

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
 Data File : VN081858.D
 Acq On : 25 Apr 2024 18:16
 Operator : JC\MD
 Sample : P2257-09
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 413B

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\82N042524W.M
 Title : SW846 8260

Signal : TIC: VN081858.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	16	22	29	rBV2	56178	87399	5.66%	0.723%
2	2.377	64	72	74	rBV6	9607	18030	1.17%	0.149%
3	3.783	301	311	319	rBV3	9655	28517	1.85%	0.236%
4	4.424	412	420	421	rBV	18179	26934	1.74%	0.223%
5	4.712	457	469	474	rBV2	11022	32741	2.12%	0.271%
6	7.224	886	896	908	rBV3	60914	167529	10.85%	1.385%
7	8.165	1047	1056	1061	rBV3	169860	418669	27.11%	3.461%
8	8.224	1061	1066	1077	rVB	335165	721210	46.69%	5.962%
9	8.577	1112	1126	1135	rBV2	214016	494489	32.01%	4.088%
10	8.671	1135	1142	1148	rBV5	22986	76031	4.92%	0.629%
11	9.100	1207	1215	1227	rVB	503031	1028580	66.59%	8.503%
12	9.271	1236	1244	1253	rBV3	25366	61918	4.01%	0.512%
13	9.659	1304	1310	1318	rVB3	9464	21968	1.42%	0.182%
14	10.565	1453	1464	1472	rBV	741560	1418152	91.81%	11.724%
15	10.635	1472	1476	1482	rVB5	13903	25344	1.64%	0.210%
16	11.865	1672	1685	1696	rBV	682879	1262917	81.76%	10.441%
17	11.965	1696	1702	1709	rVB4	7302	17630	1.14%	0.146%
18	12.065	1712	1719	1727	rBV2	25414	54983	3.56%	0.455%
19	12.153	1727	1734	1736	rBV4	8823	17157	1.11%	0.142%
20	12.206	1739	1743	1749	rBV3	13373	22855	1.48%	0.189%
21	12.418	1767	1779	1789	rBV	160813	324705	21.02%	2.684%
22	12.847	1843	1852	1862	rBV	511701	923290	59.78%	7.633%
23	12.941	1864	1868	1872	rBV3	14015	21071	1.36%	0.174%
24	13.094	1890	1894	1902	rVB10	12937	31802	2.06%	0.263%
25	13.176	1902	1908	1912	rVB5	10814	18150	1.18%	0.150%
26	13.241	1912	1919	1922	rBV3	76418	133494	8.64%	1.104%
27	13.270	1922	1924	1929	rVV2	63144	79701	5.16%	0.659%
