

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071725\
 Data File : VN087342.D
 Acq On : 17 Jul 2025 13:36
 Operator : JC\MD
 Sample : Q2620-01
 Misc : 1.00g/10.0mL/100uL/5.0mL/MSVOA_N/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 GAS-BUR-25-0010

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: VN087342.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	55	60	68	rBV	22387	37534	2.11%	0.231%
2	2.889	148	159	160	rBV4	17253	38215	2.15%	0.235%
3	4.436	414	422	431	rBV2	9444	30055	1.69%	0.185%
4	6.265	721	733	744	rBV3	22523	71919	4.04%	0.442%
5	8.147	1045	1053	1056	rBV4	8987	18317	1.03%	0.113%
6	8.200	1056	1062	1073	rVB6	12227	31709	1.78%	0.195%
7	8.424	1091	1100	1107	rBV4	12872	29057	1.63%	0.178%
8	8.559	1115	1123	1131	rBV3	10294	21370	1.20%	0.131%
9	8.941	1182	1188	1197	rVB4	11775	23768	1.34%	0.146%
10	9.082	1203	1212	1219	rBV3	15359	32356	1.82%	0.199%
11	10.547	1452	1461	1465	rBV3	24278	42874	2.41%	0.263%
12	10.612	1465	1472	1481	rVB	200946	376971	21.19%	2.316%
13	10.723	1486	1491	1498	rVB4	10699	20144	1.13%	0.124%
14	11.617	1636	1643	1649	rBV4	20238	46540	2.62%	0.286%
15	11.723	1656	1661	1667	rVB2	22306	34200	1.92%	0.210%
16	12.053	1707	1717	1727	rVV3	117208	281061	15.80%	1.726%
17	12.135	1727	1731	1736	rVB3	20103	34701	1.95%	0.213%
18	12.276	1748	1755	1759	rVB5	9091	18061	1.02%	0.111%
19	12.353	1761	1768	1780	rBV5	43241	162834	9.15%	1.000%
20	12.459	1781	1786	1792	rVB2	50951	86234	4.85%	0.530%
21	12.576	1792	1806	1818	rBV9	48380	241601	13.58%	1.484%
22	12.676	1818	1823	1824	rVV4	22180	33985	1.91%	0.209%
23	12.753	1828	1836	1838	rVV2	74849	187323	10.53%	1.151%
24	12.776	1838	1840	1845	rVB2	79467	93220	5.24%	0.573%
25	12.859	1845	1854	1860	rBV2	73689	146836	8.25%	0.902%
26	12.912	1860	1863	1868	rVB5	16730	24957	1.40%	0.153%
27	13.006	1874	1879	1884	rVB4	38013	74090	4.16%	0.455%
28	13.076	1884	1891	1895	rBV2	81700	158273	8.89%	0.972%
29	13.141	1895	1902	1909	rVV2	562752	1030005	57.89%	6.327%
30	13.206	1909	1913	1918	rVB3	64812	108779	6.11%	0.668%
31	13.294	1918	1928	1930	rBV4	57380	129103	7.26%	0.793%
32	13.335	1931	1935	1937	rVV4	31928	51462	2.89%	0.316%
33	13.370	1937	1941	1948	rVB	149764	240677	13.53%	1.478%
34	13.464	1952	1957	1961	rVV	105957	152711	8.58%	0.938%
35	13.500	1961	1963	1968	rVB4	44426	53764	3.02%	0.330%
36	13.553	1968	1972	1976	rBV3	50035	77420	4.35%	0.476%

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37	13.594	1976	1979	1982	rVB3	31846	41961	2.36%	0.258%
38	13.659	1983	1990	1993	rBV5	156811	331162	18.61%	2.034%
39	13.694	1993	1996	1999	rVV	114724	144526	8.12%	0.888%
40	13.729	1999	2002	2004	rVV	54744	56295	3.16%	0.346%
41	13.764	2004	2008	2011	rVB2	126181	163009	9.16%	1.001%
42	13.800	2011	2014	2016	rBV3	37670	43670	2.45%	0.268%
43	13.835	2016	2020	2026	rVB2	161070	262239	14.74%	1.611%
44	13.923	2026	2035	2037	rBV6	76656	191908	10.79%	1.179%
45	13.959	2037	2041	2045	rBV2	103479	164723	9.26%	1.012%
46	14.082	2057	2062	2068	rBV	1131702	1779356	100.00%	10.930%
47	14.194	2078	2081	2084	rBV3	41241	47263	2.66%	0.290%
48	14.247	2084	2090	2095	rVV5	105971	209026	11.75%	1.284%
49	14.306	2096	2100	2104	rVB3	94067	136531	7.67%	0.839%
50	14.417	2113	2119	2124	rBV4	153094	300668	16.90%	1.847%
51	14.476	2125	2129	2135	rBV8	64917	125905	7.08%	0.773%
52	14.558	2138	2143	2146	rBV5	177077	337365	18.96%	2.072%
53	14.606	2146	2151	2154	rVV3	376568	613689	34.49%	3.770%
54	14.641	2154	2157	2160	rVB2	130821	159226	8.95%	0.978%
55	14.711	2165	2169	2173	rBV2	198665	265225	14.91%	1.629%
56	14.823	2184	2188	2191	rBV4	93772	164124	9.22%	1.008%
57	14.935	2198	2207	2215	rBV2	943781	1595605	89.67%	9.801%
58	15.023	2215	2222	2225	rBV5	239282	577479	32.45%	3.547%
59	15.194	2246	2251	2256	rVB2	140588	291193	16.37%	1.789%
60	15.294	2264	2268	2273	rVB7	105988	172114	9.67%	1.057%
61	15.405	2280	2287	2296	rBV9	112524	402697	22.63%	2.474%
62	15.482	2296	2300	2309	rVB7	146478	367985	20.68%	2.260%
63	15.570	2309	2315	2324	rBV2	215940	441102	24.79%	2.710%
64	15.723	2337	2341	2344	rBV6	64232	101150	5.68%	0.621%
65	15.805	2350	2355	2365	rVB	612299	1157848	65.07%	7.112%
66	15.917	2366	2374	2382	rBV7	125645	386104	21.70%	2.372%
67	16.141	2407	2412	2418	rVB2	169520	339009	19.05%	2.082%
68	16.452	2457	2465	2467	rBV4	124974	299951	16.86%	1.843%
69	16.582	2483	2487	2495	rVB	73600	135199	7.60%	0.830%
70	16.682	2497	2504	2510	rVV2	106489	232107	13.04%	1.426%

