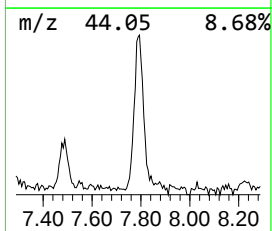
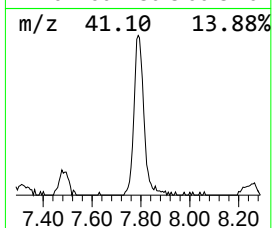
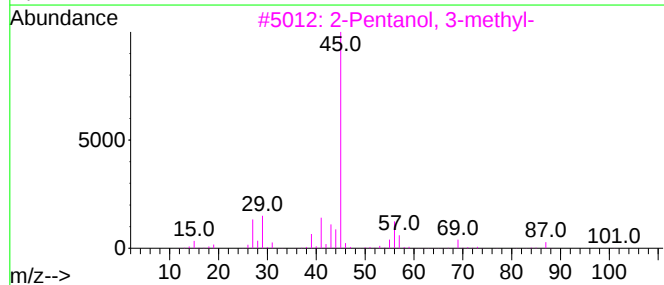
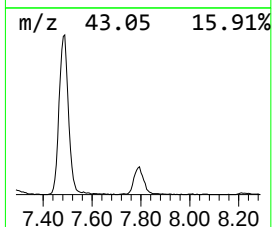
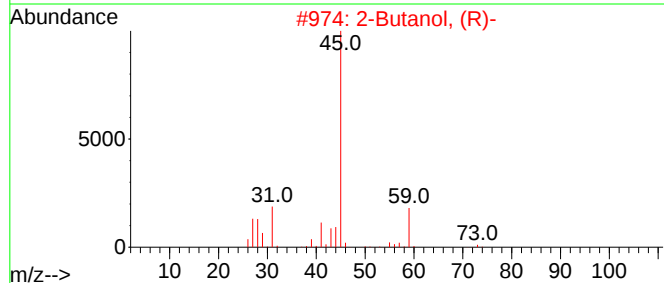
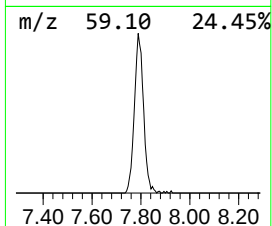
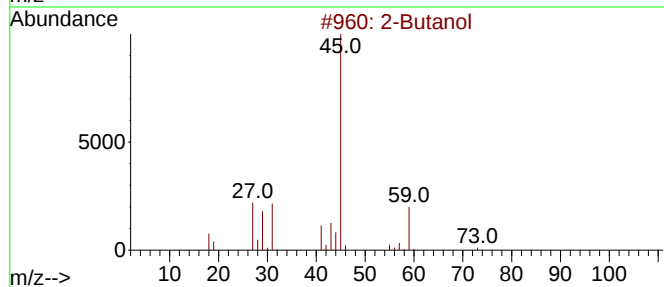
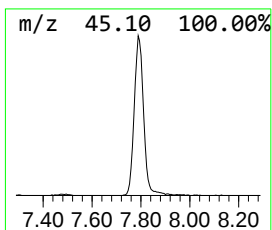
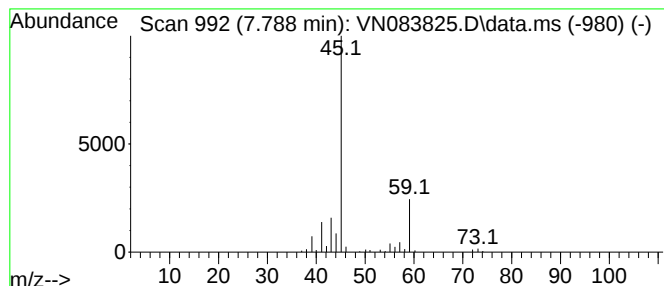
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 4 2-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.788	40.20 ug/l	340101	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol		74	C4H10O	000078-92-2	83
2	2-Butanol, (R)-		74	C4H10O	014898-79-4	74
3	2-Pentanol, 3-methyl-		102	C6H14O	000565-60-6	59
4	Isopropyl Alcohol		60	C3H8O	000067-63-0	45
5	2-Hexanol, (R)-		102	C6H14O	026549-24-6	38



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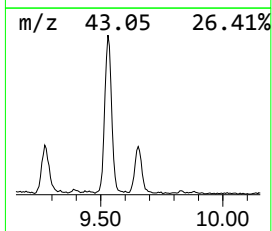
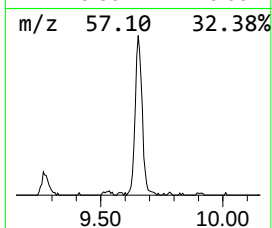
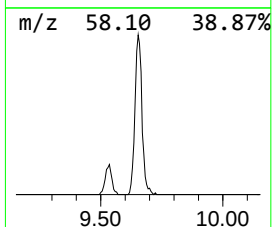
