

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072125\
 Data File : VN087373.D
 Acq On : 21 Jul 2025 12:51
 Operator : JC\MD
 Sample : Q2646-01 5X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 FRAC TANK

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\82N071625W.M
 Title : SW846 8260

Signal : TIC: VN087373.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.101	19	25	28	rBV2	14105	23887	1.44%	0.182%
2	2.683	117	124	134	rBV	13316	26566	1.61%	0.202%
3	2.859	147	154	164	rBV2	19082	47889	2.89%	0.364%
4	3.653	280	289	301	rBV	59507	153096	9.25%	1.164%
5	3.789	302	312	323	rBV	107651	310010	18.74%	2.357%
6	4.000	339	348	358	rBV5	8944	26221	1.58%	0.199%
7	4.289	390	397	406	rVB4	8399	22567	1.36%	0.172%
8	4.424	410	420	429	rVV2	26914	87940	5.31%	0.669%
9	4.512	429	435	449	rVB5	10433	32925	1.99%	0.250%
10	4.712	459	469	480	rBV2	27742	102192	6.18%	0.777%
11	6.589	779	788	799	rBV3	15389	47918	2.90%	0.364%
12	6.724	799	811	830	rVV	186736	599800	36.25%	4.560%
13	7.471	919	938	948	rBV	339494	950104	57.42%	7.222%
14	7.547	948	951	963	rVB	22435	50589	3.06%	0.385%
15	7.771	978	989	1005	rBV	638354	1654652	100.00%	12.578%
16	8.153	1044	1054	1058	rBV2	134146	322564	19.49%	2.452%
17	8.206	1058	1063	1077	rVB	197894	452389	27.34%	3.439%
18	8.565	1110	1124	1134	rBV	149800	360303	21.78%	2.739%
19	8.818	1158	1167	1174	rVB5	7170	19397	1.17%	0.147%
20	8.953	1183	1190	1199	rBV4	20454	46968	2.84%	0.357%
21	9.082	1203	1212	1222	rBV	331630	687726	41.56%	5.228%
22	9.259	1235	1242	1254	rBV3	75129	191421	11.57%	1.455%
23	9.506	1279	1284	1289	rVV4	11583	29167	1.76%	0.222%
24	9.559	1289	1293	1300	rVV	21787	42075	2.54%	0.320%
25	9.647	1300	1308	1316	rVV5	45294	113558	6.86%	0.863%
26	9.724	1316	1321	1331	rVB2	22821	45214	2.73%	0.344%
27	9.812	1331	1336	1346	rBV	18197	37848	2.29%	0.288%
28	10.547	1453	1461	1468	rBV	531867	973527	58.84%	7.401%
29	10.724	1483	1491	1499	rVB4	19336	34090	2.06%	0.259%
30	10.818	1499	1507	1514	rBV8	13750	35451	2.14%	0.269%
31	10.965	1524	1532	1545	rBV3	36215	119181	7.20%	0.906%
32	11.188	1561	1570	1579	rBV3	33898	69319	4.19%	0.527%
33	11.282	1579	1586	1602	rVV	292544	542496	32.79%	4.124%
34	11.847	1674	1682	1691	rBV	456602	819883	49.55%	6.233%
35	11.941	1694	1698	1703	rVB2	11668	17888	1.08%	0.136%
36	12.047	1703	1716	1724	rBV5	28480	82327	4.98%	0.626%

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37	12.376	1760	1772	1773	rBV5	26707	43388	2.62%	0.330%
38	12.829	1842	1849	1859	rVB	367304	628903	38.01%	4.781%
39	13.076	1885	1891	1895	rBV	26155	48795	2.95%	0.371%
40	13.141	1895	1902	1910	rVB4	40286	91085	5.50%	0.692%
41	13.323	1925	1933	1939	rBV6	89387	256110	15.48%	1.947%
42	13.459	1948	1956	1965	rBV3	88044	191070	11.55%	1.452%
43	13.770	2002	2009	2018	rVB	480561	832331	50.30%	6.327%
44	13.965	2037	2042	2046	rBV4	23265	48829	2.95%	0.371%
45	14.082	2057	2062	2067	rBV2	87913	140817	8.51%	1.070%
46	14.247	2083	2090	2095	rBV7	16345	43563	2.63%	0.331%
47	14.306	2095	2100	2104	rBV5	43898	91727	5.54%	0.697%
48	14.417	2116	2119	2126	rVB3	22868	36234	2.19%	0.275%
49	14.553	2138	2142	2146	rBV6	19687	37201	2.25%	0.283%
50	14.606	2147	2151	2154	rVV3	30868	47643	2.88%	0.362%
51	14.635	2154	2156	2159	rVV3	23960	27029	1.63%	0.205%
52	14.670	2160	2162	2165	rVB2	18599	16741	1.01%	0.127%
53	14.712	2165	2169	2173	rVB6	21675	27745	1.68%	0.211%
54	14.900	2196	2201	2202	rBV3	20011	21062	1.27%	0.160%
55	14.935	2202	2207	2213	rVB2	126933	194907	11.78%	1.482%
56	15.023	2215	2222	2227	rBV6	48816	141552	8.55%	1.076%
57	15.188	2244	2250	2256	rVB2	37481	70630	4.27%	0.537%
58	15.288	2263	2267	2274	rVB8	15165	28766	1.74%	0.219%
59	15.476	2297	2299	2307	rVB7	22528	46058	2.78%	0.350%
60	15.564	2309	2314	2318	rBV3	42550	71377	4.31%	0.543%
61	15.670	2329	2332	2337	rVB6	12309	17400	1.05%	0.132%
62	15.806	2349	2355	2366	rVB	135344	250431	15.13%	1.904%
63	15.917	2366	2374	2381	rBV9	25208	76469	4.62%	0.581%
64	16.100	2399	2405	2406	rBV4	14352	28090	1.70%	0.214%
65	16.141	2407	2412	2422	rVB8	50113	111729	6.75%	0.849%
66	16.288	2432	2437	2440	rBV7	12136	25816	1.56%	0.196%
67	16.376	2447	2452	2456	rVB7	11109	20805	1.26%	0.158%
68	16.429	2456	2461	2462	rBV5	14637	23152	1.40%	0.176%
69	16.470	2464	2468	2472	rVV7	25855	51101	3.09%	0.388%
70	16.511	2472	2475	2480	rVB7	22335	38626	2.33%	0.294%
71	16.582	2482	2487	2497	rVB6	27321	53048	3.21%	0.403%
72	16.670	2497	2502	2510	rVB7	25857	62111	3.75%	0.472%
73	16.758	2510	2517	2518	rBV7	16366	33305	2.01%	0.253%