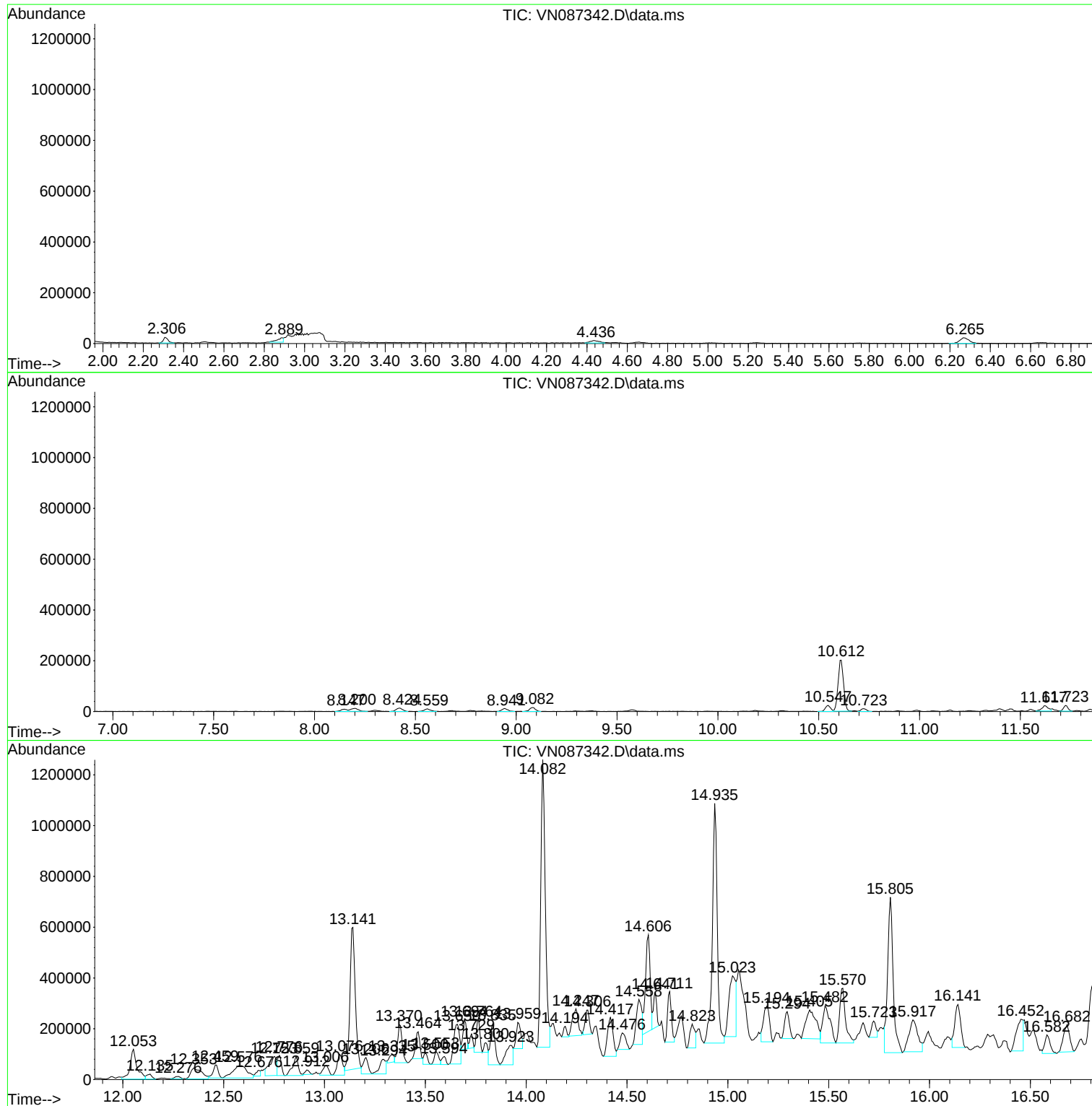
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ClientSampleId :
GAS-BUR-25-0010

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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Instrument :
MSVOA_N
ClientSampleId :
GAS-BUR-25-0010

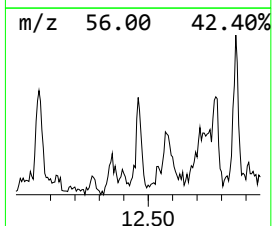
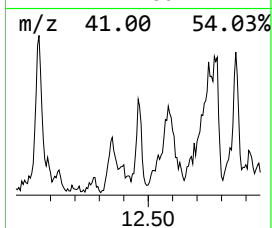
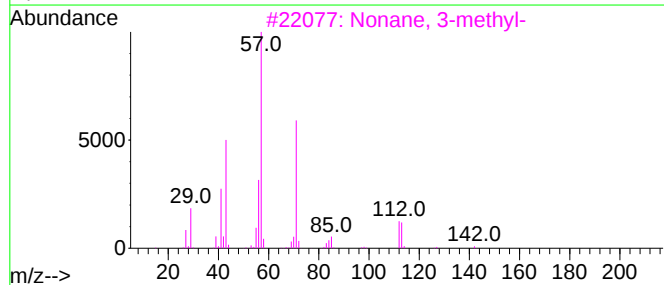
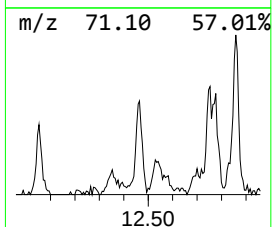
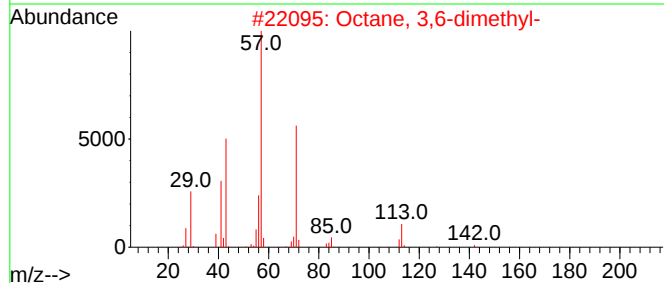
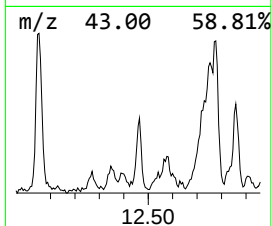
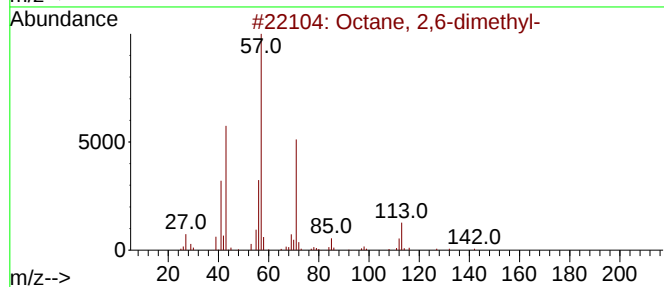
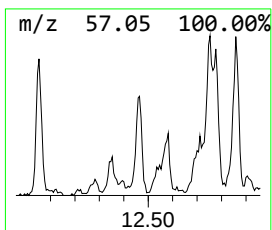
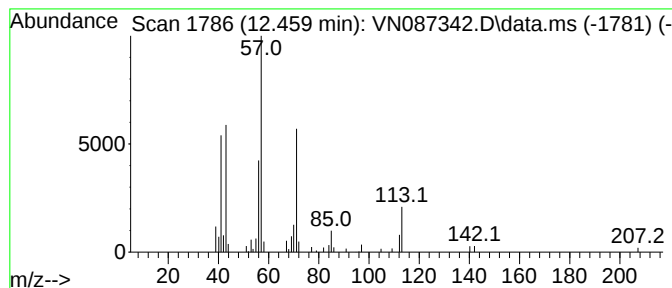
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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