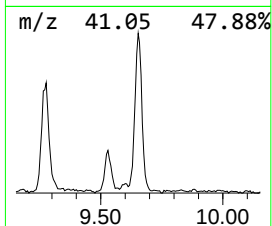
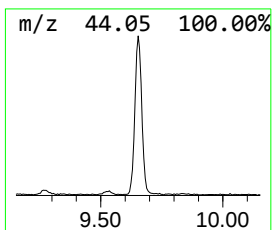
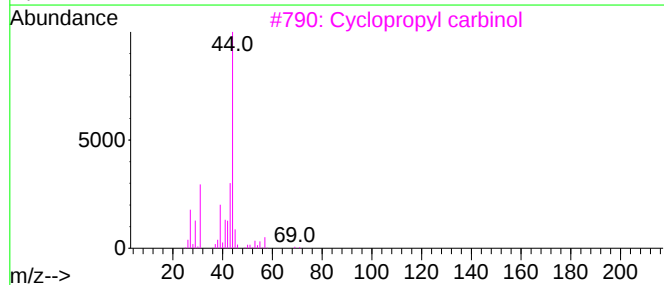
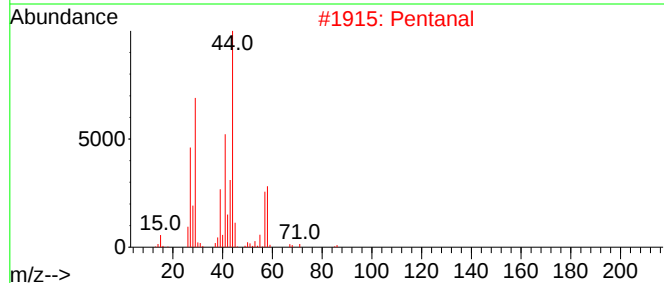
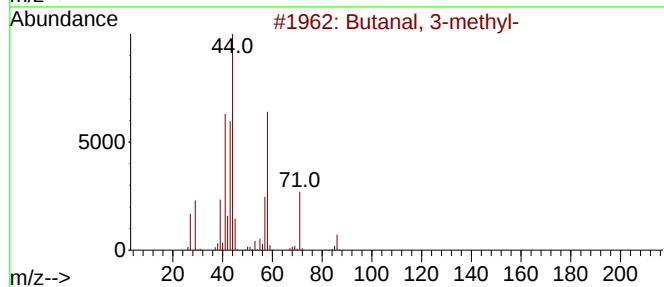
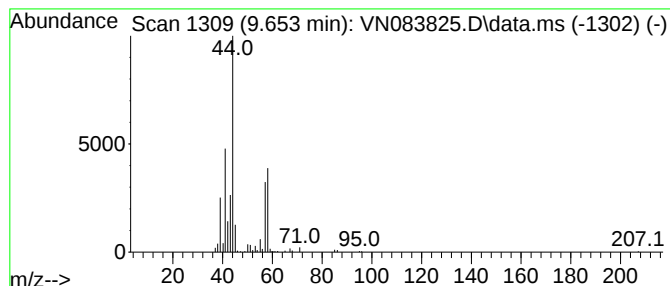
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Quant Title : SW846 8260

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

Peak Number 5 Butanal, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.653	24.41 ug/l	313787	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3-methyl-	86	C5H10O	000590-86-3	83
2			Pentanal	86	C5H10O	000110-62-3	72
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	50
4			Urea, trimethyl-	102	C4H10N2O	000632-14-4	42
5			Ethylene oxide	44	C2H4O	000075-21-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083825.D
Acq On : 12 Sep 2024 12:08
Operator : JC\MD
Sample : P3913-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