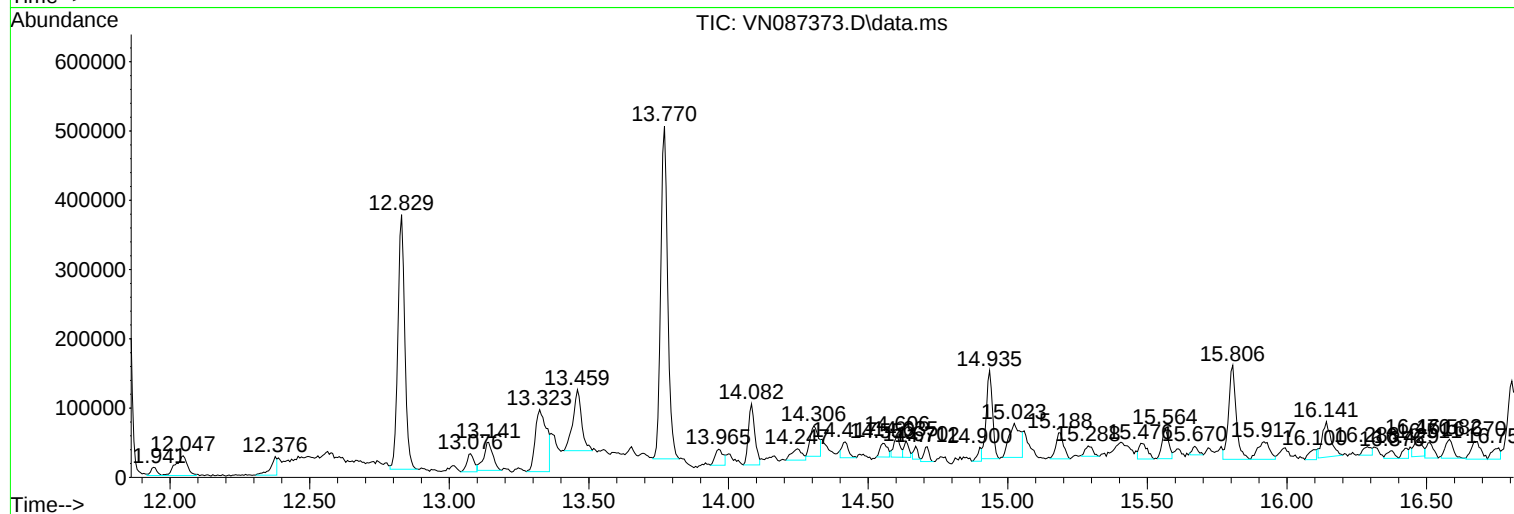
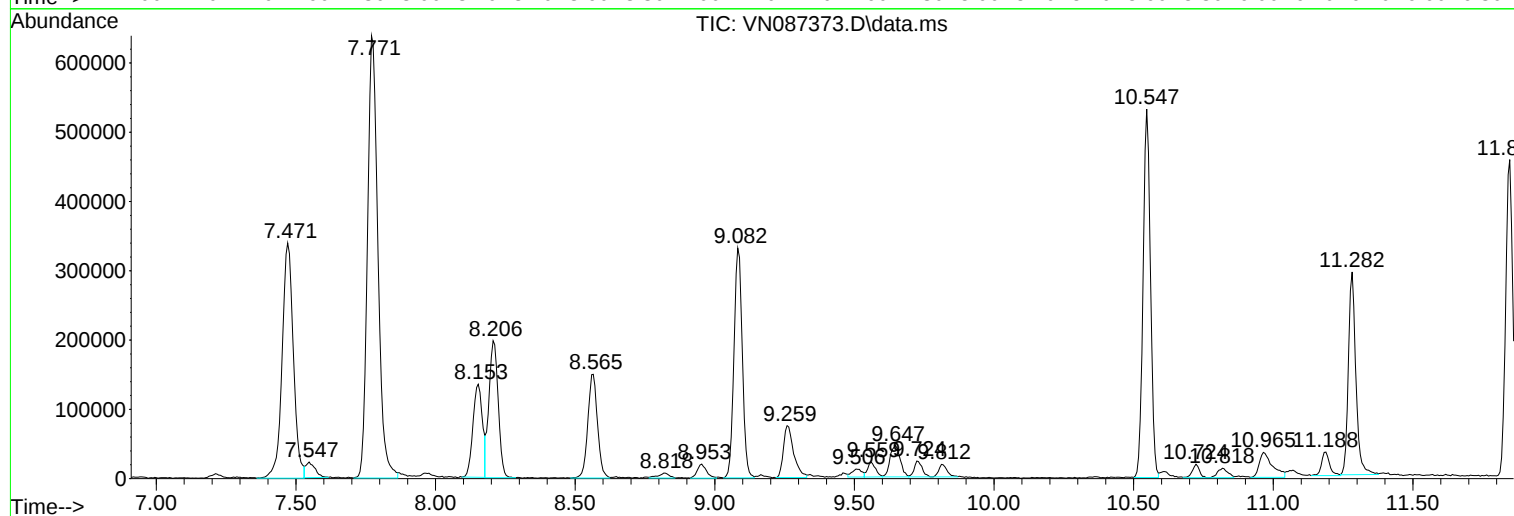
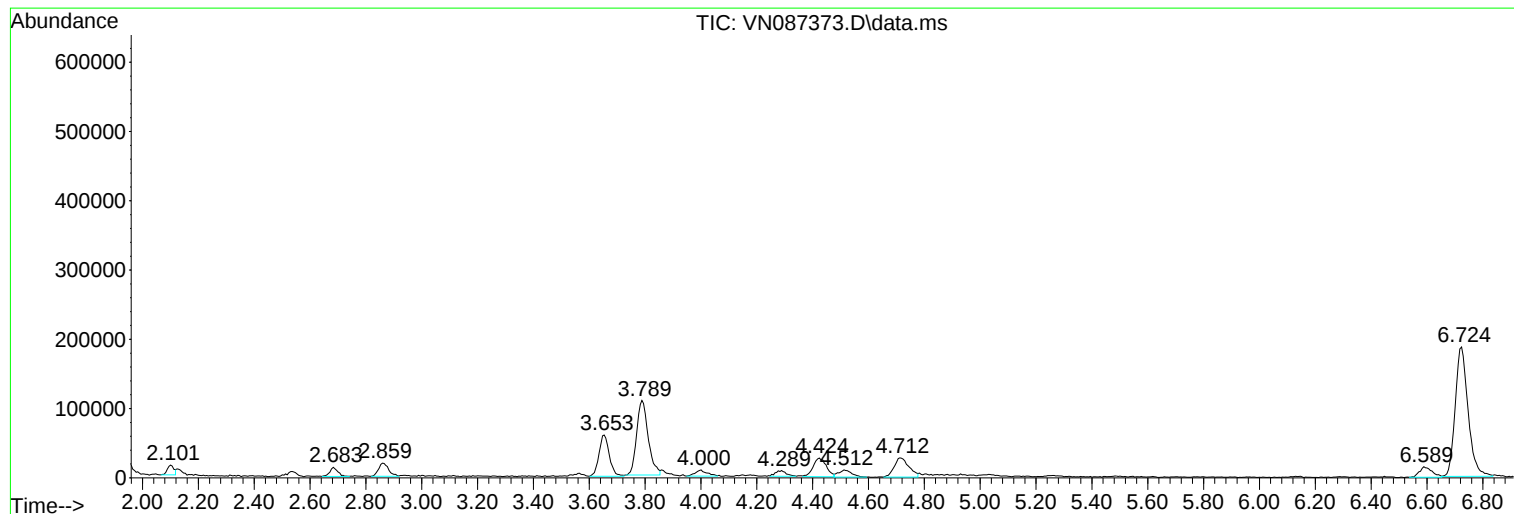
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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