Peak Number 1 Octane, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.459	126.07 ug/l	86234	Chlorobenzene-d5	11.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
2			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	72
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	64
4			Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	50
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	50



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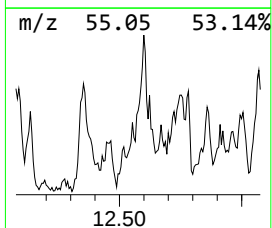
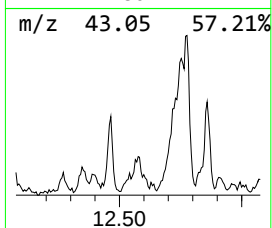
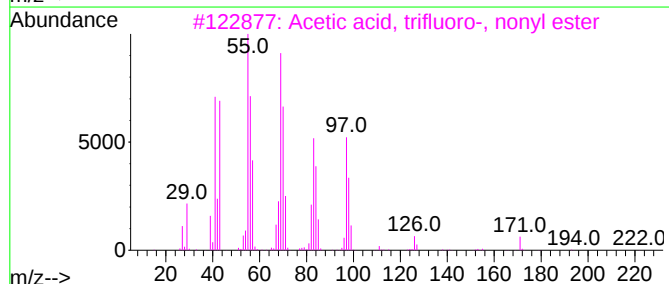
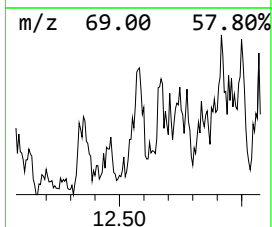
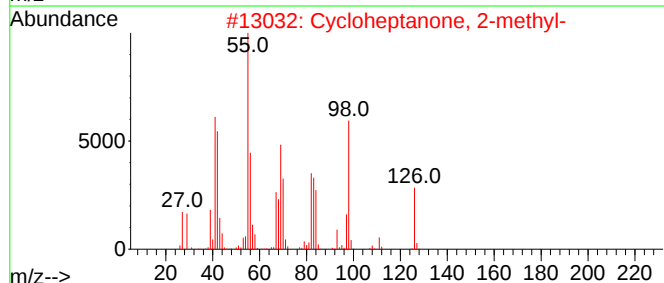
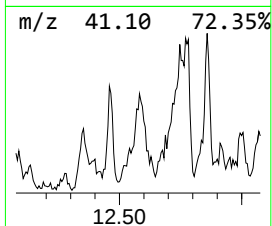
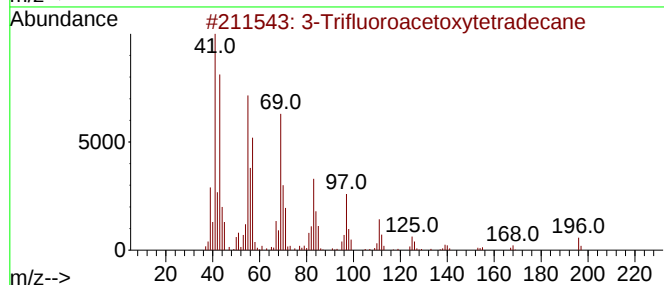
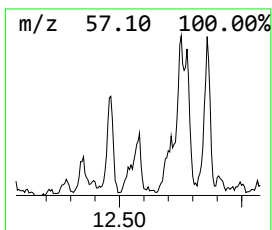
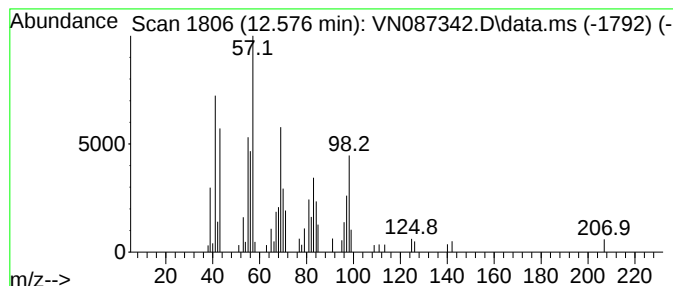
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Trifluoroacetyltetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.576	353.22 ug/l	241601	Chlorobenzene-d5	11.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Trifluoroacetyltetradecane	310	C16H29F3O2	1010245-47-5	72
2			Cycloheptanone, 2-methyl-	126	C8H14O	000932-56-9	60
3			Acetic acid, trifluoro-, nonyl e...	240	C11H19F3O2	030767-14-7	59
4			1-Tetradecene	196	C14H28	001120-36-1	58
5			Decyl trifluoroacetate	254	C12H21F3O2	000333-88-0	58