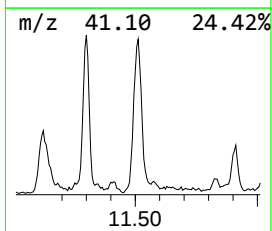
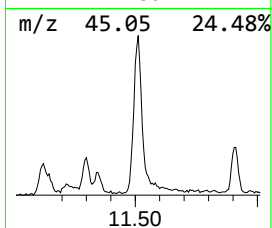
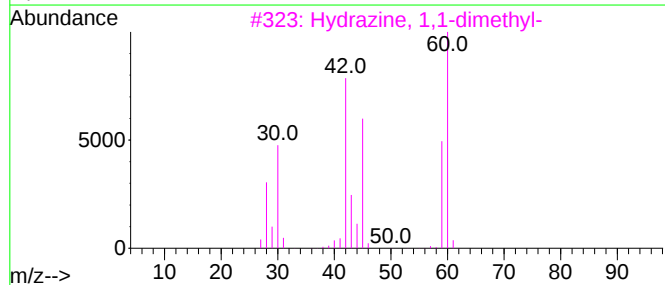
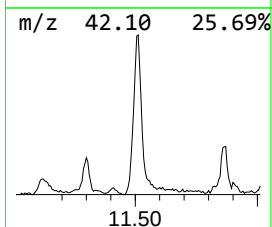
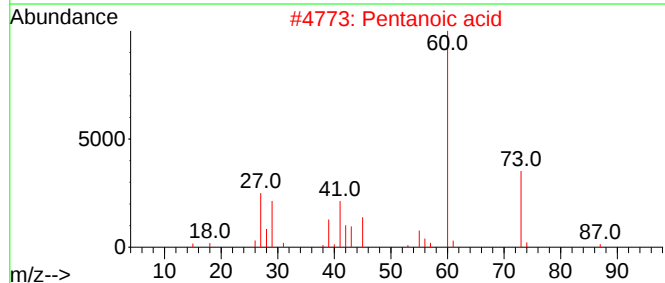
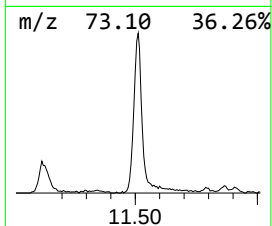
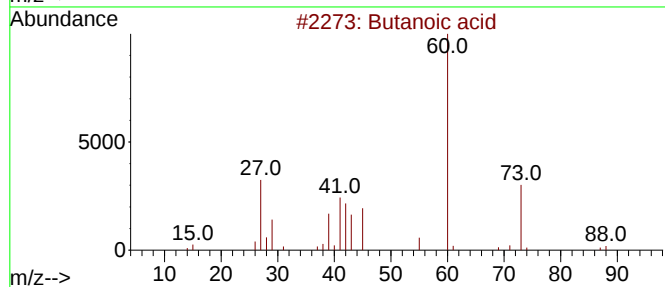
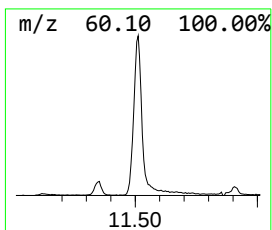
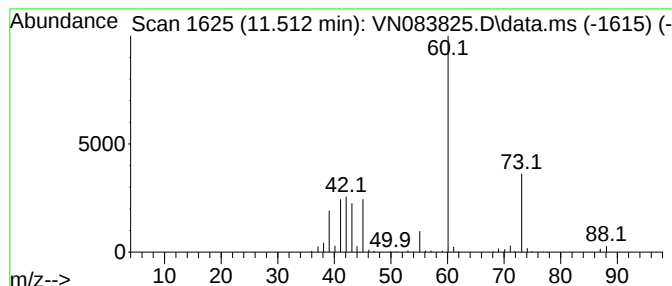
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ClientSampleId :
9424-D-F-82924-D

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Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.512	29.60 ug/l	601922	Chlorobenzene-d5		11.865	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Butanoic acid		88	C4H8O2	000107-92-6	90
2	Pentanoic acid		102	C5H10O2	000109-52-4	45
3	Hydrazine, 1,1-dimethyl-		60	C2H8N2	000057-14-7	9
4	4-Bromobutyric acid		166	C4H7BrO2	002623-87-2	9
5	Hexanoic acid		116	C6H12O2	000142-62-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083825.D