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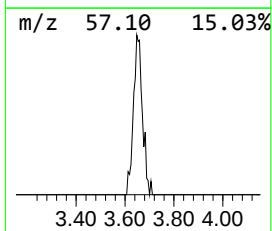
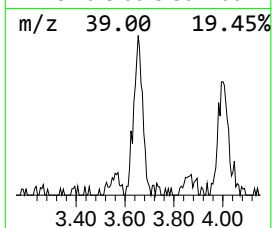
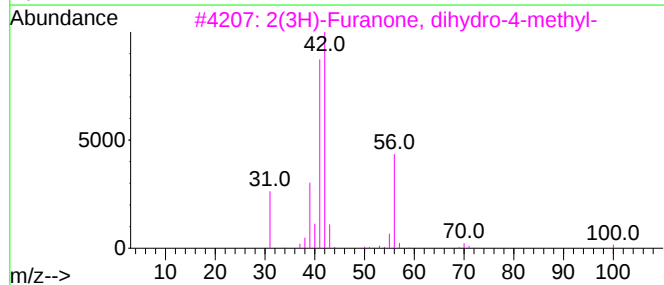
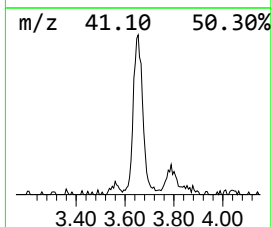
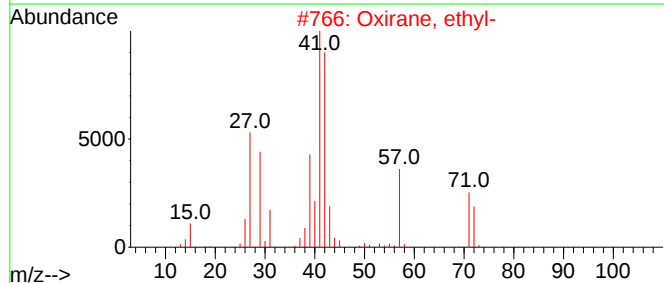
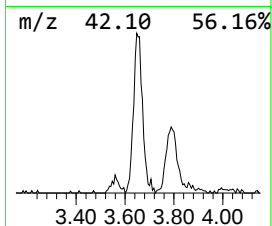
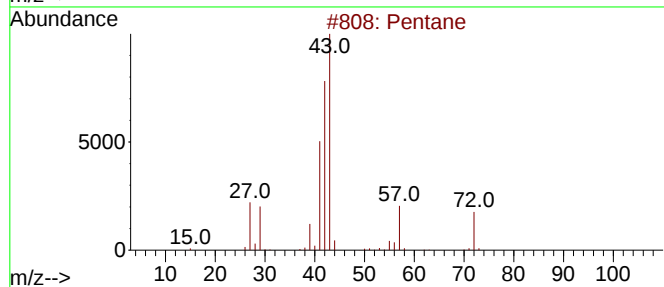
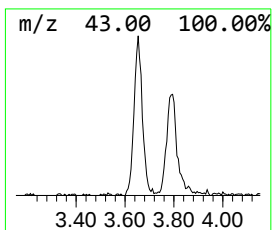
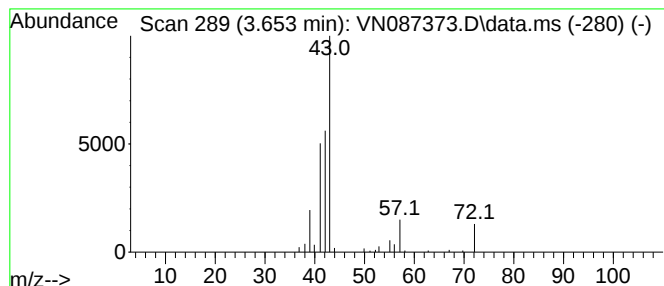
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.653	16.92 ug/l	153096	Pentafluorobenzene	8.206

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane		72	C5H12	000109-66-0	86
2	Oxirane, ethyl-		72	C4H8O	000106-88-7	53
3	2(3H)-Furanone, dihydro-4-methyl-		100	C5H8O2	001679-49-8	28
4	Diaziridine,3,3-dimethyl-		72	C3H8N2	004901-76-2	9
5	3-Buten-1-ol		72	C4H8O	000627-27-0	9



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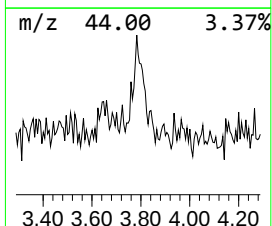
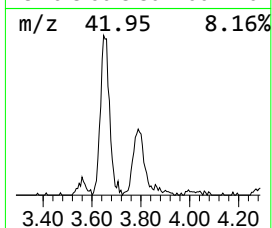
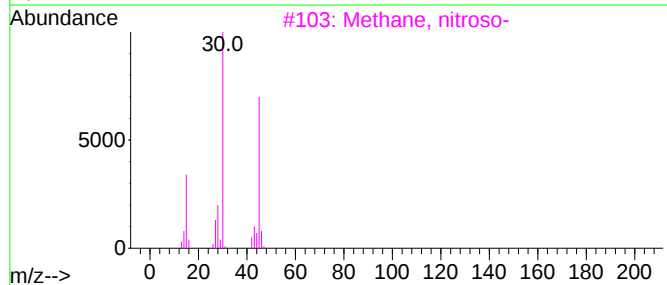
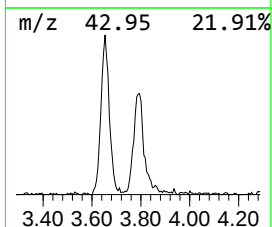
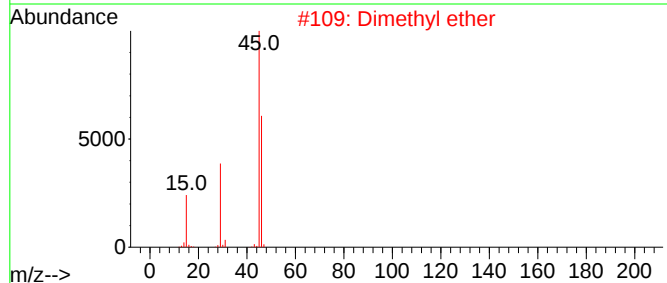
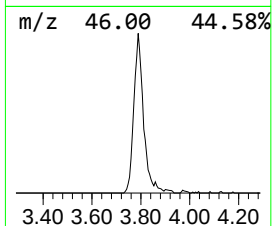
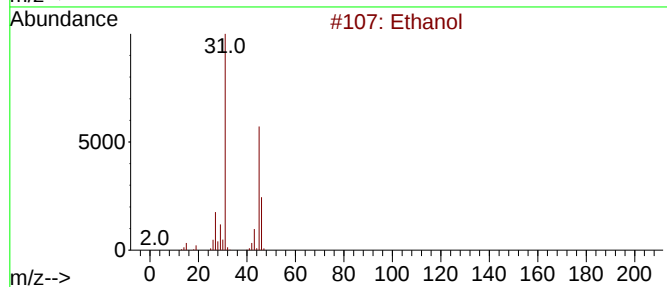
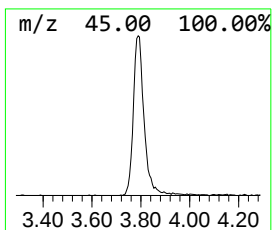
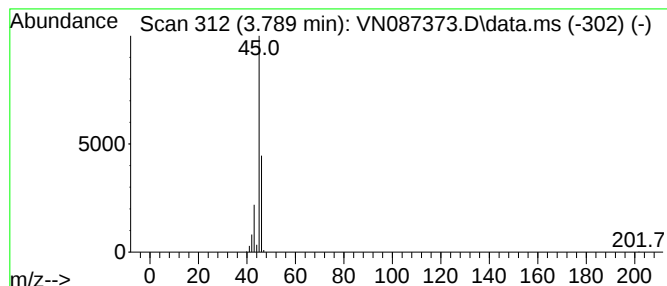
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	34.26 ug/l	310010	Pentafluorobenzene	8.206