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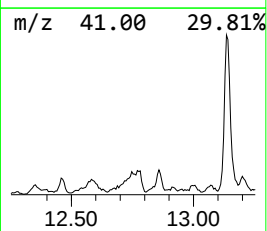
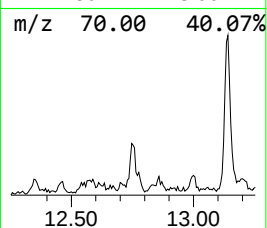
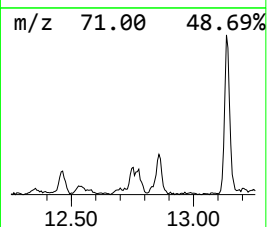
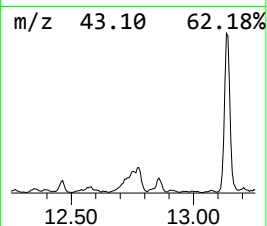
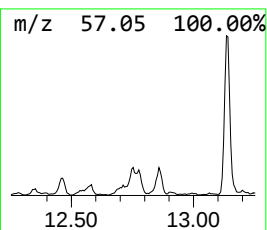
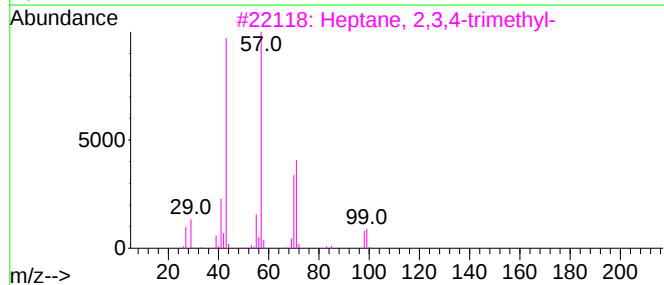
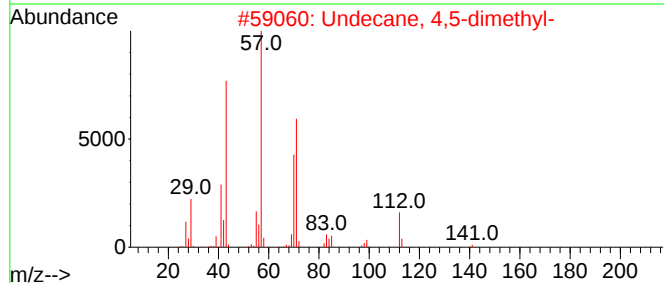
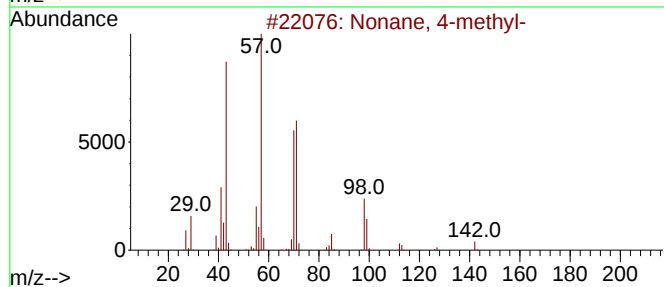
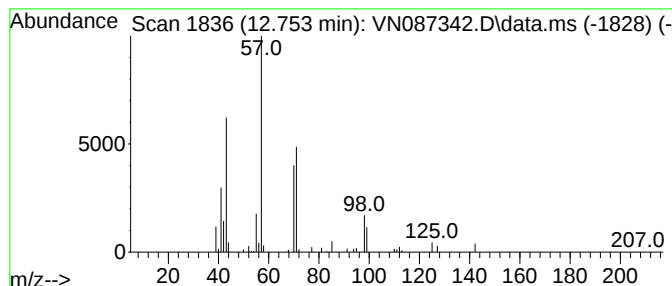
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Peak Number 3 Nonane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.753	273.86 ug/l	187323	Chlorobenzene-d5	11.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 4-methyl-	142	C10H22	017301-94-9	91
2			Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	64
3			Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	56
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	50



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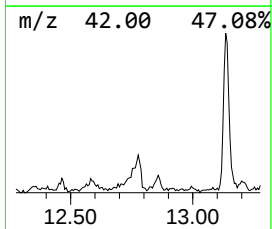
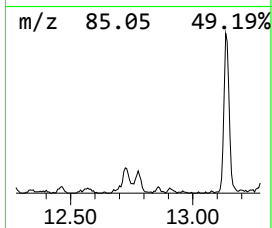
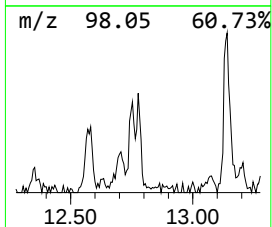
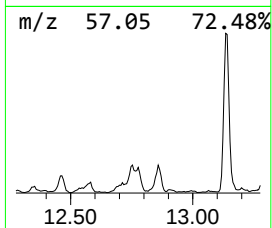
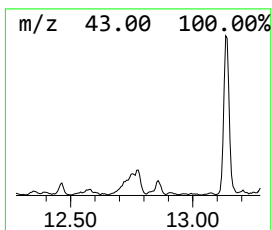
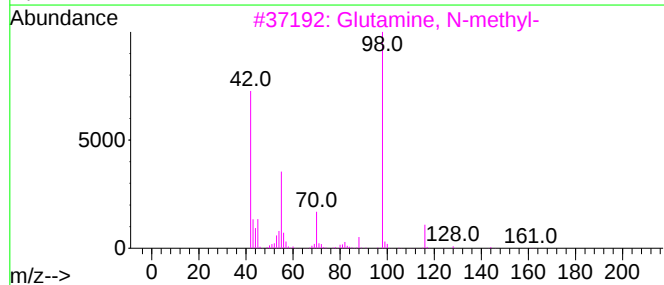
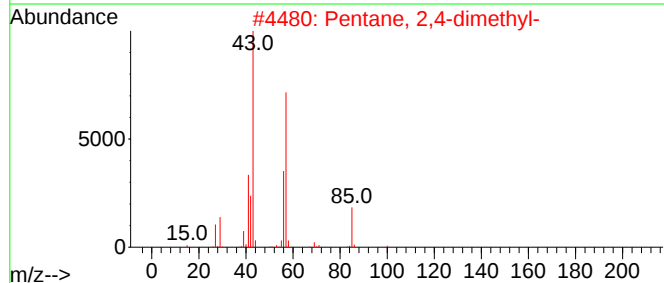
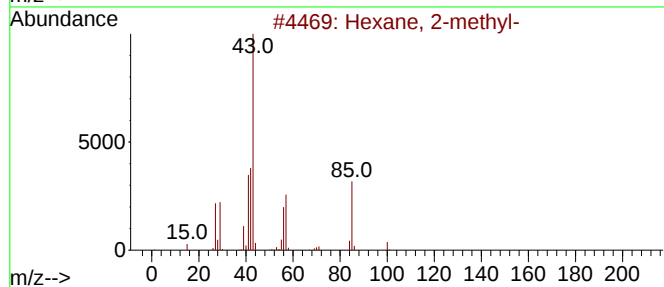
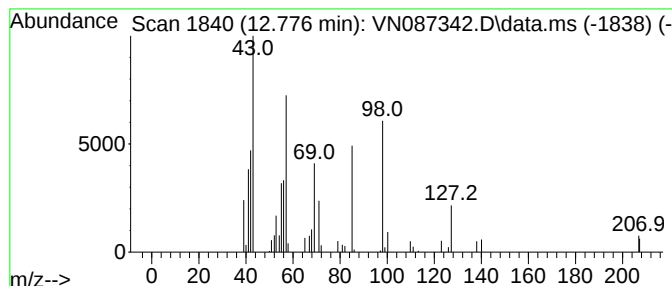
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown12.776 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.776	136.29 ug/l	93220	Chlorobenzene-d5	11.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2-methyl-	100	C7H16	000591-76-4	32
2			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	16
3			Glutamine, N-methyl-	161	C6H11NO4	1000130-17-1	16
4			Oxalic acid, allyl isohexyl ester	214	C11H18O4	1000309-23-3	14
5			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071725\
Data File : VN087342.D
Acq On : 17 Jul 2025 13:36
Operator : JC\MD
Sample : Q2620-01
Misc : 1.00g/10.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GAS-BUR-25-0010