28	13.335	1929	1935	1942	rVB	832465	1273153	82.43%	10.525%
29	13.482	1956	1960	1965	rBV3	40631	67481	4.37%	0.558%
30	13.529	1965	1968	1975	rVB6	17339	36658	2.37%	0.303%
31	13.682	1979	1994	2004	rVB10	21582	100332	6.50%	0.829%
32	13.794	2004	2013	2020	rBV	588167	1044108	67.60%	8.632%
33	13.870	2020	2026	2035	rVV	975531	1544599	100.00%	12.770%
34	13.953	2035	2040	2046	rVB4	28122	46097	2.98%	0.381%
35	14.188	2068	2080	2084	rBV7	15588	42831	2.77%	0.354%
36	14.253	2086	2091	2096	rVB4	14756	24378	1.58%	0.202%

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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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37	14.753	2170	2176	2181	rBV3	42088	85341	5.53%	0.706%
38	15.394	2281	2285	2290	rVV2	21699	33232	2.15%	0.275%
39	15.459	2292	2296	2304	rVB6	14739	30284	1.96%	0.250%
40	15.617	2313	2323	2336	rBV3	90689	212384	13.75%	1.756%
41	16.117	2401	2408	2414	rBV7	10541	19855	1.29%	0.164%

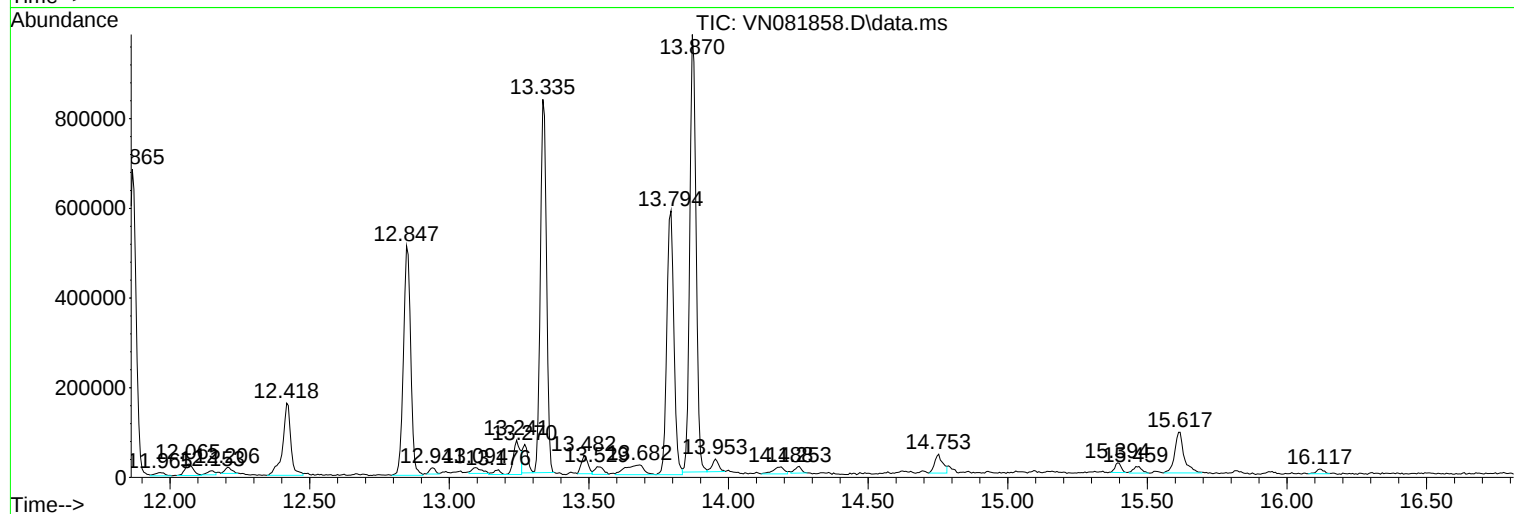
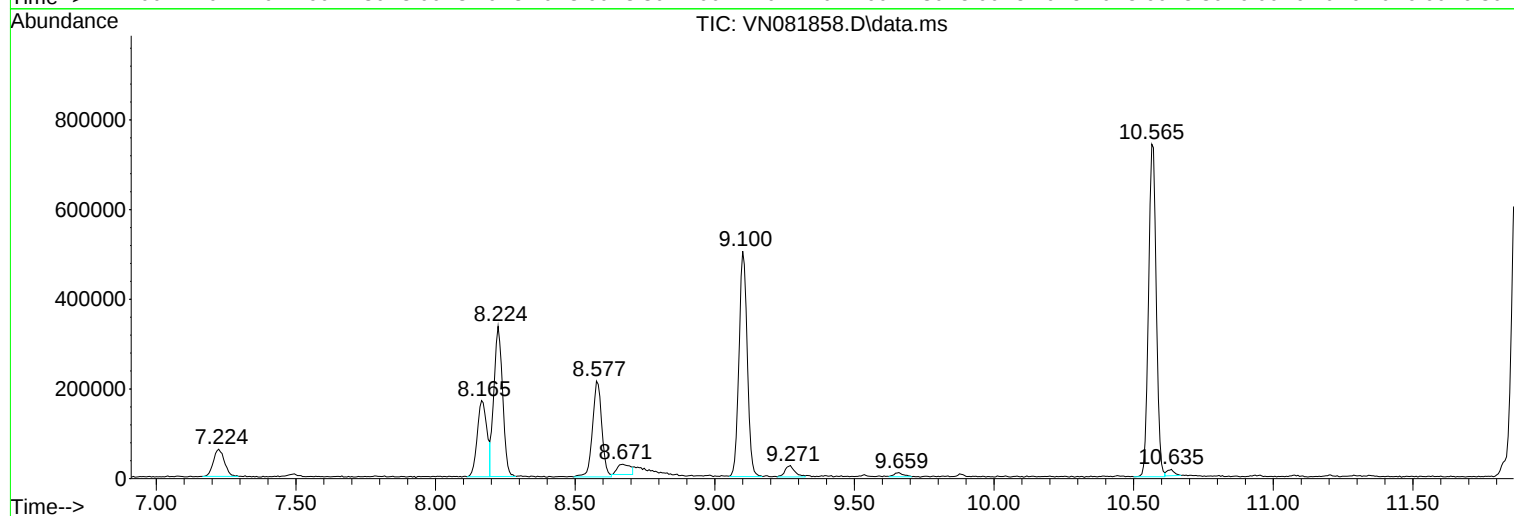
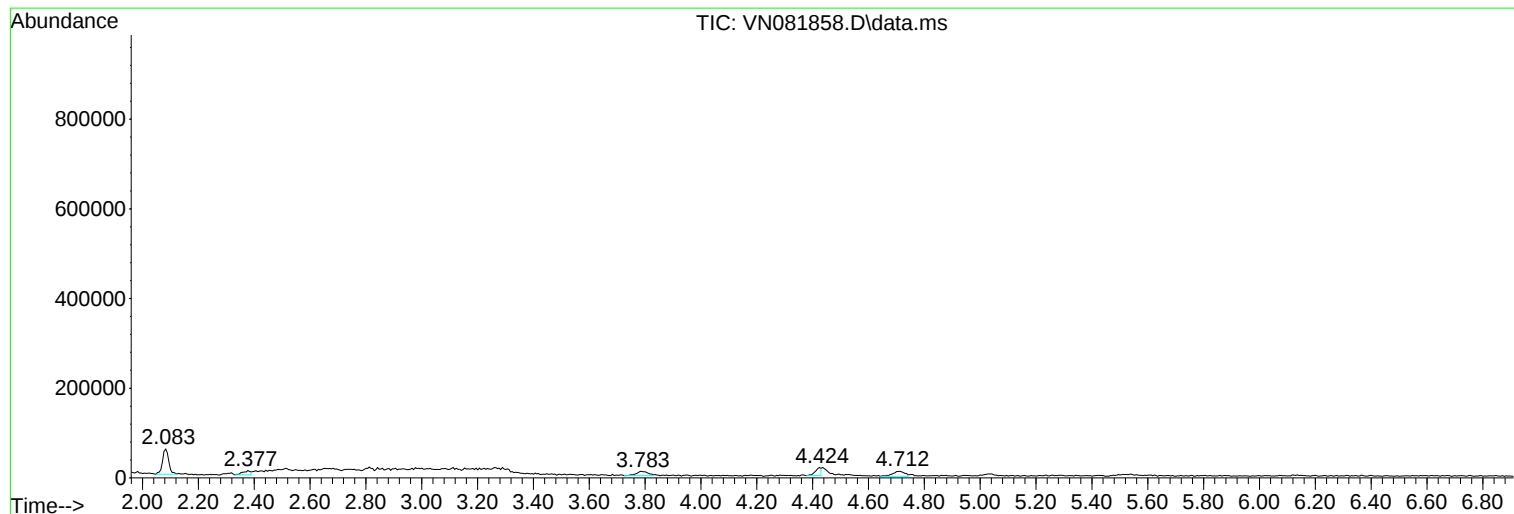
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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



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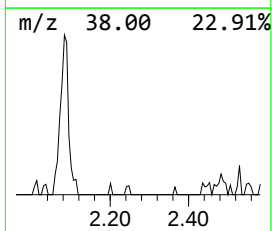
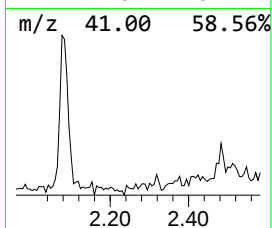
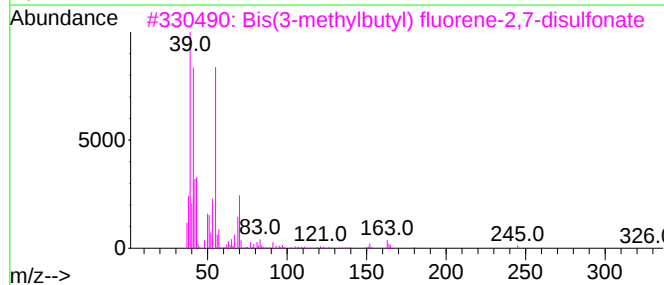
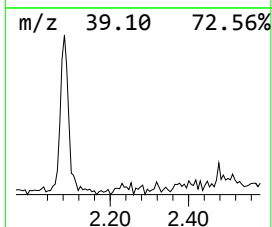
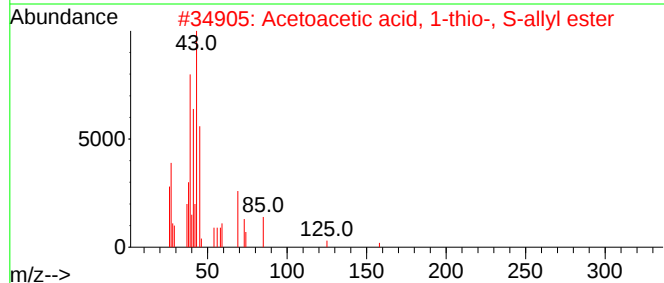
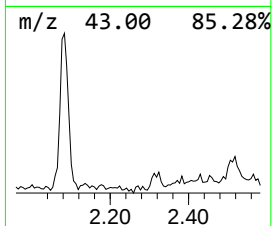
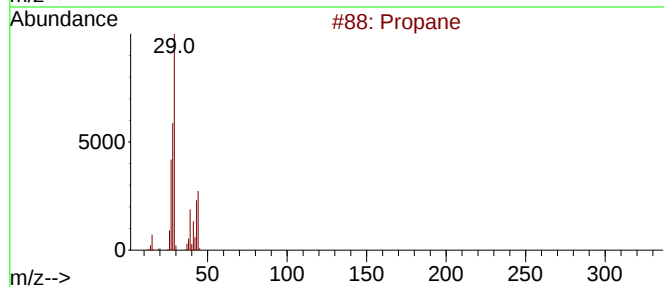
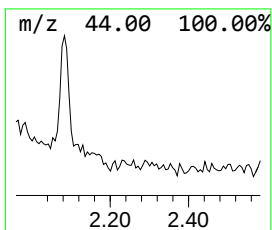
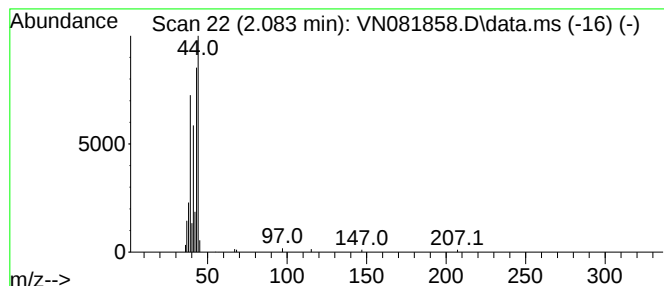
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	6.06 ug/l	87399	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	78
2			Acetoacetic acid, 1-thio-, S-all...	158	C7H10O2S	015780-65-1	50