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4



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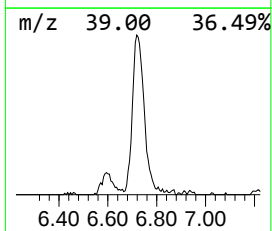
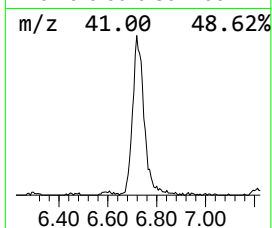
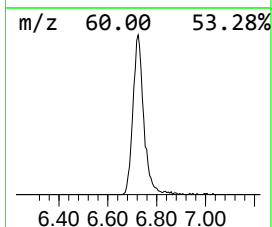
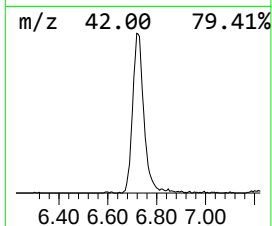
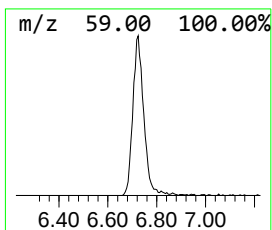
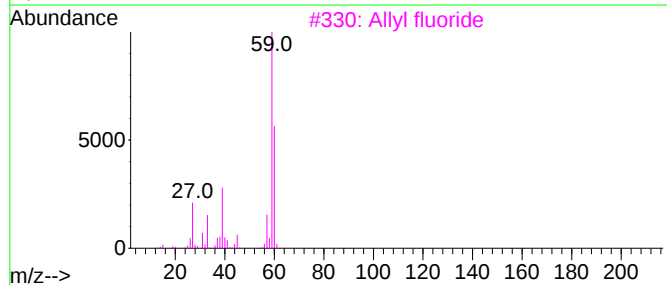
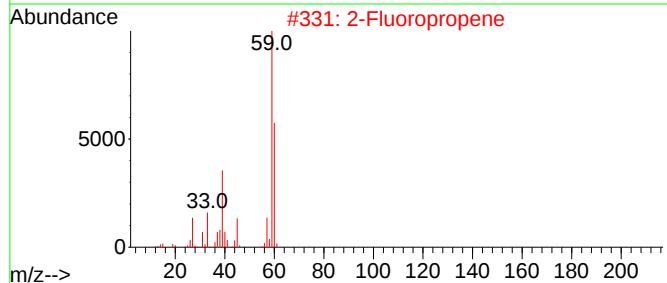
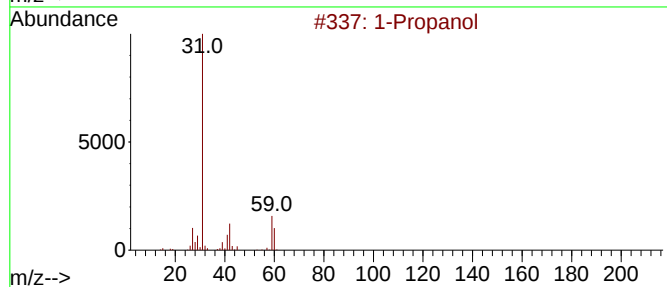
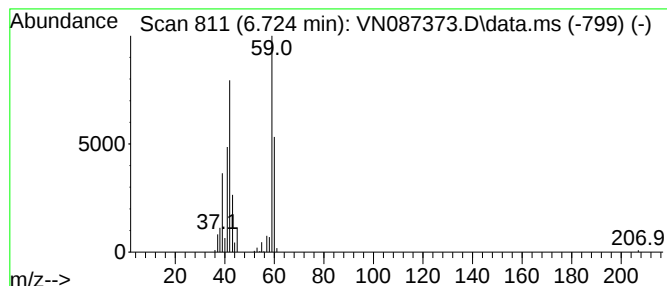
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Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.724	66.29 ug/l	599800	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	78
2			2-Fluoropropene	60	C3H5F	001184-60-7	49
3			Allyl fluoride	60	C3H5F	000818-92-8	43
4			Isoxazolidine, 4-ethyl-2,5-dimet...	129	C7H15NO	056728-13-3	28
5			Isoxazolidine, 5-ethyl-2,4-dimet...	129	C7H15NO	056728-14-4	23



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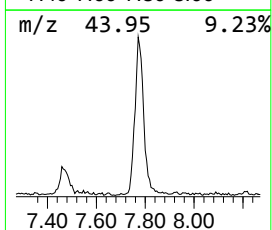
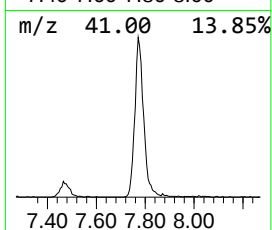
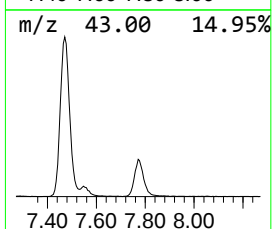
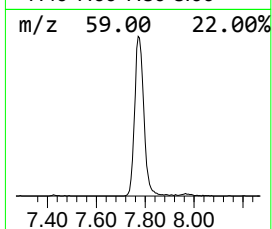
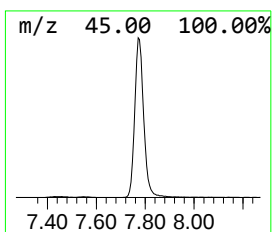
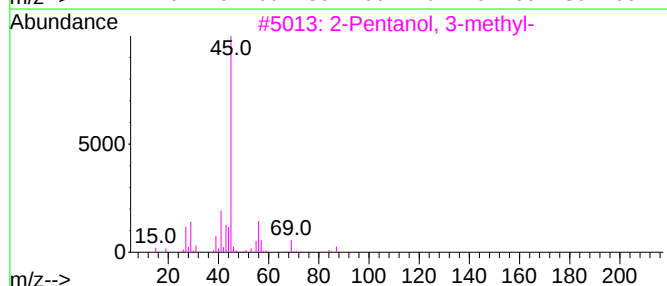
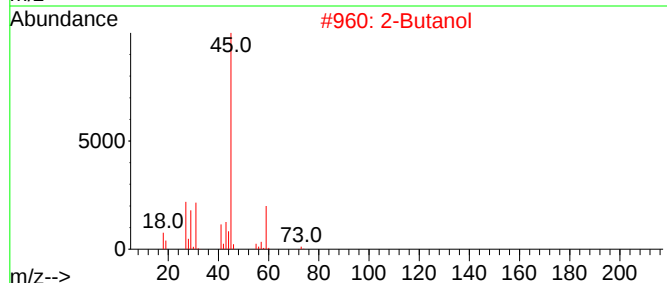
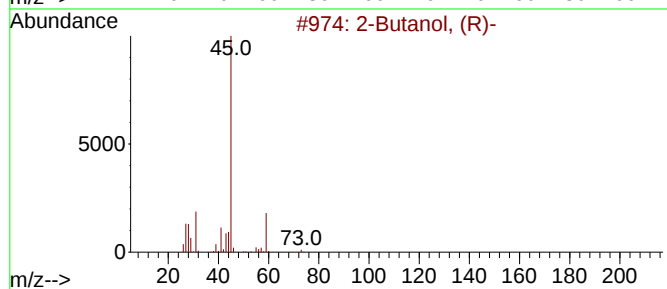
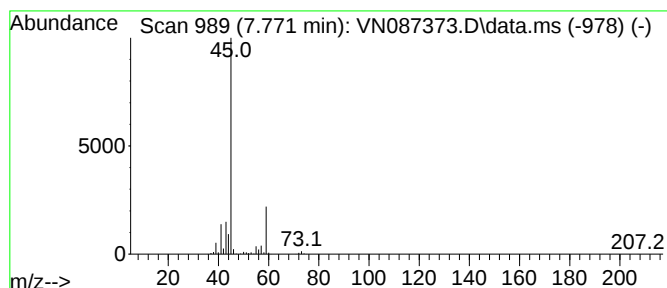
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Quant Title : SW846 8260

