

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031425\
 Data File : VN085992.D
 Acq On : 14 Mar 2025 16:21
 Operator : JC\MD
 Sample : Q1575-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW3

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\82N021825W.M
 Title : SW846 8260

Signal : TIC: VN085992.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.277	549	565	587	rBV	33348	139043	4.33%	0.760%
2	7.224	885	896	907	rBV2	98038	280062	8.73%	1.531%
3	8.165	1041	1056	1060	rBV	120188	277697	8.66%	1.518%
4	8.224	1060	1066	1075	rVV	225569	514514	16.04%	2.813%
5	8.324	1075	1083	1094	rVB	288255	689710	21.50%	3.771%
6	8.447	1096	1104	1110	rBV3	25457	55652	1.73%	0.304%
7	8.577	1119	1126	1135	rVB2	116643	259536	8.09%	1.419%
8	8.759	1141	1157	1168	rBV	1359792	3208180	100.00%	17.539%
9	8.847	1168	1172	1182	rVB4	19502	48263	1.50%	0.264%
10	9.100	1204	1215	1228	rBV	326811	680986	21.23%	3.723%
11	9.588	1287	1298	1303	rBV3	152622	367379	11.45%	2.008%
12	9.641	1303	1307	1314	rVB2	122474	226290	7.05%	1.237%
13	9.723	1314	1321	1328	rBV	105003	220766	6.88%	1.207%
14	9.859	1335	1344	1349	rBV7	12820	33186	1.03%	0.181%
15	10.012	1359	1370	1380	rBV	891128	1722382	53.69%	9.416%
16	10.141	1380	1392	1406	rBV	1364027	2845633	88.70%	15.557%
17	10.323	1415	1423	1432	rBV4	57239	148031	4.61%	0.809%
18	10.494	1438	1452	1457	rBV	177331	331971	10.35%	1.815%
19	10.565	1457	1464	1477	rVB	488043	920153	28.68%	5.031%
20	10.747	1487	1495	1503	rVB7	24822	71105	2.22%	0.389%
21	10.912	1517	1523	1529	rBV5	20643	47310	1.47%	0.259%
22	11.006	1529	1539	1545	rVV4	51157	144701	4.51%	0.791%
23	11.170	1559	1567	1573	rBV3	38027	82938	2.59%	0.453%
24	11.241	1573	1579	1587	rVV	149823	276240	8.61%	1.510%
25	11.865	1674	1685	1691	rBV	439029	832715	25.96%	4.552%
26	11.923	1691	1695	1700	rVB2	36023	61401	1.91%	0.336%
27	12.106	1720	1726	1732	rBV4	33458	57017	1.78%	0.312%
28	12.582	1795	1807	1817	rBV9	12750	41814	1.30%	0.229%
29	12.688	1820	1825	1829	rVV2	17703	32652	1.02%	0.179%
30	12.847	1839	1852	1860	rVV2	347216	808384	25.20%	4.419%
31	12.923	1860	1865	1871	rVV7	15463	37608	1.17%	0.206%
32	12.988	1871	1876	1879	rVV2	37265	69392	2.16%	0.379%
33	13.029	1879	1883	1889	rVB	42722	73318	2.29%	0.401%
34	13.194	1901	1911	1915	rBV3	30312	72453	2.26%	0.396%
35	13.417	1942	1949	1957	rVB	73305	134646	4.20%	0.736%
36	13.529	1963	1968	1974	rBV	24461	39831	1.24%	0.218%

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37	13.641	1974	1987	1996	rBV2	110187	239855	7.48%	1.311%
38	13.788	2001	2012	2017	rVV	416376	740729	23.09%	4.050%
39	13.835	2017	2020	2030	rVV	141227	261050	8.14%	1.427%
40	13.947	2034	2039	2042	rVV2	36752	54157	1.69%	0.296%
41	13.994	2042	2047	2063	rVB3	104157	237543	7.40%	1.299%
42	14.129	2063	2070	2074	rBV6	23613	54000	1.68%	0.295%
43	14.182	2075	2079	2085	rVB4	22701	42611	1.33%	0.233%
44	14.270	2085	2094	2098	rBV5	20855	48998	1.53%	0.268%
45	14.329	2098	2104	2111	rVV2	62838	114419	3.57%	0.626%
46	14.441	2118	2123	2128	rVV3	38366	67594	2.11%	0.370%
47	14.506	2128	2134	2143	rVB7	17492	44612	1.39%	0.244%
48	14.623	2149	2154	2156	rBV2	40411	61510	1.92%	0.336%
49	14.653	2156	2159	2165	rVB	46109	73554	2.29%	0.402%
50	14.735	2167	2173	2182	rBV3	59820	128895	4.02%	0.705%
51	14.923	2200	2205	2210	rBV4	28135	50390	1.57%	0.275%
52	15.047	2216	2226	2232	rVB5	34255	100016	3.12%	0.547%
53	15.429	2286	2291	2299	rVB4	13560	33489	1.04%	0.183%
54	15.605	2315	2321	2328	rVB5	18885	41664	1.30%	0.228%
55	16.335	2437	2445	2450	rVB4	19099	43380	1.35%	0.237%