3			Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	47
4			2H-Pyran-2-one	96	C5H4O2	000504-31-4	28
5			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	25



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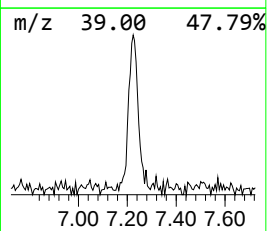
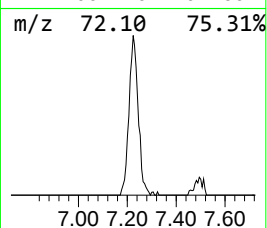
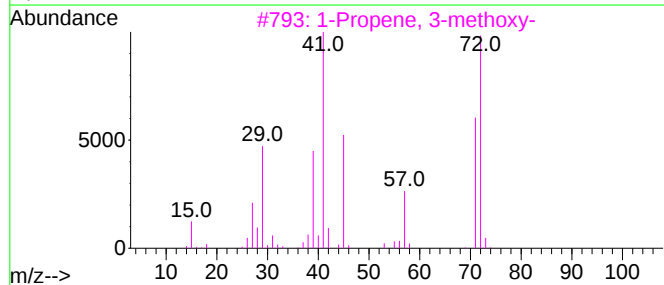
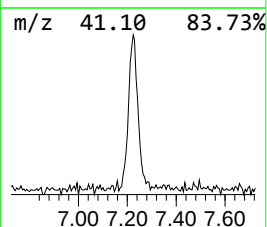
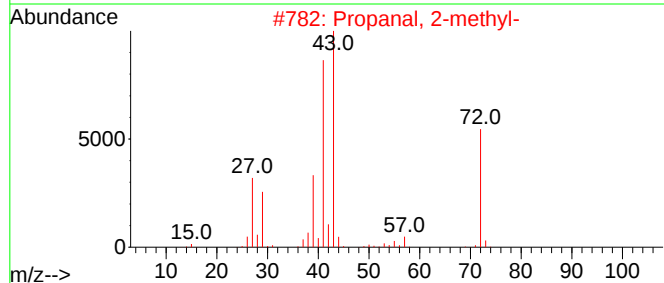
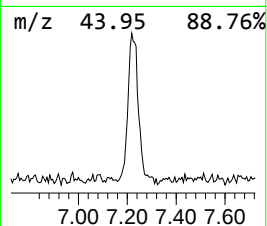
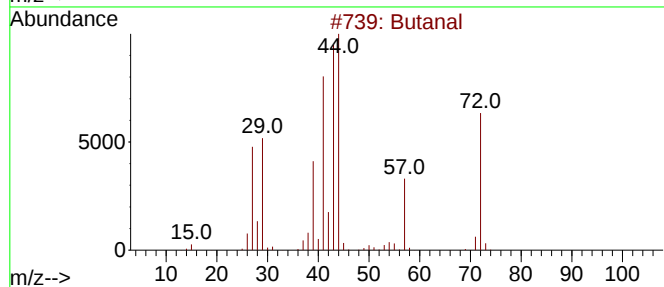
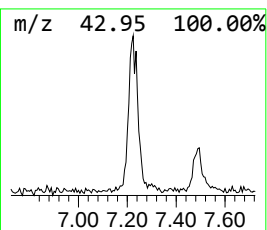
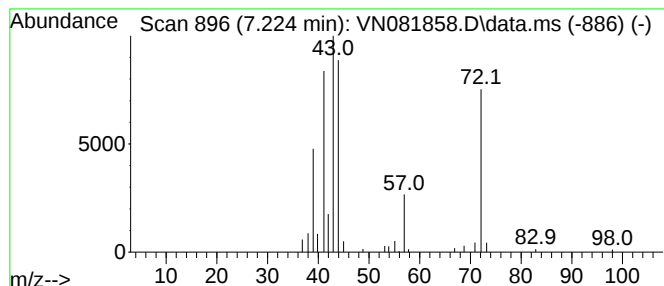
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Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	11.61 ug/l	167529	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	91
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	58
3		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5		2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	38