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

Peak Number 4 2-Butanol, (R)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.771	182.88 ug/l	1654650	Pentafluorobenzene	8.206

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-	74	C4H10O	014898-79-4	83	
2	2-Butanol	74	C4H10O	000078-92-2	83	
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	59	
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	42	
5	2-Hexanol	102	C6H14O	000626-93-7	38	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072125\
Data File : VN087373.D
Acq On : 21 Jul 2025 12:51
Operator : JC\MD
Sample : Q2646-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FRAC TANK

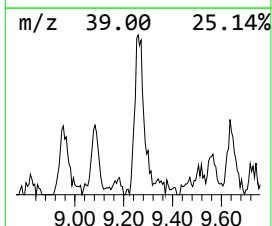
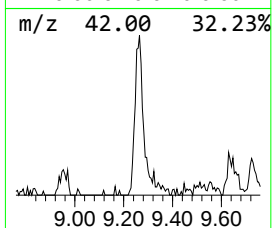
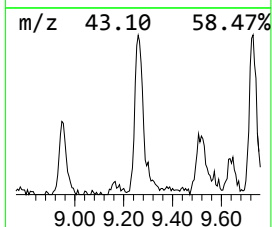
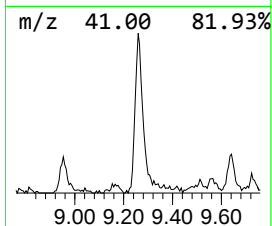
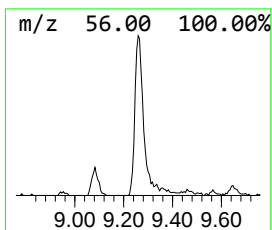
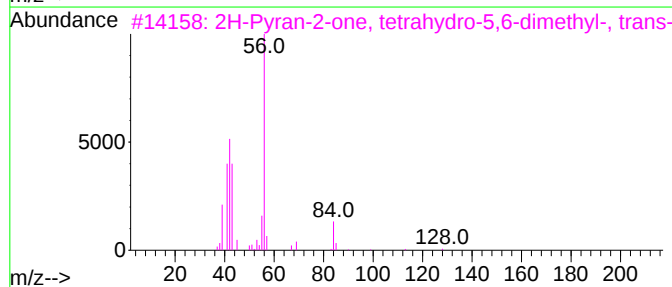
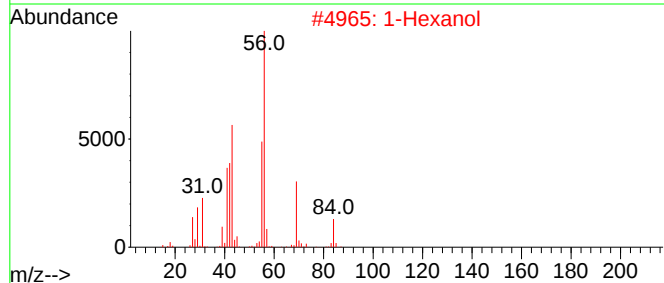
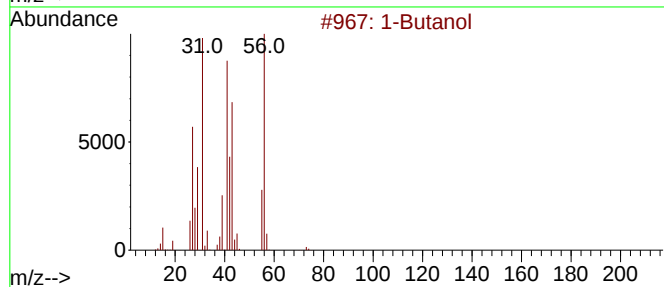
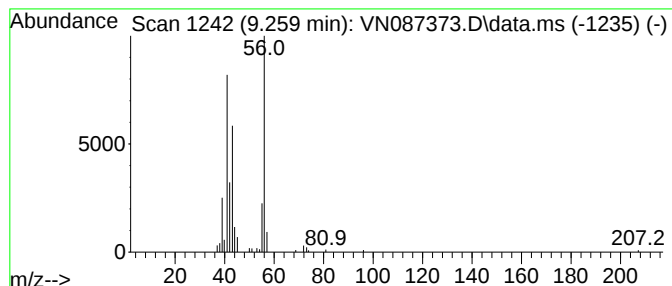
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Quant Title : SW846 8260

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

Peak Number 5 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.259	13.92 ug/l	191421	1,4-Difluorobenzene	9.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			1-Hexanol	102	C6H14O	000111-27-3	38
3			2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	36
4			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	36
5			Cyclobutane	56	C4H8	000287-23-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072125\
Data File : VN087373.D
Acq On : 21 Jul 2025 12:51
Operator : JC\MD
Sample : Q2646-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FRAC TANK