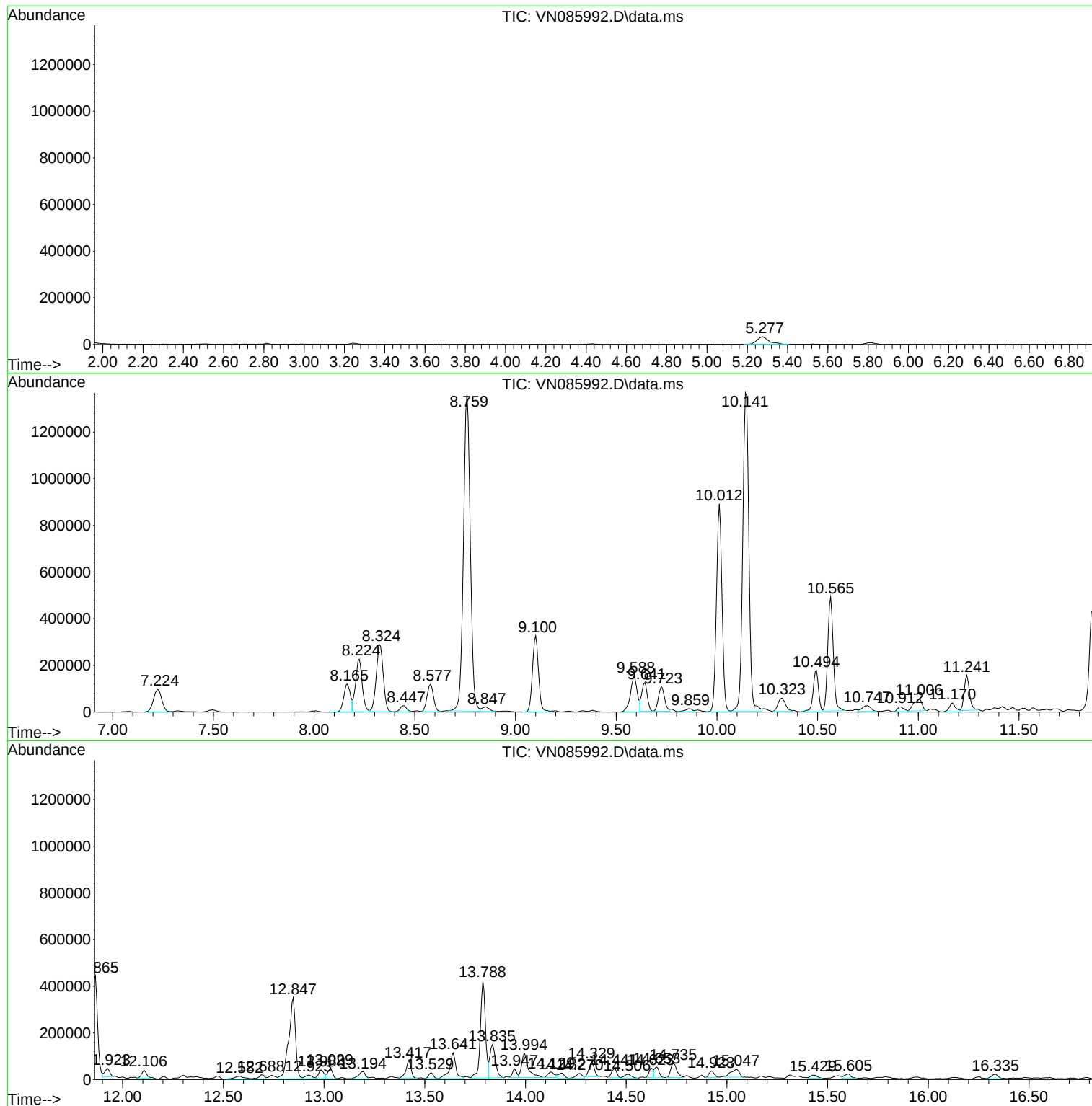
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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