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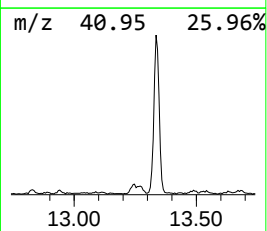
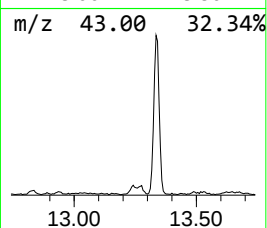
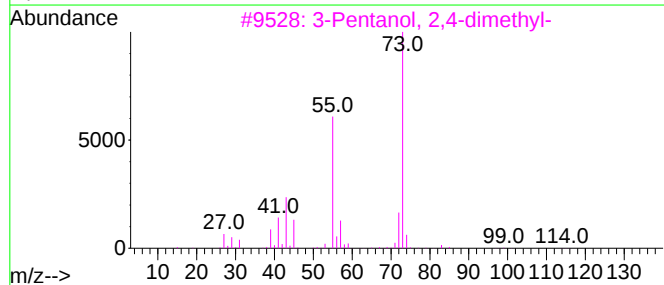
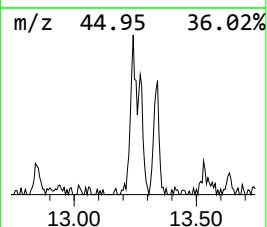
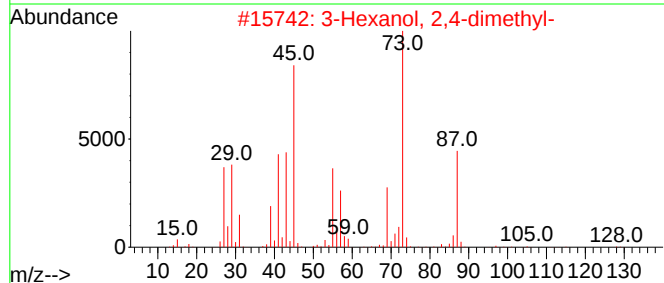
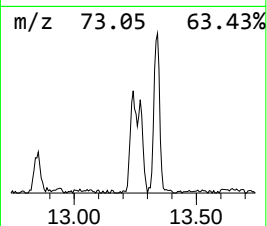
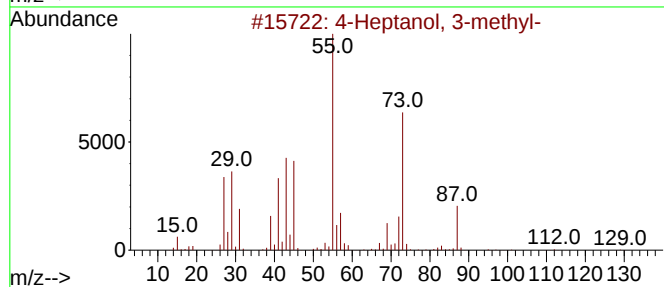
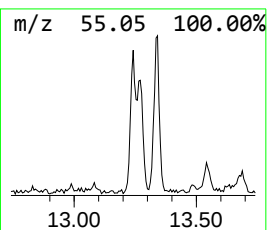
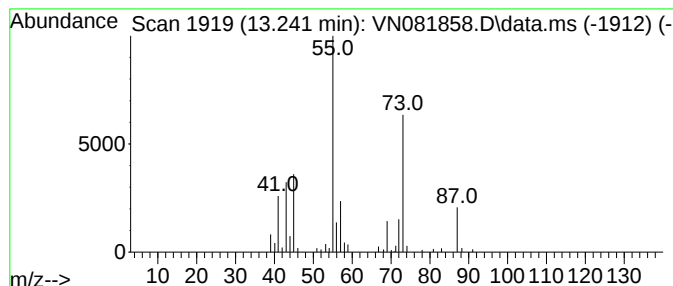
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-Heptanol, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.241	6.39 ug/l	133494	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	83
2		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	50
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	47
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	43
5		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38