Acq On : 12 Sep 2024 12:08
Operator : JC\MD
Sample : P3913-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-D-F-82924-D

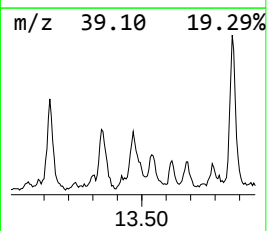
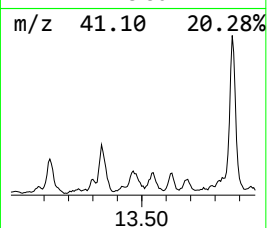
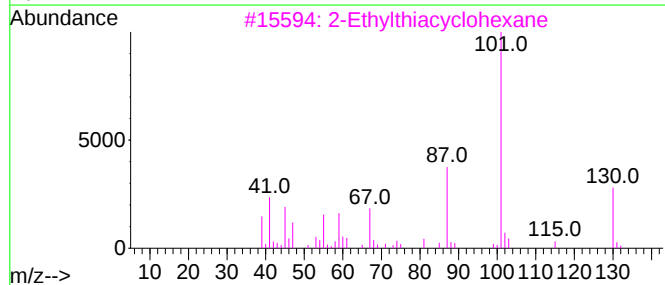
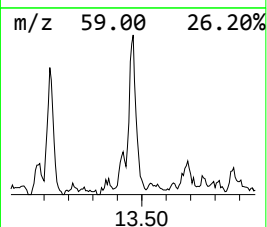
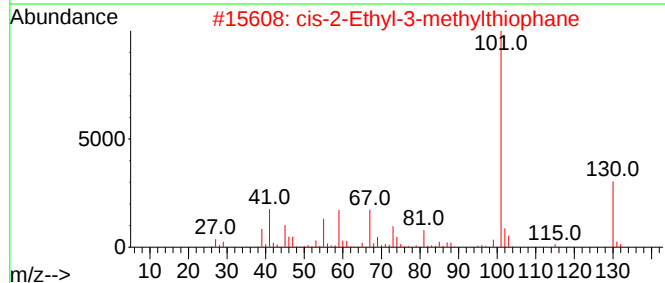
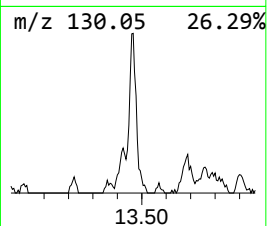
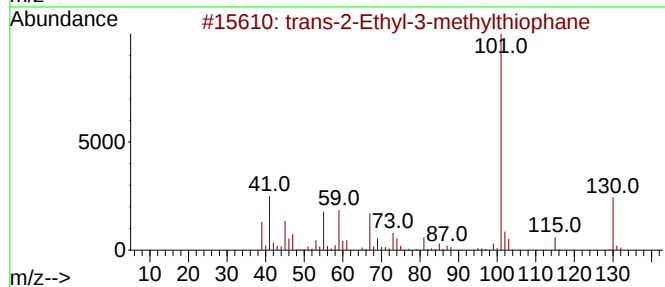
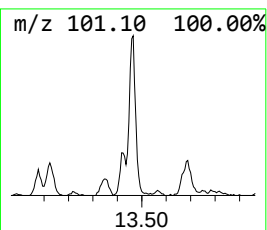
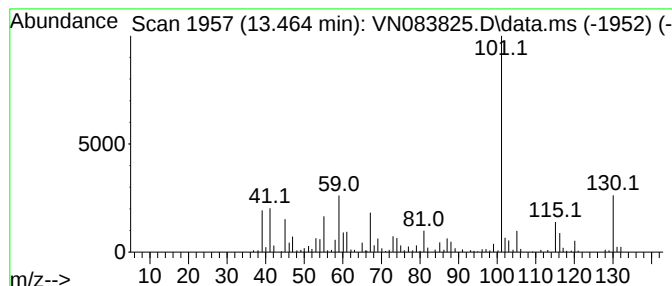
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Quant Title : SW846 8260

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

Peak Number 7 trans-2-Ethyl-3-methylthiop... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.464	19.81 ug/l	478372	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2-Ethyl-3-methylthiophane	130	C7H14S	061568-36-3	76
2			cis-2-Ethyl-3-methylthiophane	130	C7H14S	061568-37-4	70