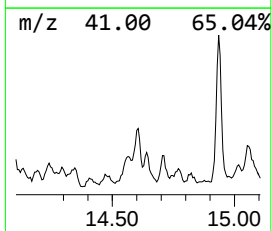
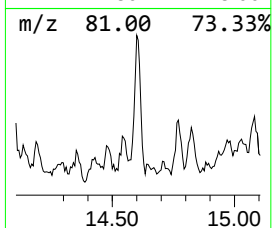
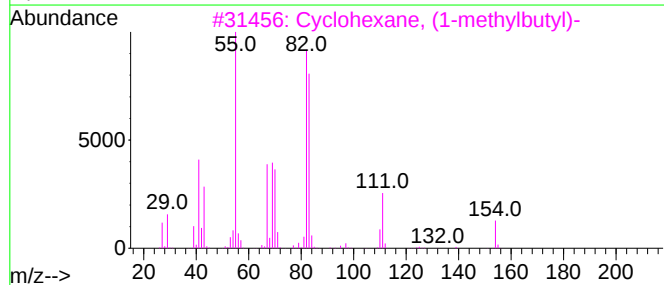
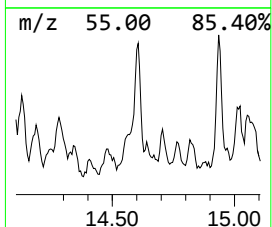
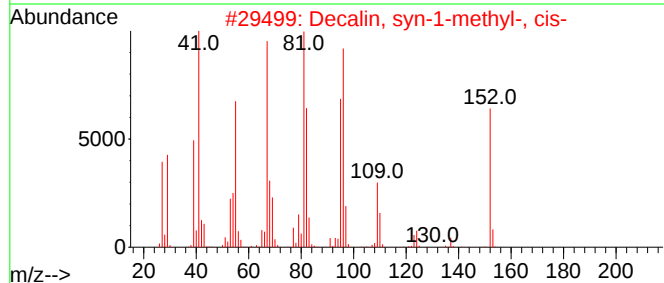
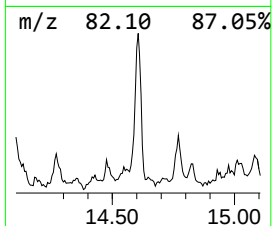
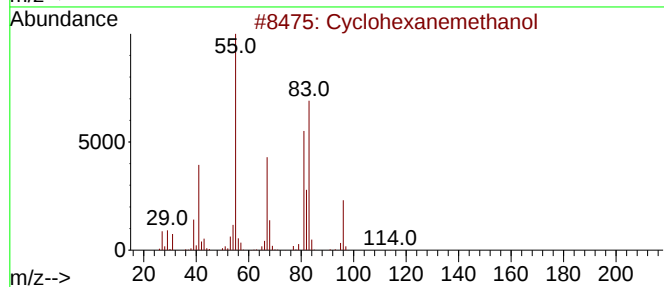
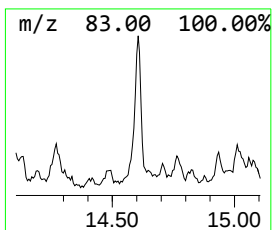
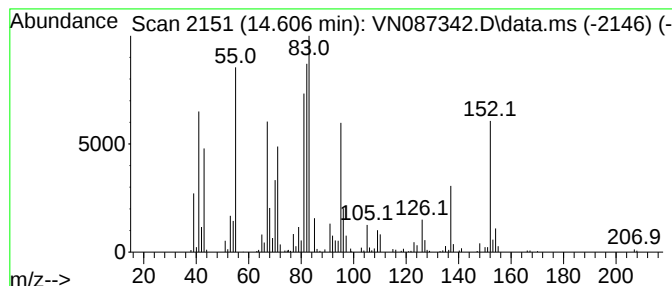
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Quant Title : SW846 8260

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

Peak Number 5 unknown14.605 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.605	188.24 ug/l	613689	1,4-Dichlorobenzene-d4	13.776

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol	114	C7H14O	000100-49-2	43
2			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	43
3			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	38
4			Pulegone	152	C10H16O	000089-82-7	38
5			Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071725\
Data File : VN087342.D
Acq On : 17 Jul 2025 13:36
Operator : JC\MD
Sample : Q2620-01
Misc : 1.00g/10.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GAS-BUR-25-0010