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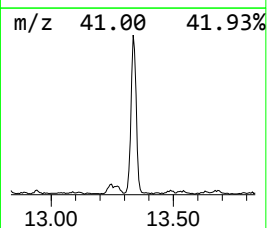
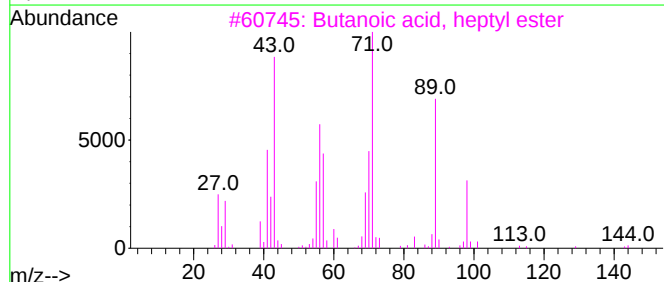
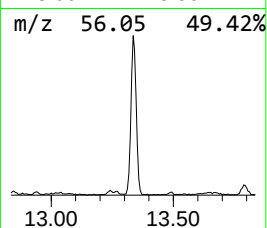
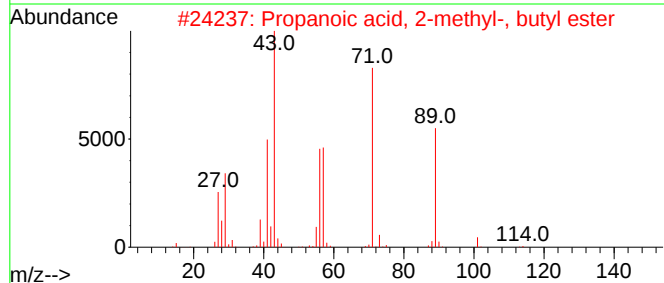
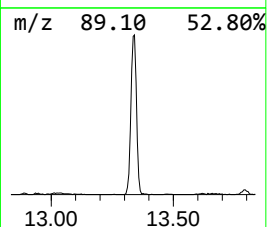
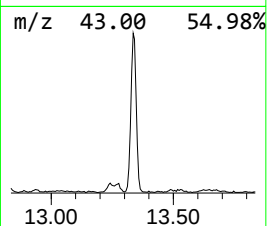
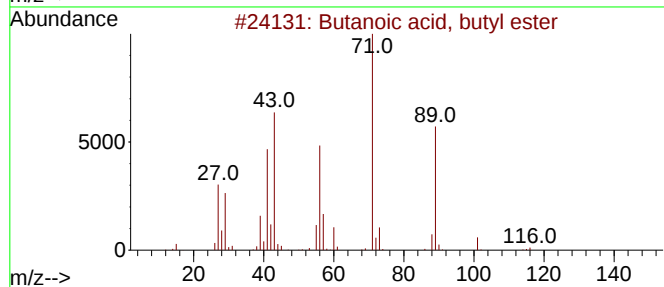
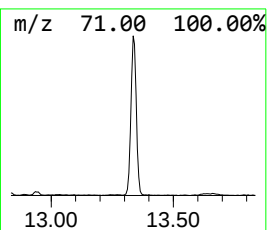
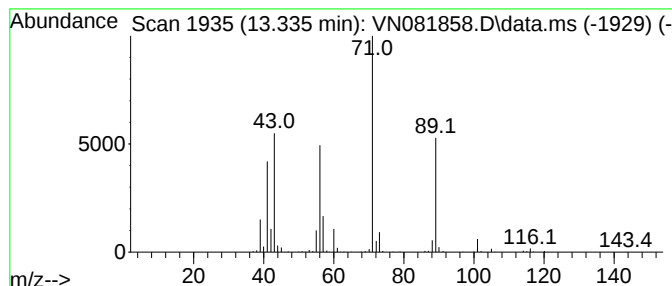
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	60.97 ug/l	1273150	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
3			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
4			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64



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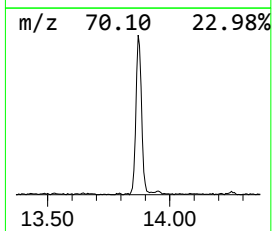
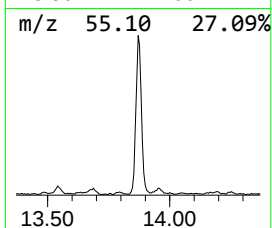
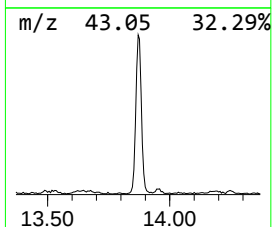
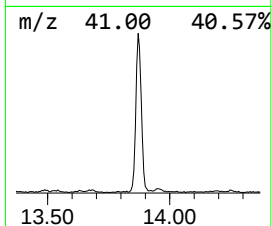