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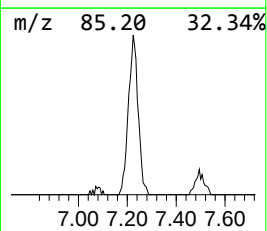
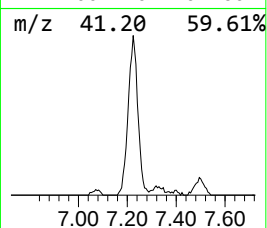
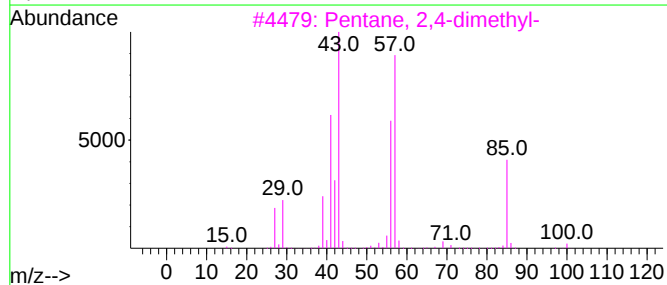
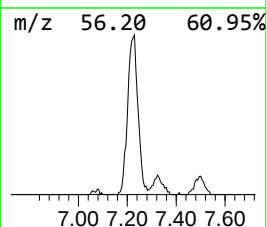
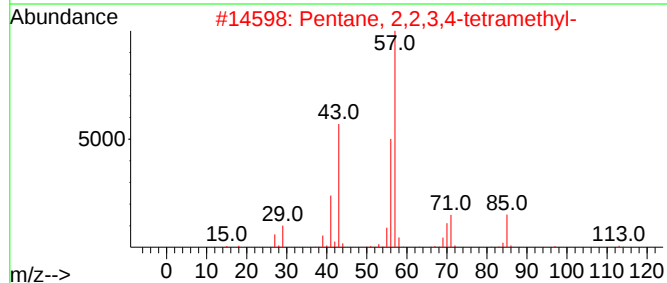
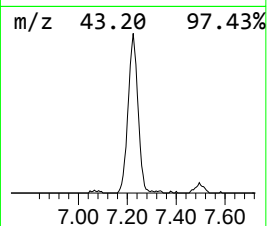
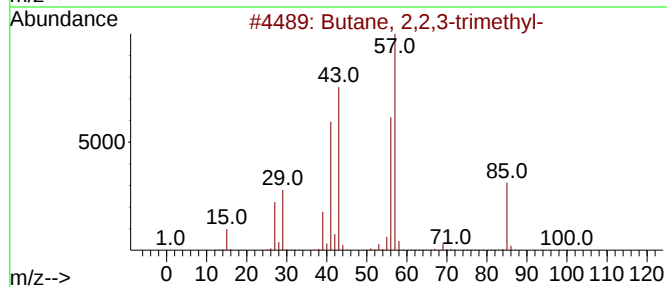
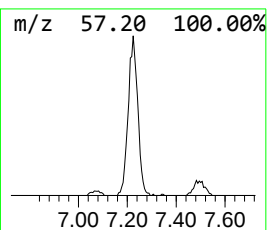
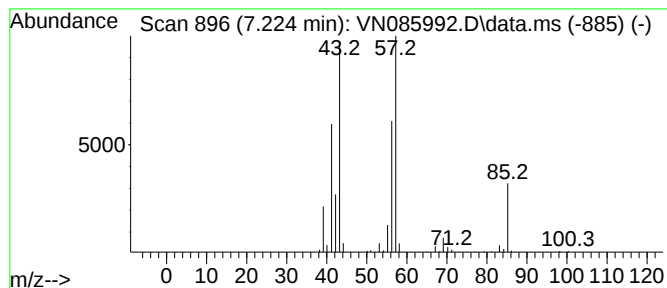
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,2,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	27.22 ug/l	280062	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
2			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	64
3			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	64
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	53
5			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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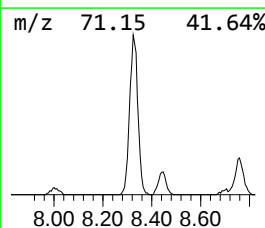
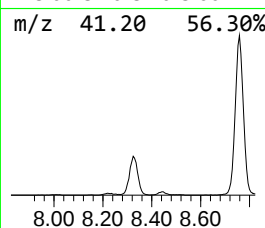
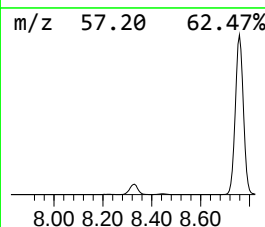
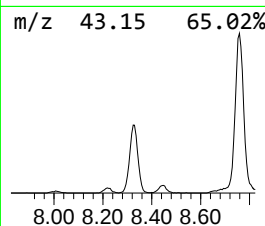
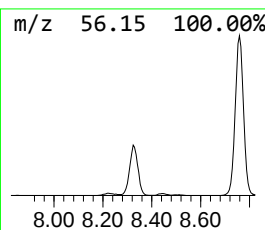
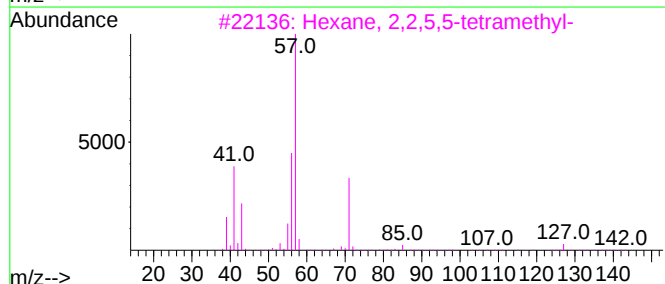
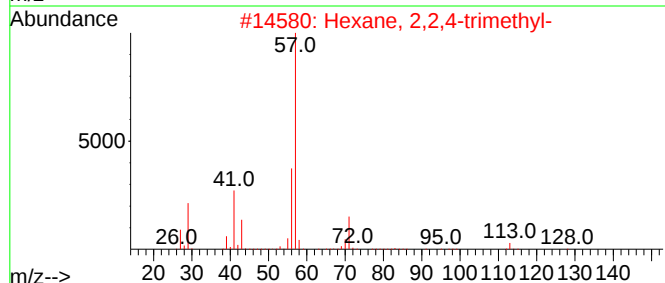
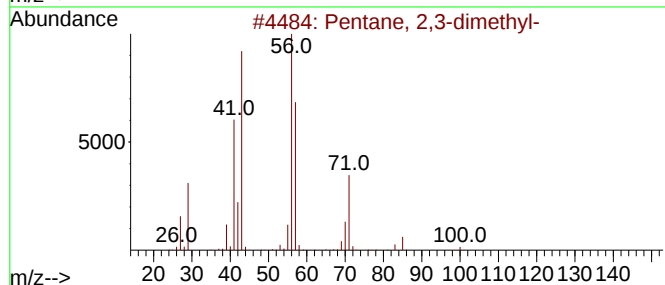
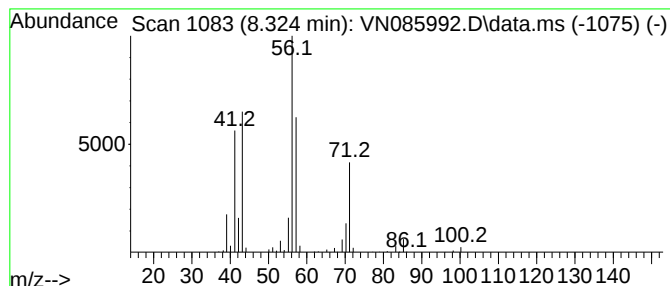
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.324	67.03 ug/l	689710	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	78
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	72
4			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	52
5			1,4-Dioxaspiro[2.4]heptan-5-one,...	142	C7H10O3	126091-79-0	42