3			2-Ethylthiacyclohexane	130	C7H14S	001613-52-1	68
4			1,2,4-Thiadiazole, 5-amino-	101	C2H3N3S	007552-07-0	58
5			2-Amino-2-thiazoline-4-carboxyli...	146	C4H6N2O2S	002150-55-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083825.D
Acq On : 12 Sep 2024 12:08
Operator : JC\MD
Sample : P3913-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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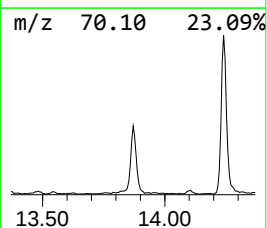
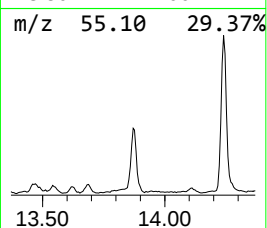
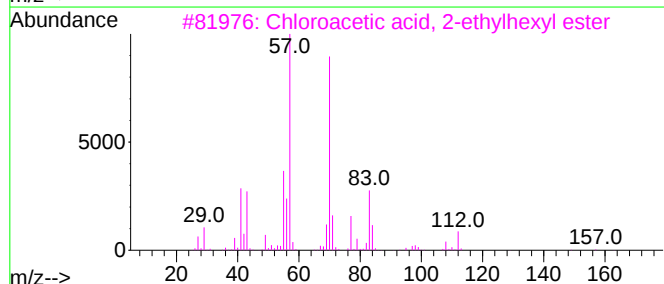
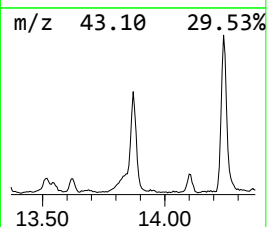
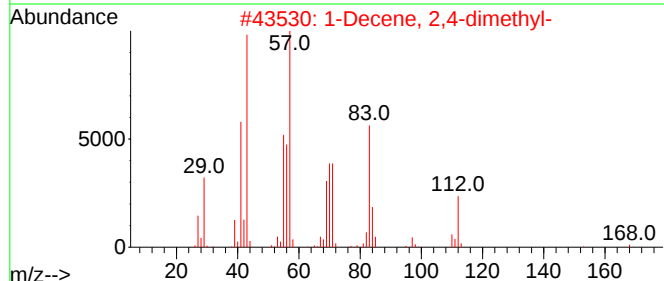
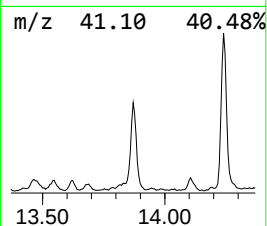
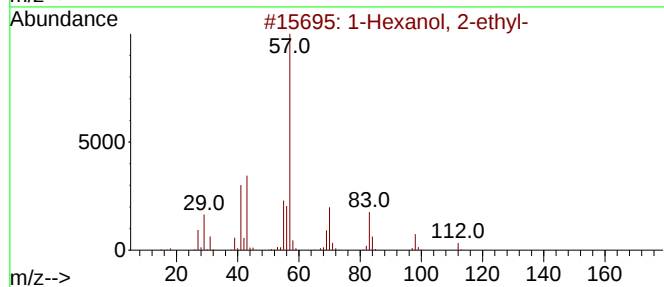
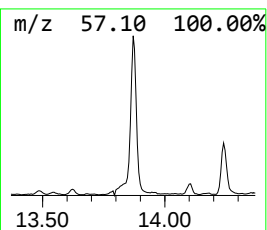
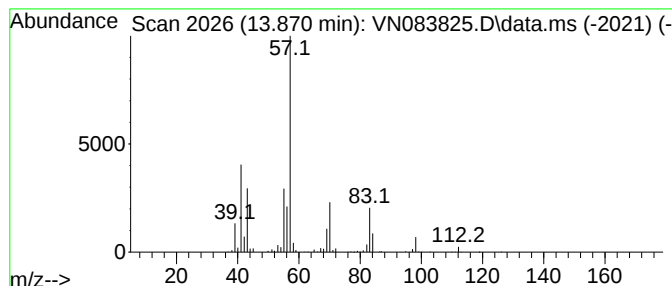
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Quant Title : SW846 8260

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	31.92 ug/l	770947	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