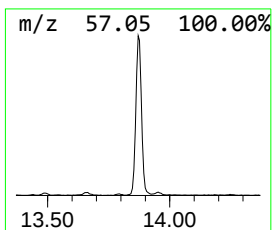
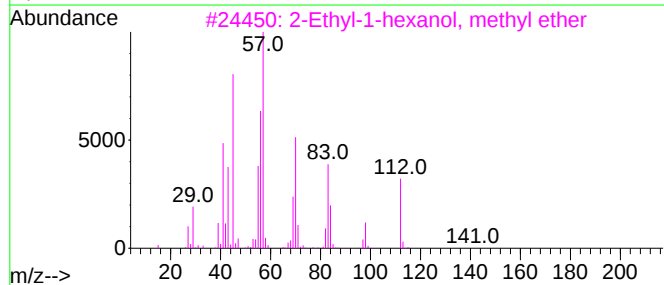
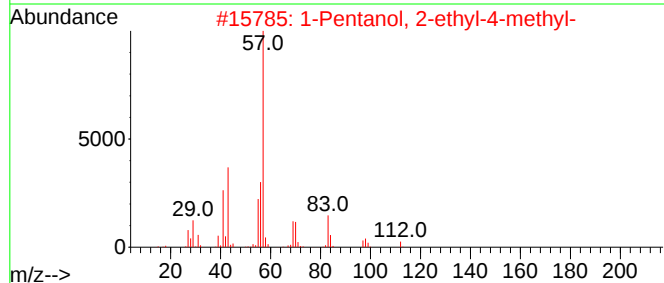
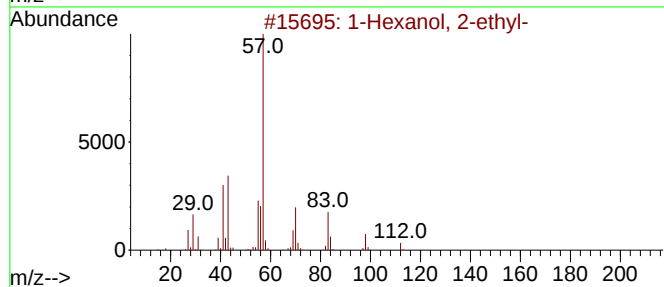
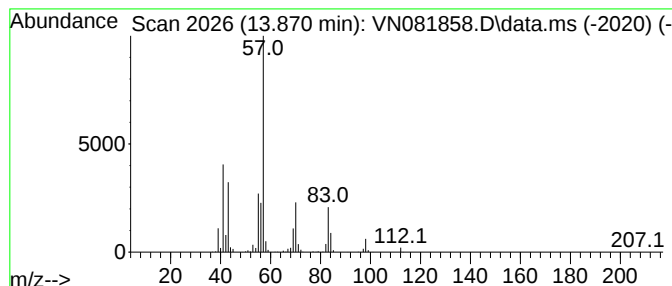
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	73.97 ug/l	1544600	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-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081858.D
Acq On : 25 Apr 2024 18:16
Operator : JC\MD
Sample : P2257-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
413B

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
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
Propane	2.083	6.1	ug/l	87399	1	8.224	721210	50.0
Butanal	7.224	11.6	ug/l	167529	1	8.224	721210	50.0
4-Heptanol, 3-m...	13.241	6.4	ug/l	133494	4	13.794	1044110	50.0
Butanoic acid, ...	13.335	61.0	ug/l	1273150	4	13.794	1044110	50.0
1-Hexanol, 2-et...	13.871	74.0	ug/l	1544600	4	13.794	1044110	50.0