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Instrument :
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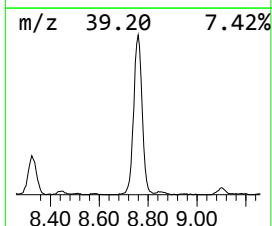
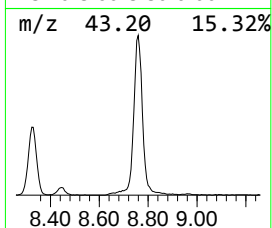
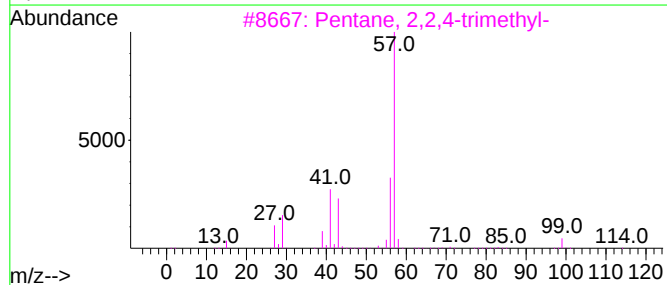
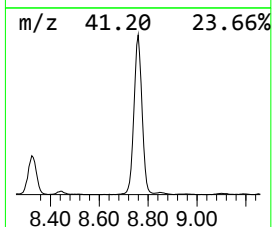
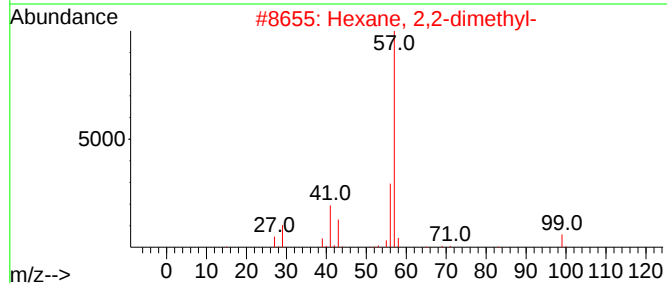
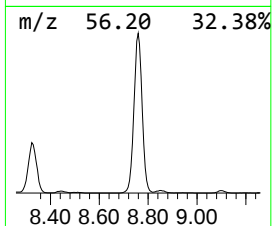
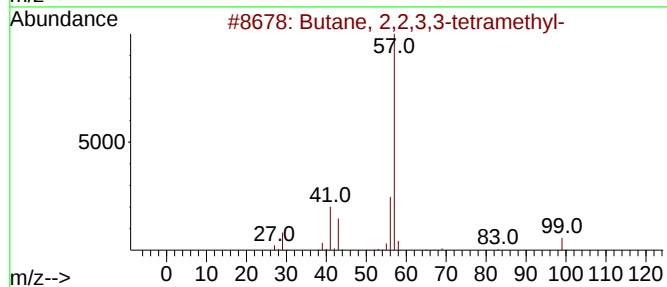
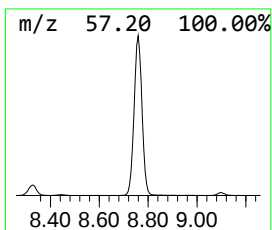
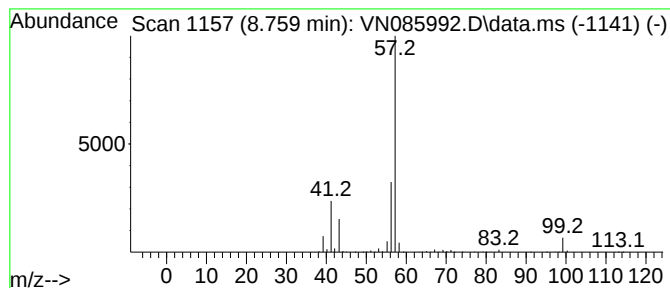
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.759	235.55 ug/l	3208180	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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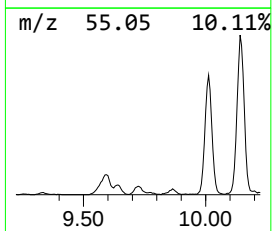
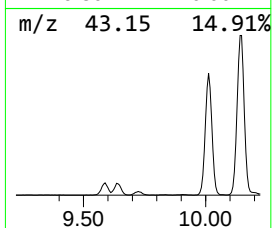
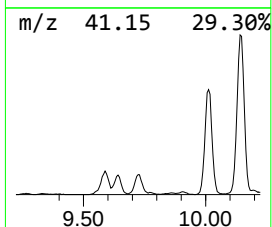
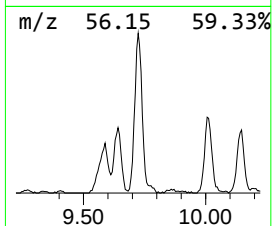
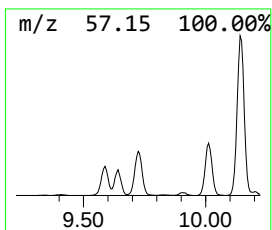
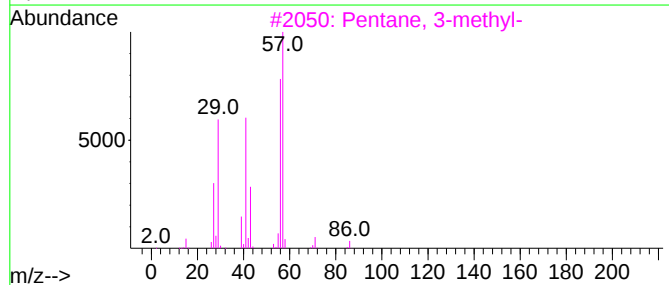
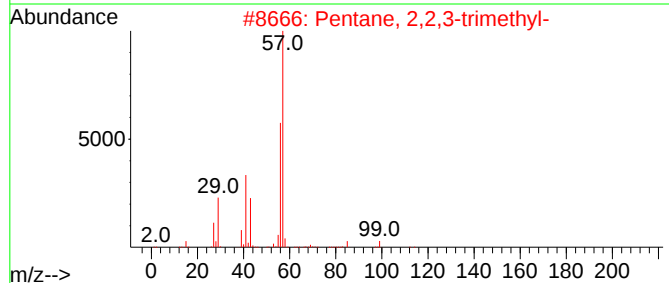
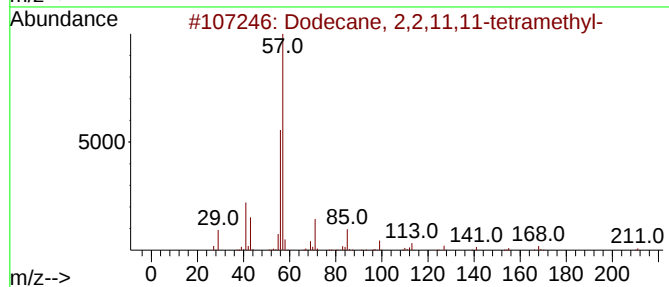
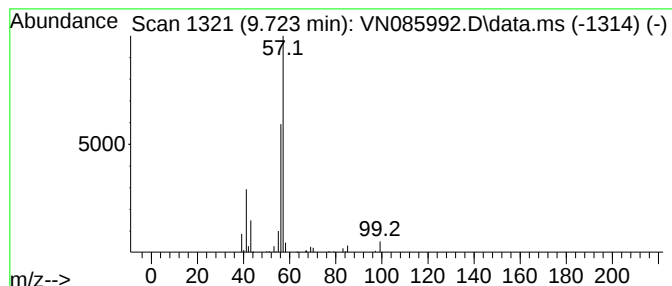
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