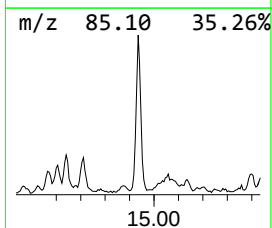
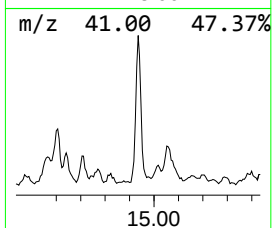
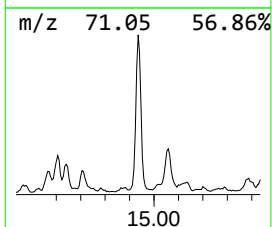
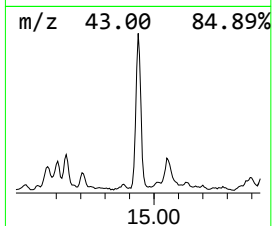
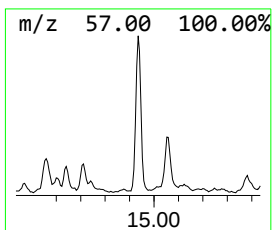
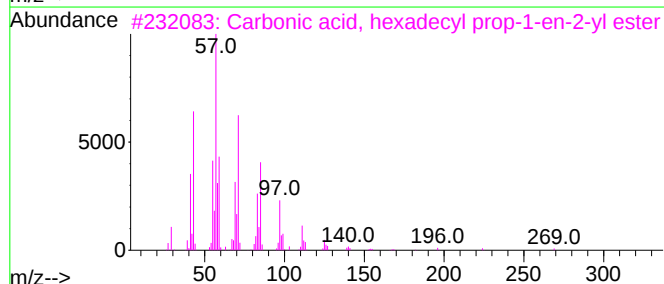
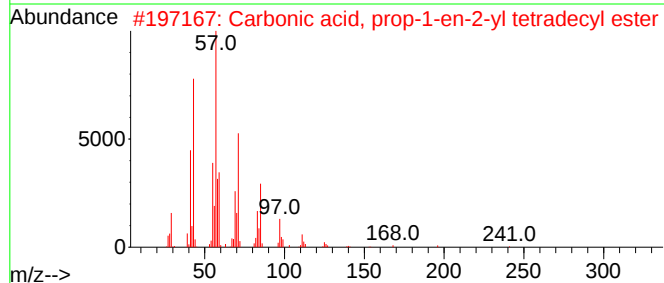
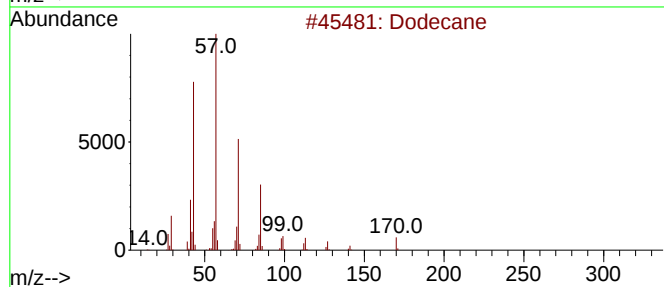
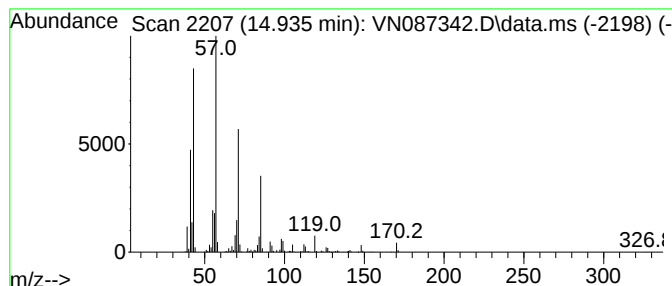
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	489.42 ug/l	1595610	1,4-Dichlorobenzene-d4	13.776

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	80
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	78
4			Tetradecane	198	C14H30	000629-59-4	78
5			Tridecane	184	C13H28	000629-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071725\
Data File : VN087342.D
Acq On : 17 Jul 2025 13:36
Operator : JC\MD
Sample : Q2620-01
Misc : 1.00g/10.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GAS-BUR-25-0010

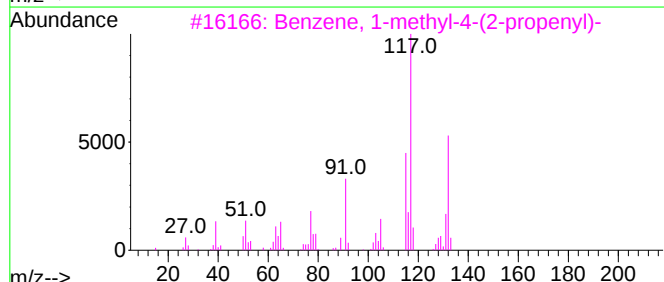
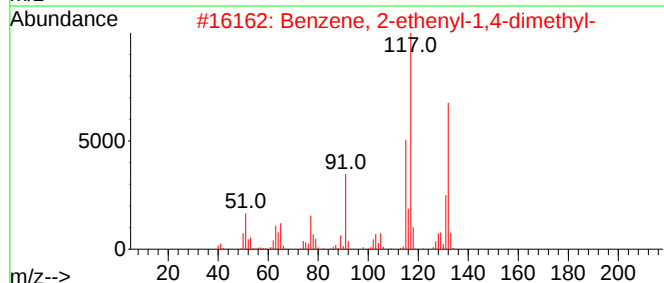
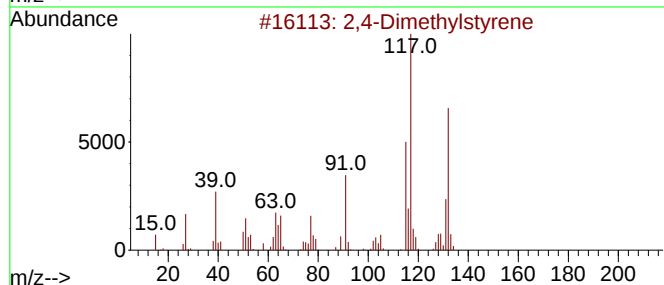
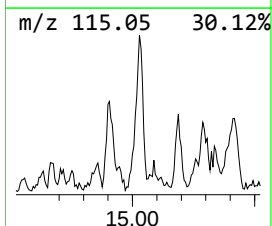
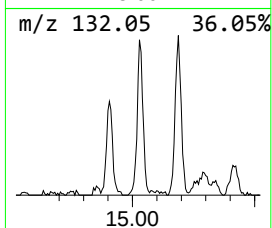
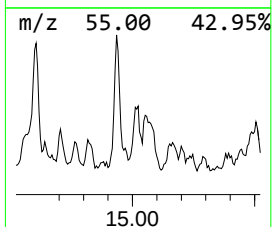
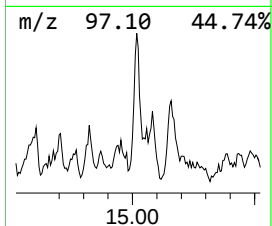
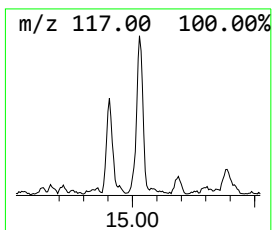
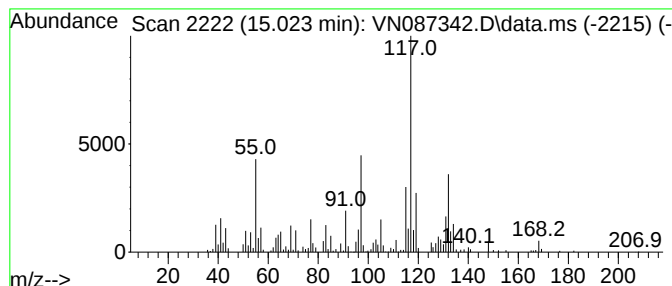
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Quant Title : SW846 8260

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

Peak Number 7 2,4-Dimethylstyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.023	177.13 ug/l	577479	1,4-Dichlorobenzene-d4	13.776

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylstyrene	132	C10H12	002234-20-0	90
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	86
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	64
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071725\
Data File : VN087342.D
Acq On : 17 Jul 2025 13:36
Operator : JC\MD
Sample : Q2620-01
Misc : 1.00g/10.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GAS-BUR-25-0010