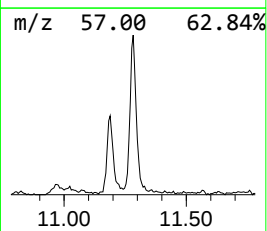
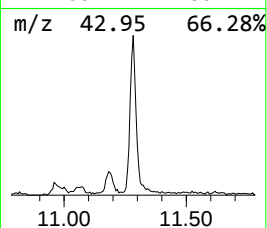
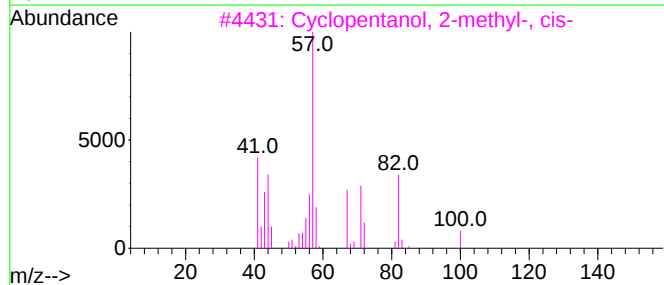
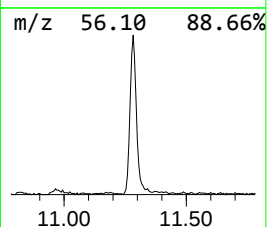
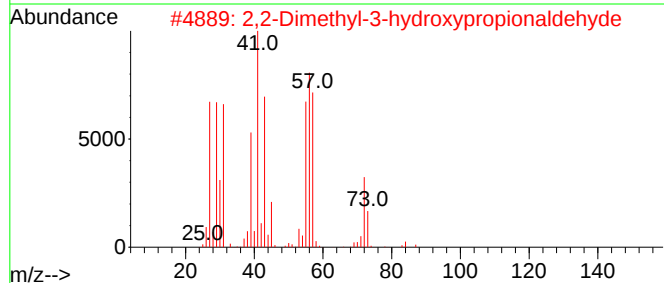
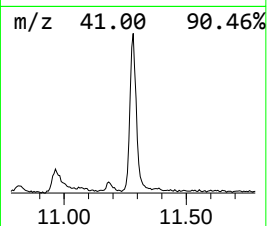
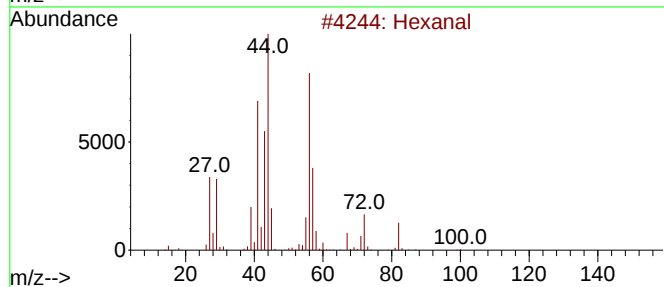
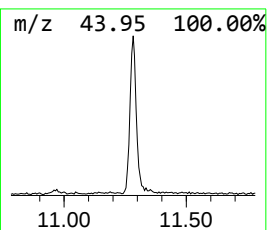
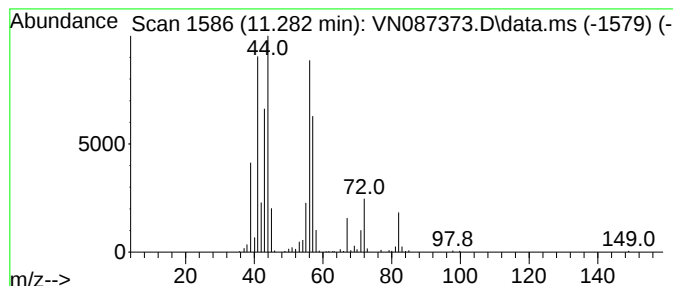
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Quant Title : SW846 8260

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

Peak Number 6 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.282	33.08 ug/l	542496	Chlorobenzene-d5	11.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	81
2			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
3			Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	35
4			Urea, trimethyl-	102	C4H10N2O	000632-14-4	25
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072125\
Data File : VN087373.D
Acq On : 21 Jul 2025 12:51
Operator : JC\MD
Sample : Q2646-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

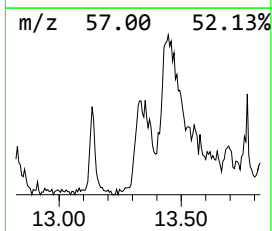
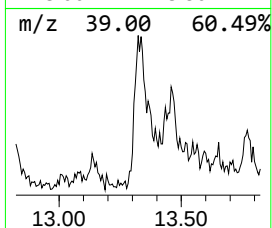
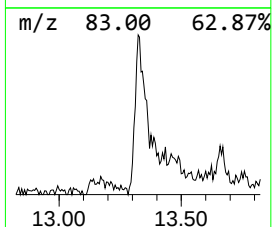
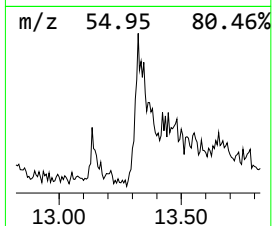
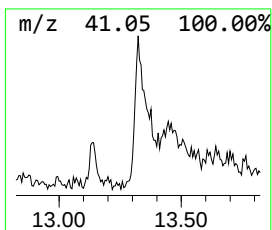
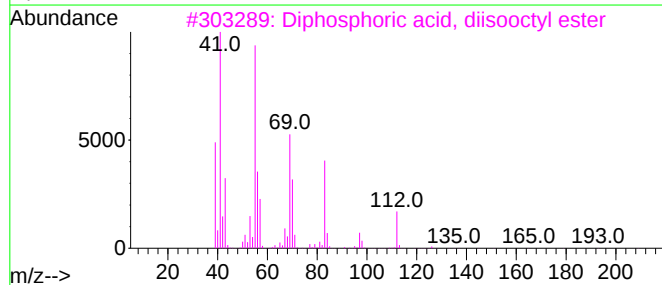
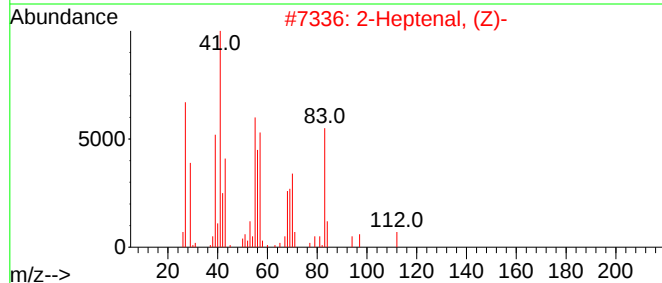
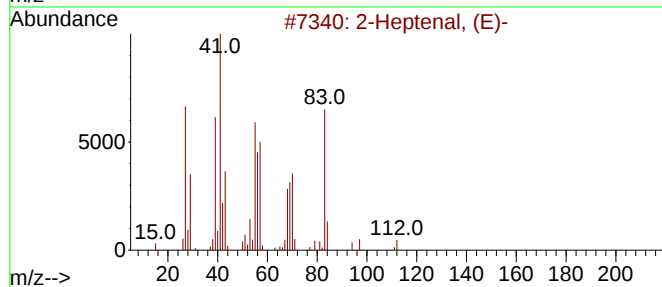
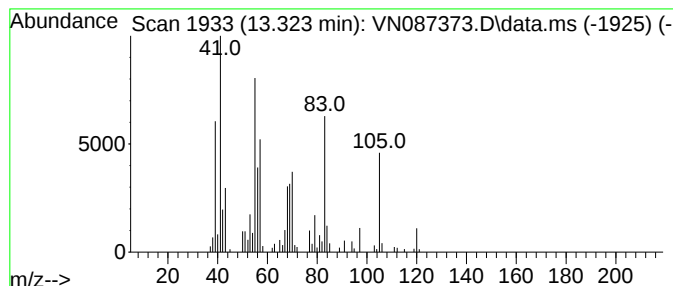
Instrument :
MSVOA_N
ClientSampleId :
FRAC TANK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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