Peak Number 4 Dodecane, 2,2,11,11-tetrame... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.723	16.21 ug/l	220766	1,4-Difluorobenzene	9.100

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	72
2		Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	64
3		Pentane, 3-methyl-	86	C6H14	000096-14-0	59
4		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	56
5		Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	50



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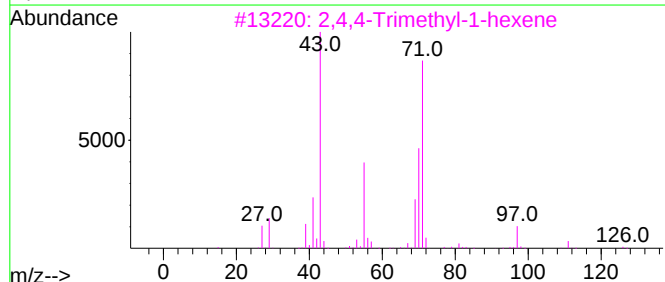
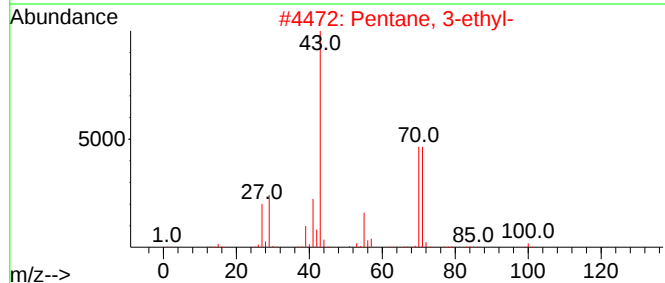
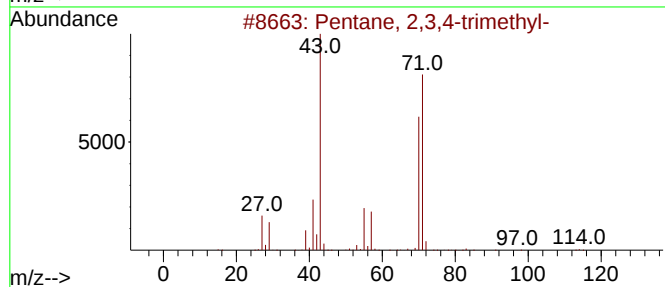
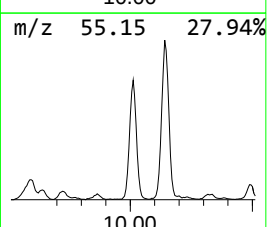
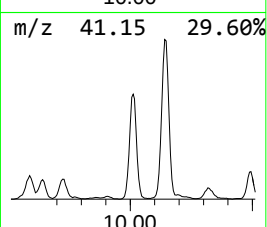
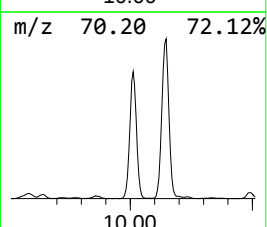
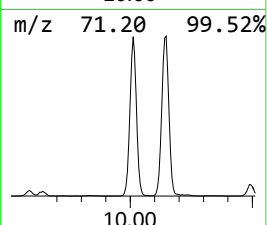
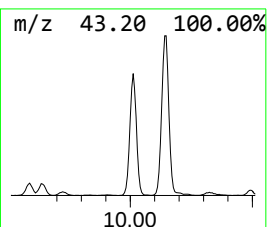
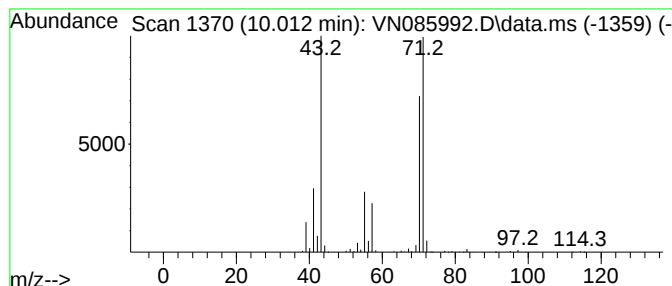
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.012	126.46 ug/l	1722380	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	74
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031425\
Data File : VN085992.D
Acq On : 14 Mar 2025 16:21
Operator : JC\MD
Sample : Q1575-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3