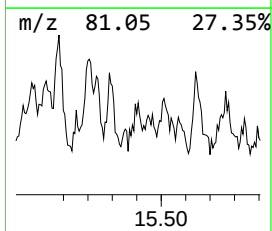
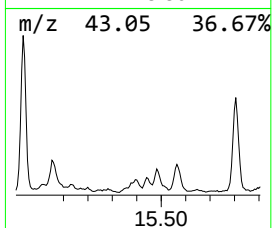
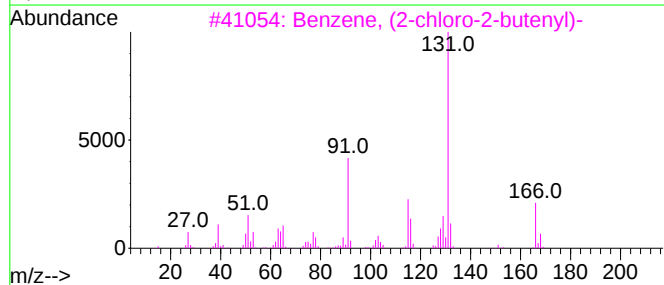
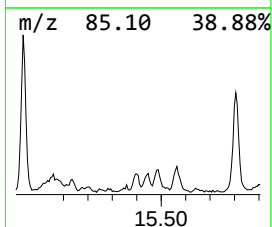
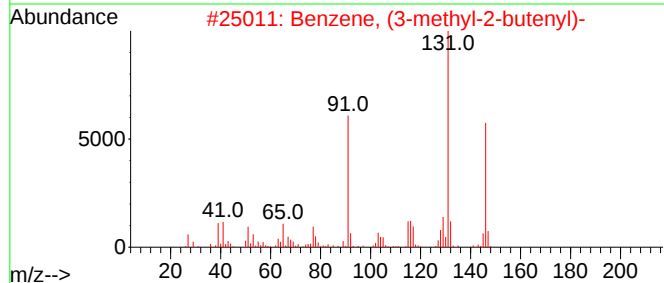
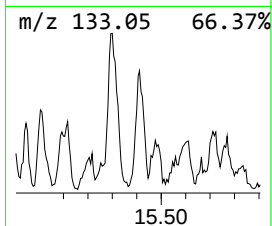
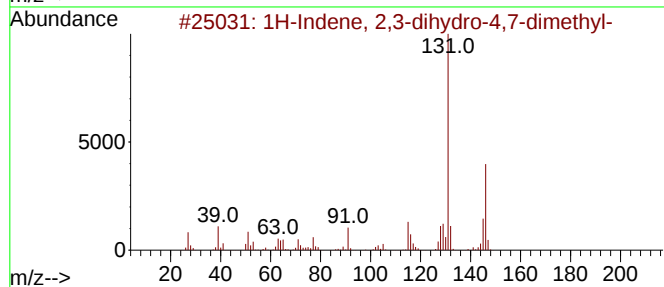
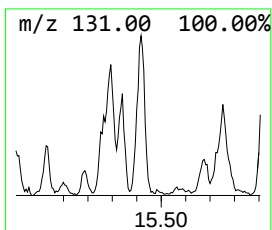
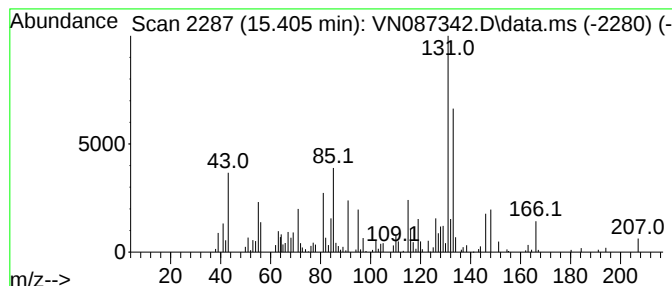
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.406 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.406	123.52 ug/l	402697	1,4-Dichlorobenzene-d4	13.776

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	46		
2	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	46		
3	Benzene, (2-chloro-2-butenyl)-	166	C10H11Cl	054411-12-0	46		
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	41		
5	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	41		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071725\
Data File : VN087342.D
Acq On : 17 Jul 2025 13:36
Operator : JC\MD
Sample : Q2620-01
Misc : 1.00g/10.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GAS-BUR-25-0010

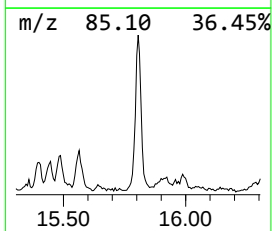
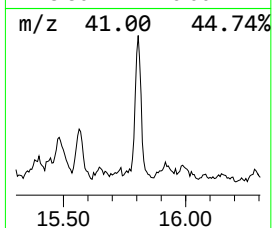
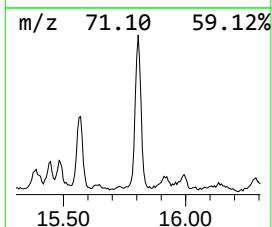
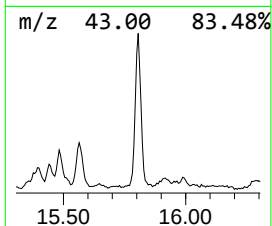
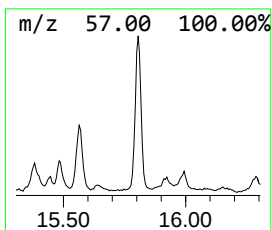
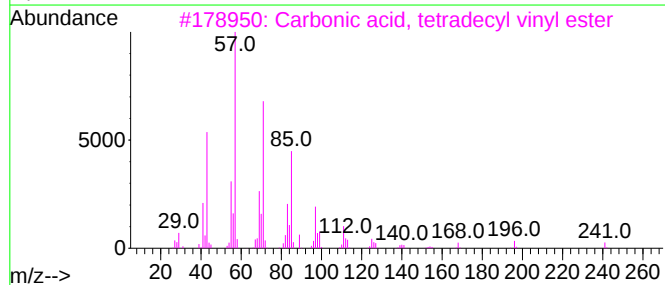
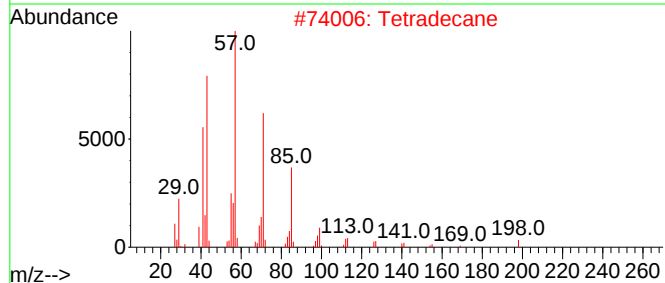
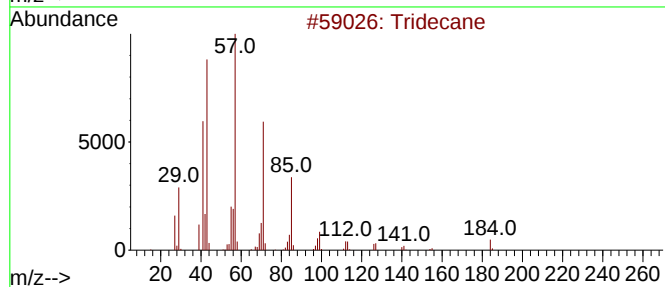
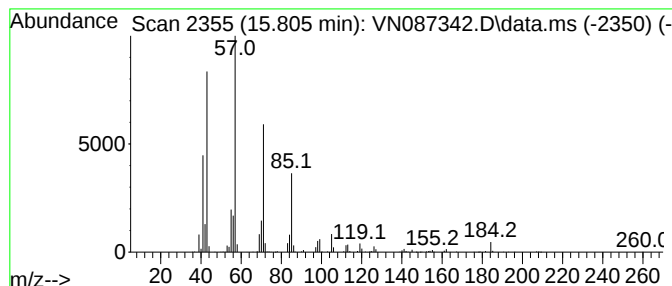
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.806	355.15 ug/l	1157850	1,4-Dichlorobenzene-d4	13.776