Peak Number 7 2-Heptenal, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.323	15.39 ug/l	256110	1,4-Dichlorobenzene-d4	13.770	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptenal, (E)-	112	C7H12O	018829-55-5	86
2	2-Heptenal, (Z)-	112	C7H12O	057266-86-1	78
3	Diphosphoric acid, diisooctyl ester	402	C16H36O7P2	072101-07-6	64
4	4-Pentenal	84	C5H8O	002100-17-6	49
5	2-Pentyn-1-ol	84	C5H8O	006261-22-9	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072125\
Data File : VN087373.D
Acq On : 21 Jul 2025 12:51
Operator : JC\MD
Sample : Q2646-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FRAC TANK

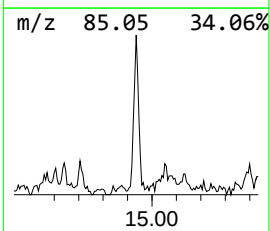
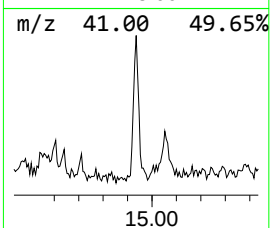
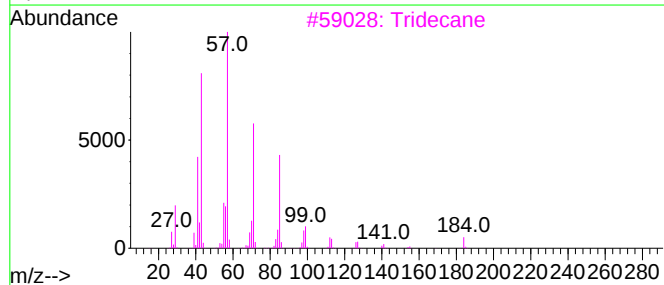
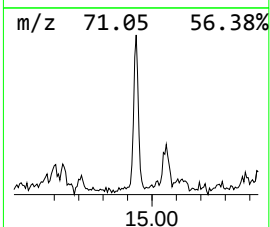
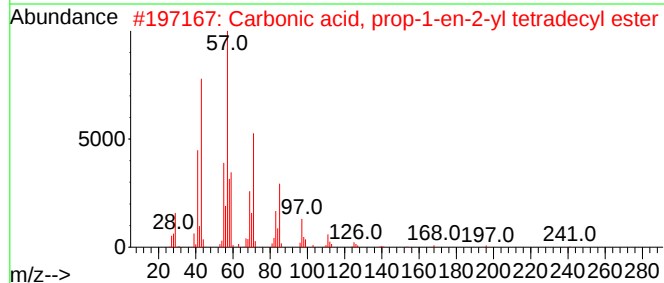
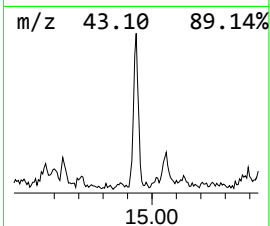
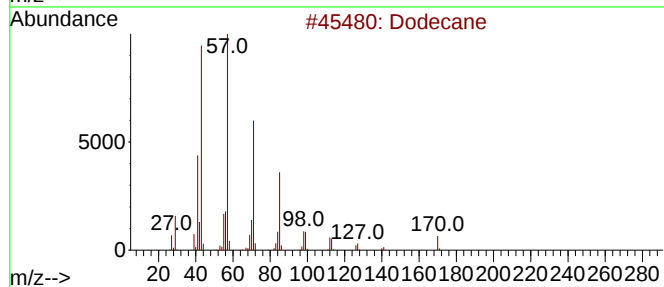
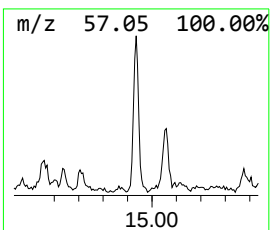
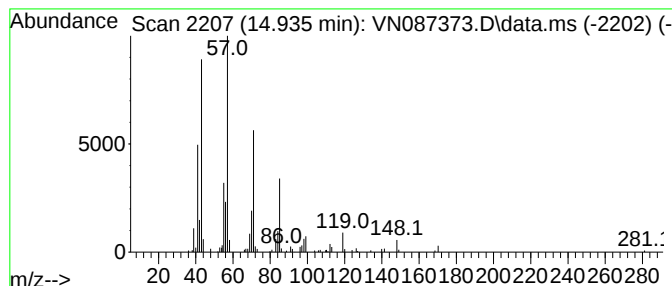
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Quant Title : SW846 8260

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

Peak Number 8 Dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	11.71 ug/l	194907	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	87
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	86
3			Tridecane	184	C13H28	000629-50-5	72
4			Tetradecane	198	C14H30	000629-59-4	72
5			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072125\
Data File : VN087373.D
Acq On : 21 Jul 2025 12:51
Operator : JC\MD
Sample : Q2646-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FRAC TANK

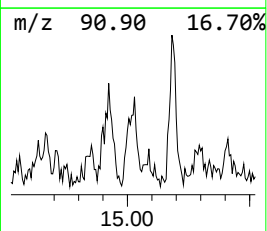
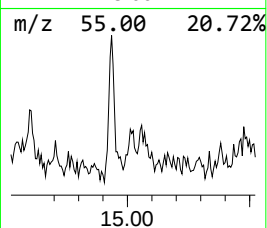
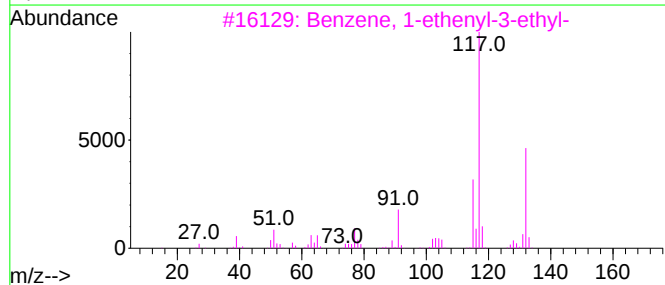
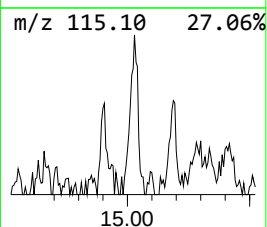
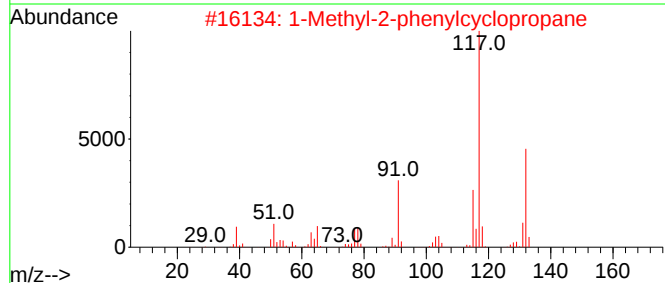
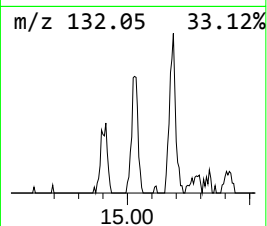
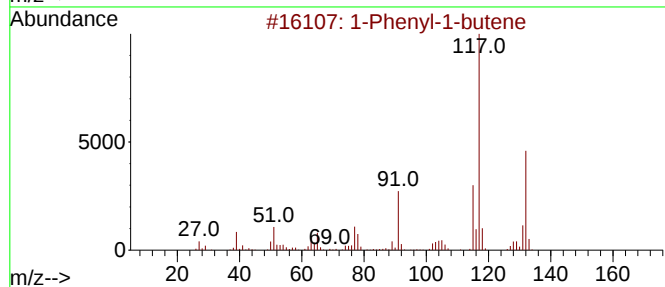
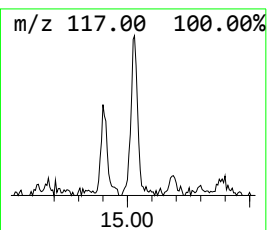
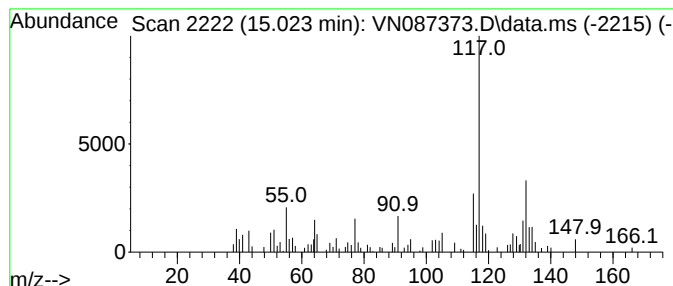
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Quant Title : SW846 8260