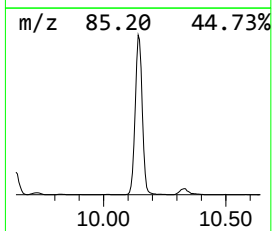
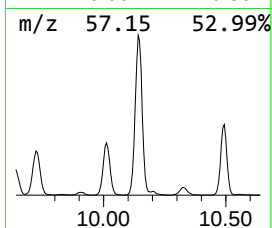
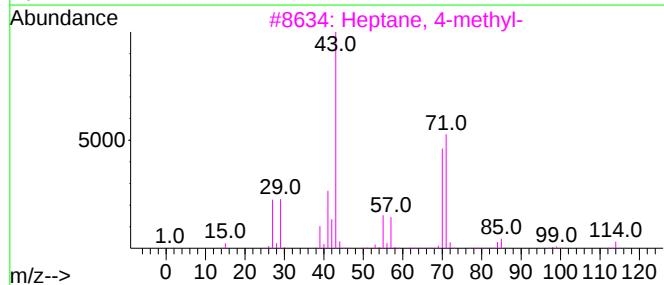
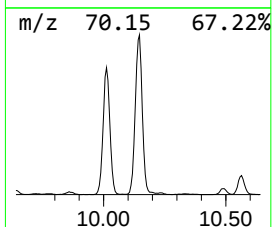
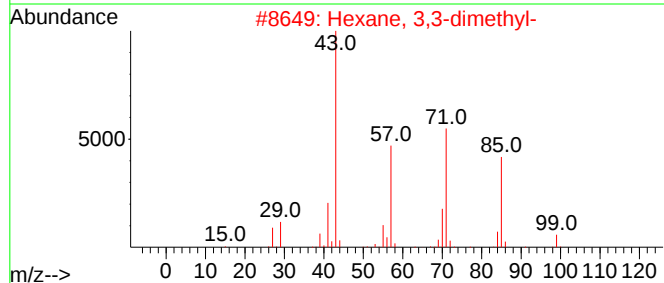
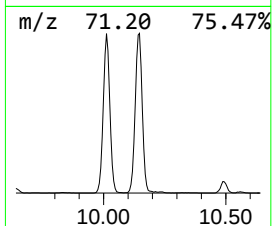
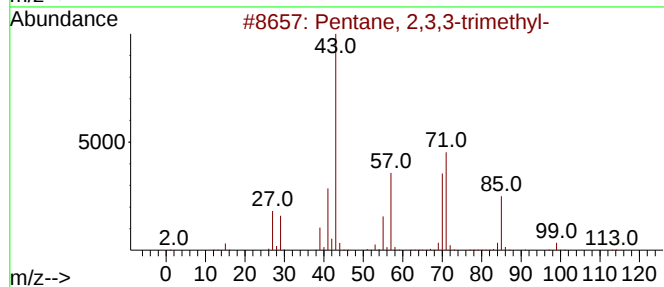
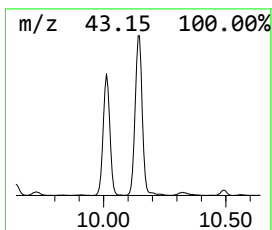
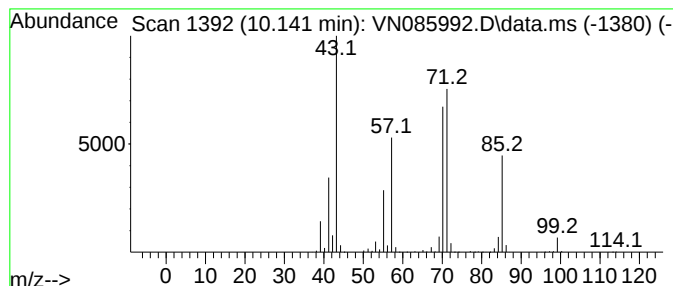
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.141	208.94 ug/l	2845630	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	72
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	56
5			Pyrrolidine	71	C4H9N	000123-75-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031425\
Data File : VN085992.D
Acq On : 14 Mar 2025 16:21
Operator : JC\MD
Sample : Q1575-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3