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Tetradecane	198	C14H30	000629-59-4	86
3			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86
4			Dodecane	170	C12H26	000112-40-3	80
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071725\
Data File : VN087342.D
Acq On : 17 Jul 2025 13:36
Operator : JC\MD
Sample : Q2620-01
Misc : 1.00g/10.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GAS-BUR-25-0010

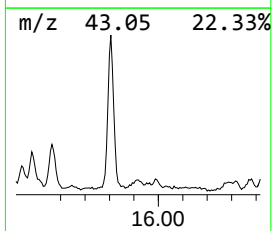
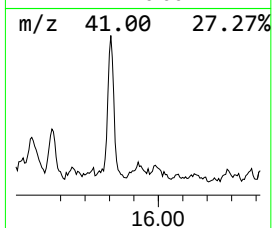
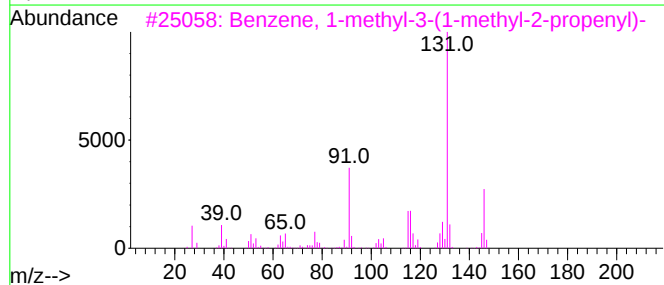
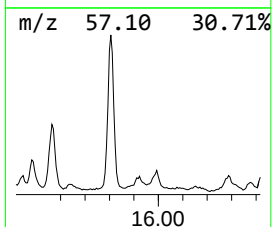
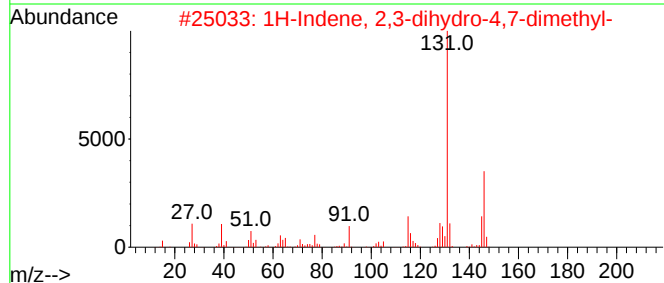
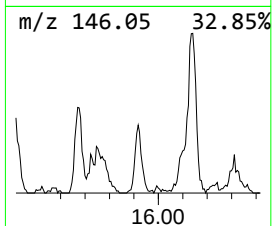
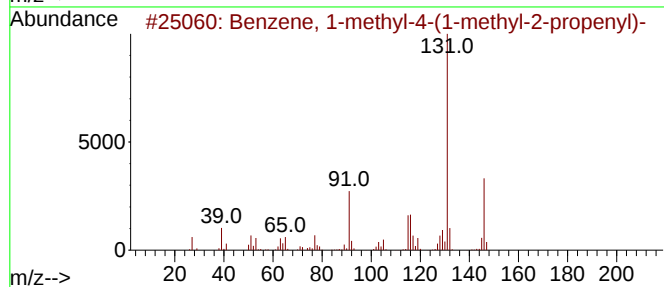
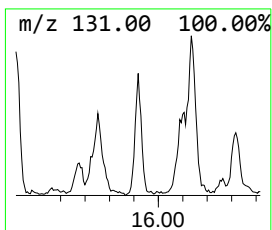
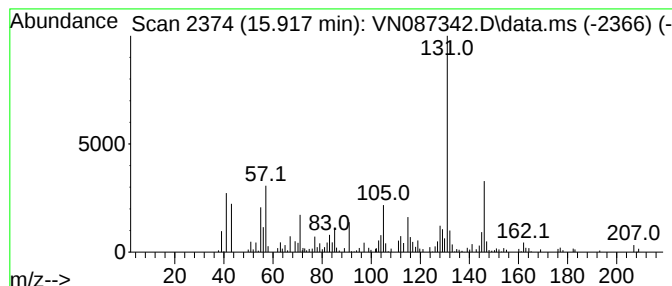
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-methyl-4-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.917	118.43 ug/l	386104	1,4-Dichlorobenzene-d4	13.776

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	90
2			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
3			Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	81
4			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	81
5			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071725\
Data File : VN087342.D
Acq On : 17 Jul 2025 13:36
Operator : JC\MD
Sample : Q2620-01
Misc : 1.00g/10.0mL/100uL/5.0mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GAS-BUR-25-0010

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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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3-Trifluoroacet...	12.576	353.2	ug/l	241601	3	11.847	34200	50.0
Nonane, 4-methyl-	12.753	273.9	ug/l	187323	3	11.847	34200	50.0
unknown12.776	12.776	136.3	ug/l	93220	3	11.847	34200	50.0
unknown14.605	14.605	188.2	ug/l	613689	4	13.776	163009	50.0
Dodecane	14.935	489.4	ug/l	1595610	4	13.776	163009	50.0
2,4-Dimethylsty...	15.023	177.1	ug/l	577479	4	13.776	163009	50.0
unknown15.406	15.406	123.5	ug/l	402697	4	13.776	163009	50.0
Tridecane	15.806	355.1	ug/l	1157850	4	13.776	163009	50.0
Benzene, 1-meth...	15.917	118.4	ug/l	386104	4	13.776	163009	50.0