3			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	53
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083825.D
Acq On : 12 Sep 2024 12:08
Operator : JC\MD
Sample : P3913-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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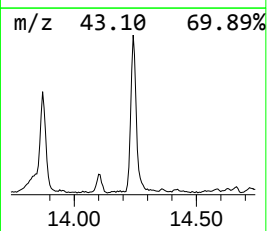
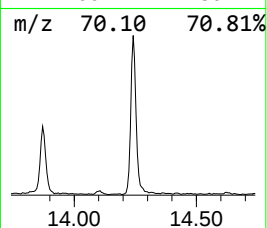
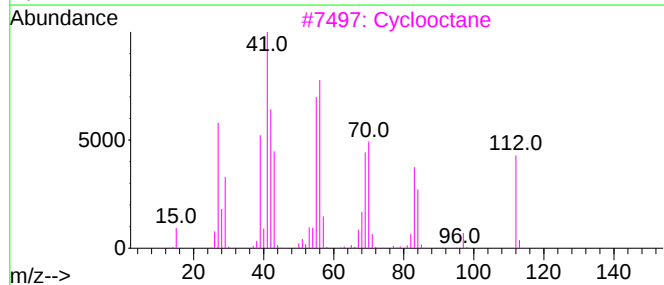
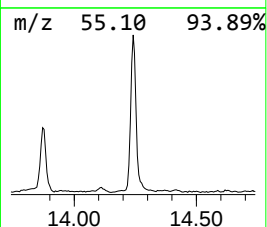
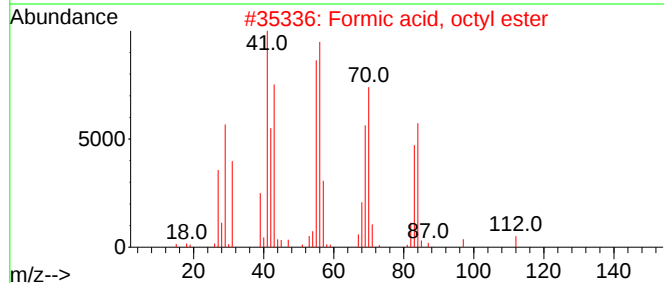
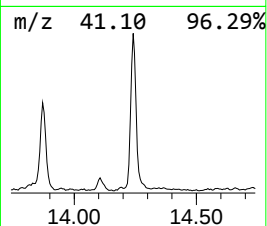
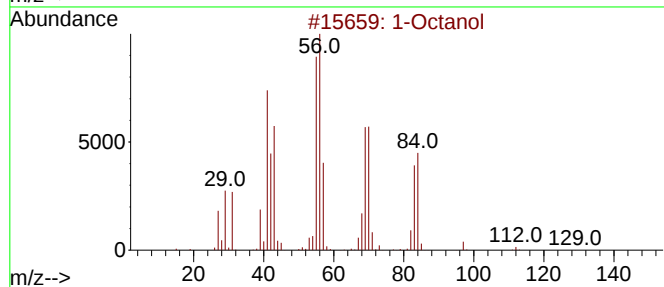
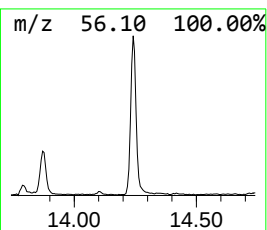
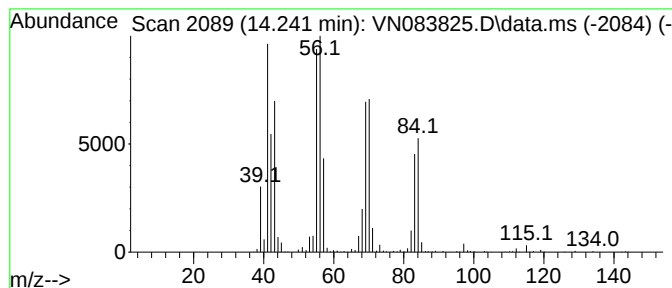
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Quant Title : SW846 8260

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

Peak Number 9 1-Octanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.241	53.10 ug/l	1282320	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	91