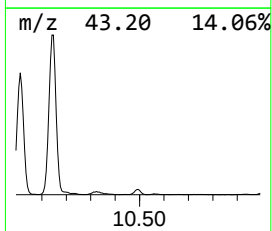
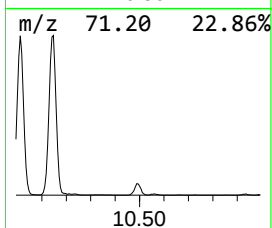
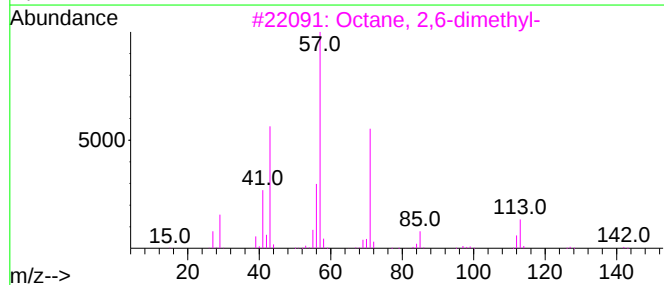
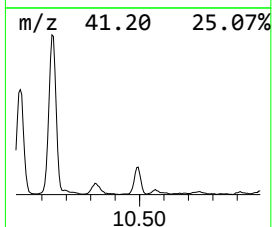
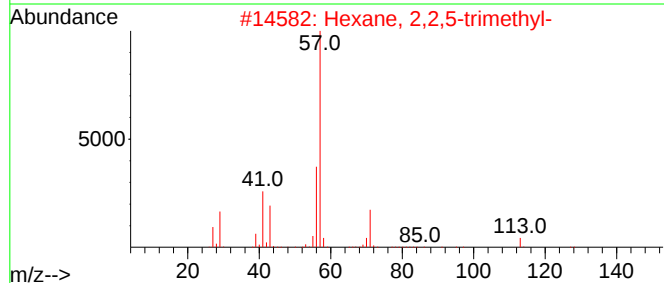
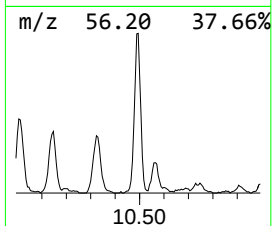
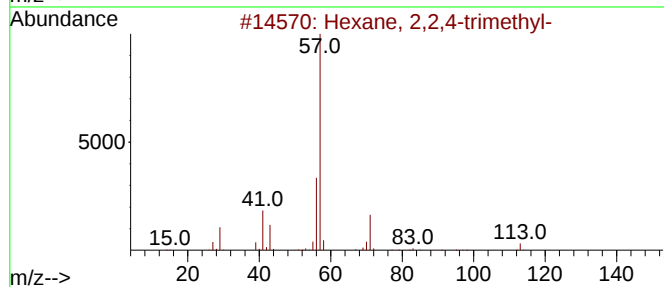
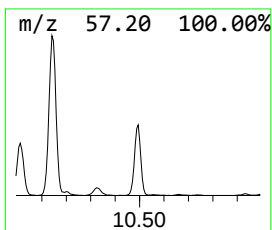
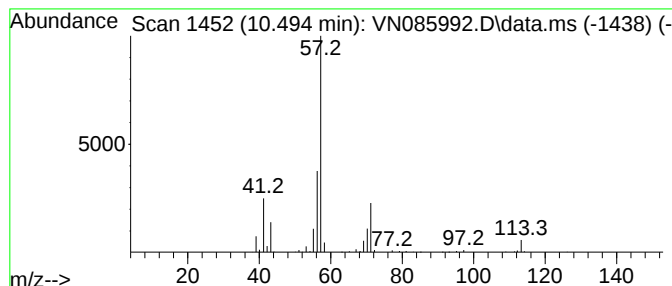
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Quant Title : SW846 8260

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

Peak Number 7 Hexane, 2,2,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.494	19.93 ug/l	331971	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	78
2			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	78
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	59
5			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031425\
Data File : VN085992.D
Acq On : 14 Mar 2025 16:21
Operator : JC\MD
Sample : Q1575-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3