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

Peak Number 9 1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.023	8.50 ug/l	141552	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	81
2			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	74
5			Indan, 1-methyl-	132	C10H12	000767-58-8	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072125\
Data File : VN087373.D
Acq On : 21 Jul 2025 12:51
Operator : JC\MD
Sample : Q2646-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FRAC TANK

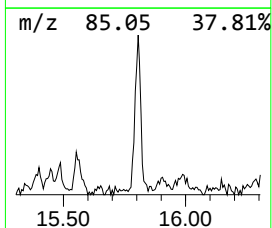
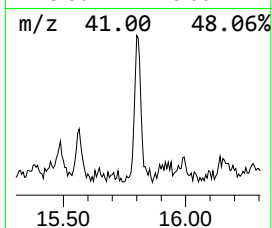
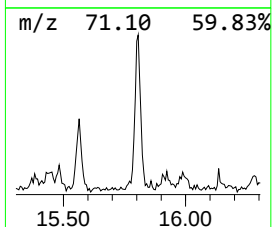
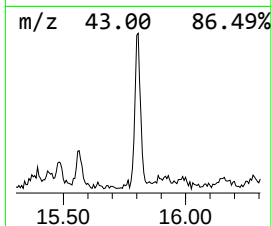
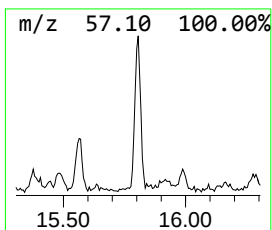
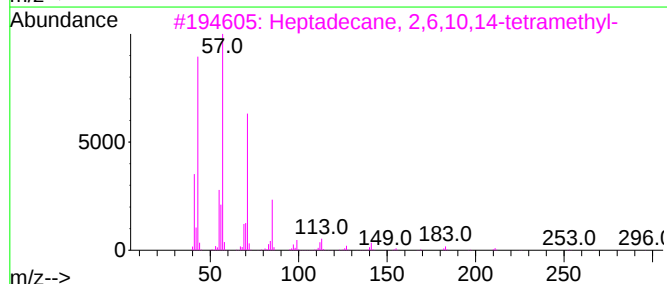
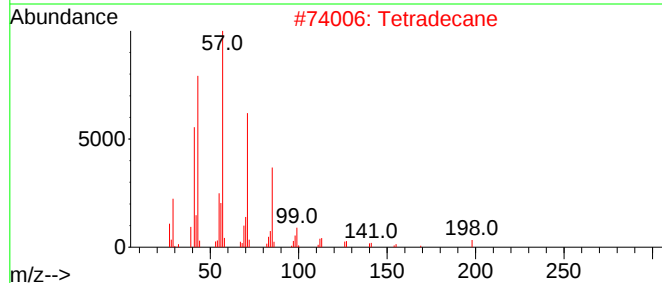
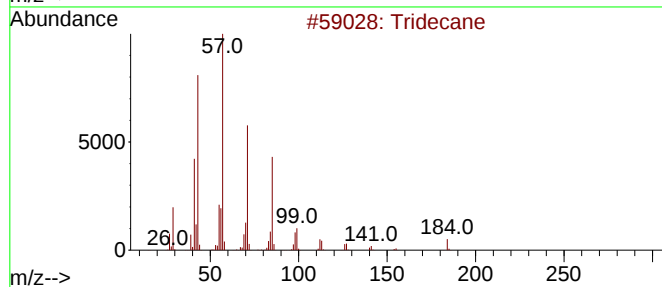
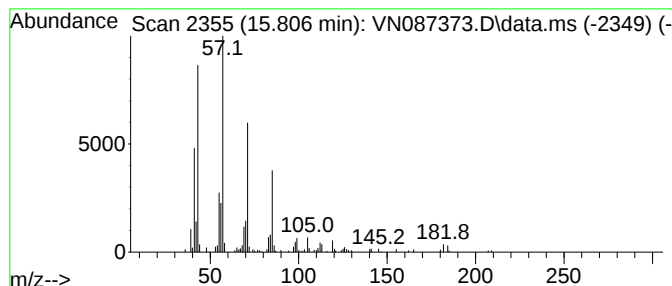
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Quant Title : SW846 8260

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

Peak Number 10 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.806	15.04 ug/l	250431	1,4-Dichlorobenzene-d4	13.770

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	93
2		Tetradecane	198	C14H30	000629-59-4	72
3		Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	72
4		Dodecane	170	C12H26	000112-40-3	64
5		Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN072125\
Data File : VN087373.D
Acq On : 21 Jul 2025 12:51
Operator : JC\MD
Sample : Q2646-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FRAC TANK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.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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Ethanol	3.789	34.3	ug/l	310010	1	8.206	452389	50.0
1-Propanol	6.724	66.3	ug/l	599800	1	8.206	452389	50.0
2-Butanol, (R)-	7.771	182.9	ug/l	1654650	1	8.206	452389	50.0
1-Butanol	9.259	13.9	ug/l	191421	2	9.088	687726	50.0
Hexanal	11.282	33.1	ug/l	542496	3	11.847	819883	50.0
2-Heptenal, (E)-	13.323	15.4	ug/l	256110	4	13.770	832331	50.0
Dodecane	14.935	11.7	ug/l	194907	4	13.770	832331	50.0
1-Phenyl-1-butene	15.023	8.5	ug/l	141552	4	13.770	832331	50.0
Tridecane	15.806	15.0	ug/l	250431	4	13.770	832331	50.0