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3			Cyclooctane	112	C8H16	000292-64-8	87
4			Octyl chloroformate	192	C9H17ClO2	007452-59-7	78
5			1-Octene	112	C8H16	000111-66-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083825.D
Acq On : 12 Sep 2024 12:08
Operator : JC\MD
Sample : P3913-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-D-F-82924-D

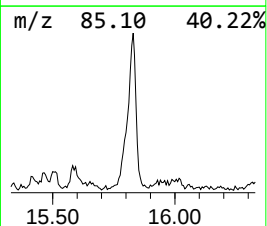
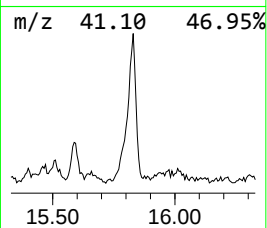
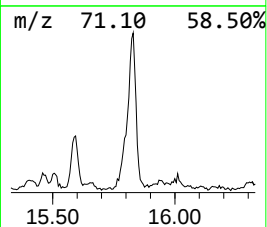
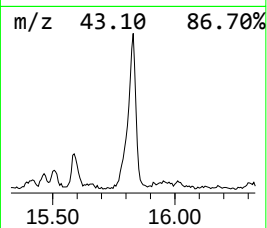
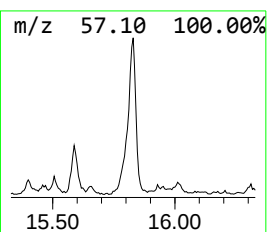
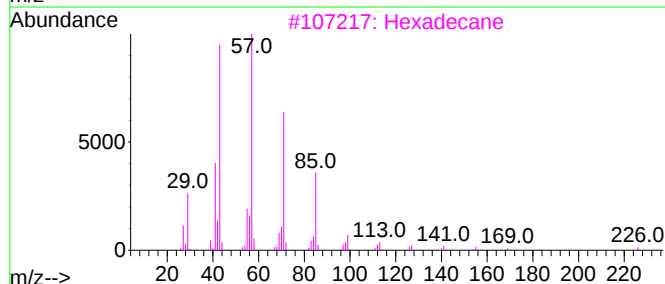
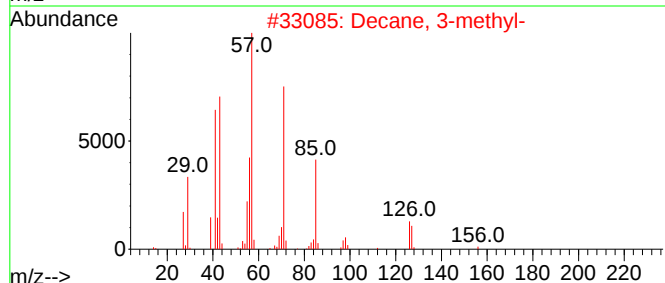
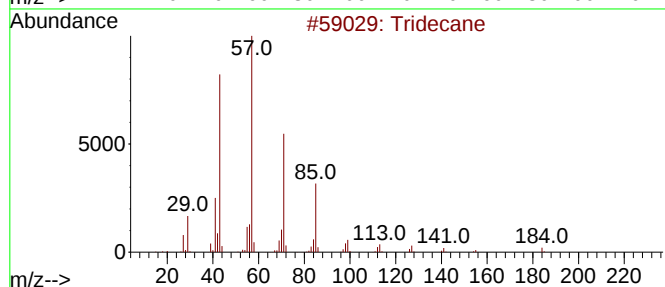
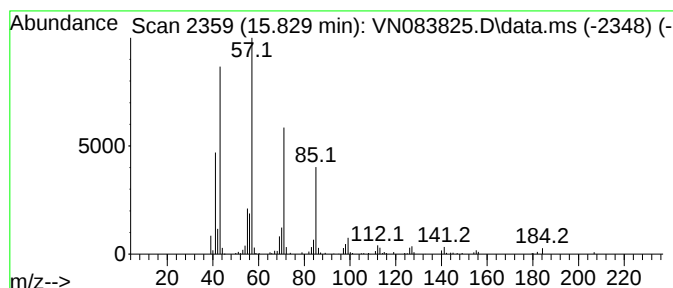
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Quant Title : SW846 8260

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

Peak Number 10 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.829	19.83 ug/l	478800	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	94
2			Decane, 3-methyl-	156	C11H24	013151-34-3	87
3			Hexadecane	226	C16H34	000544-76-3	86
4			Tritetracontane	605	C43H88	007098-21-7	83
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083825.D
Acq On : 12 Sep 2024 12:08
Operator : JC\MD
Sample : P3913-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-D-F-82924-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Butanal	7.224	33.2	ug/l	280912	1	8.224	423029	50.0
2-Butanol	7.788	40.2	ug/l	340101	1	8.224	423029	50.0
Butanal, 3-methyl-	9.653	24.4	ug/l	313787	2	9.100	642859	50.0
Butanoic acid	11.512	29.6	ug/l	601922	3	11.865	1016900	50.0
trans-2-Ethyl-3...	13.464	19.8	ug/l	478372	4	13.794	1207470	50.0
1-Hexanol, 2-et...	13.870	31.9	ug/l	770947	4	13.794	1207470	50.0
1-Octanol	14.241	53.1	ug/l	1282320	4	13.794	1207470	50.0
Tridecane	15.829	19.8	ug/l	478800	4	13.794	1207470	50.0