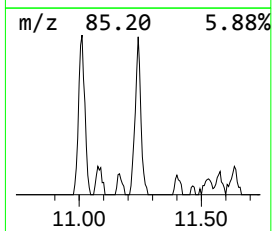
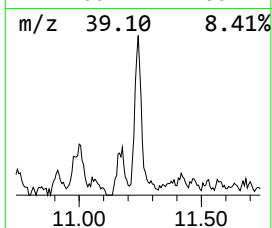
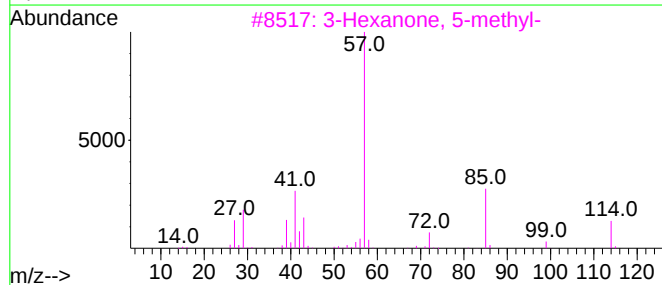
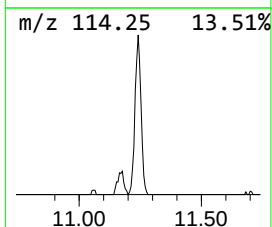
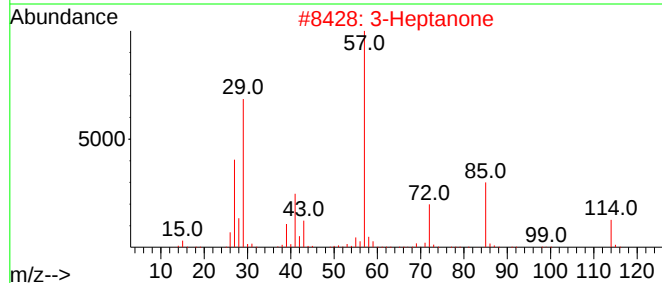
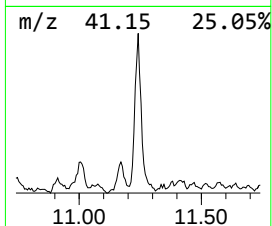
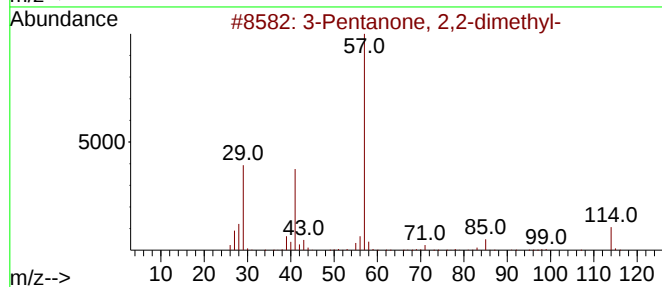
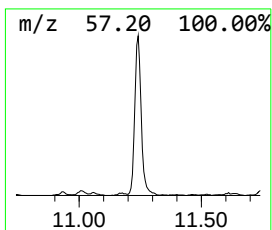
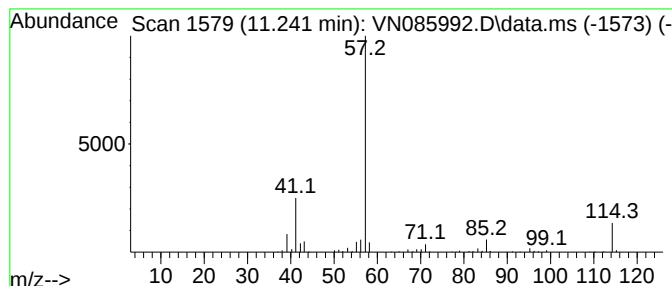
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

Peak Number 8 3-Pentanone, 2,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.241	16.59 ug/l	276240	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	86
2			3-Heptanone	114	C7H14O	000106-35-4	53
3			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	53
4			2,2,5,5-Tetramethyl-3-hexanone	156	C10H20O	000868-91-7	42
5			3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031425\
Data File : VN085992.D
Acq On : 14 Mar 2025 16:21
Operator : JC\MD
Sample : Q1575-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3

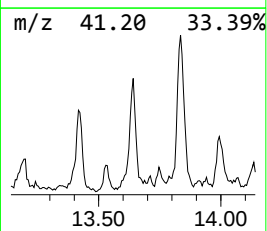
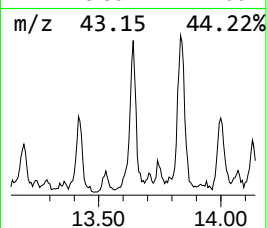
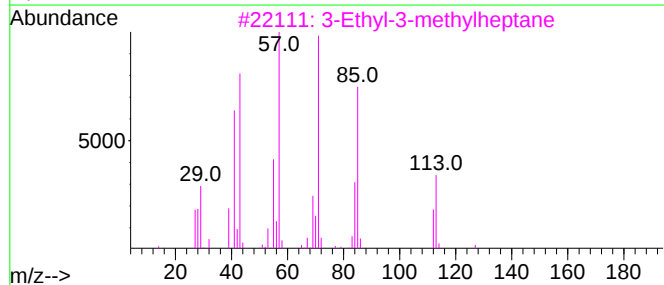
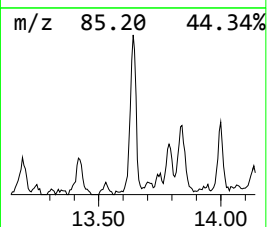
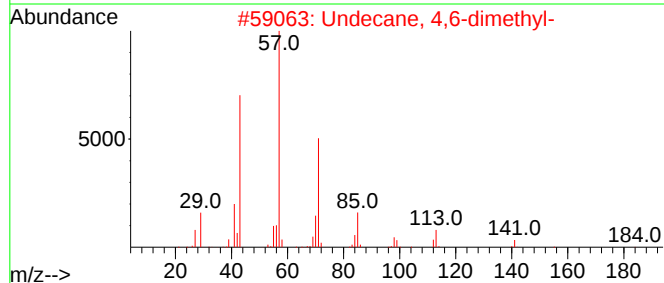
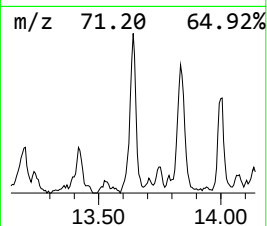
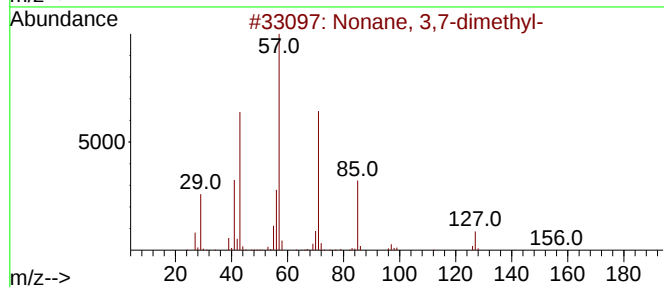
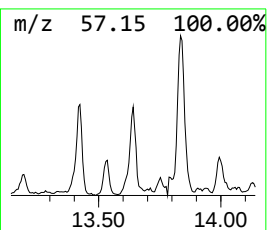
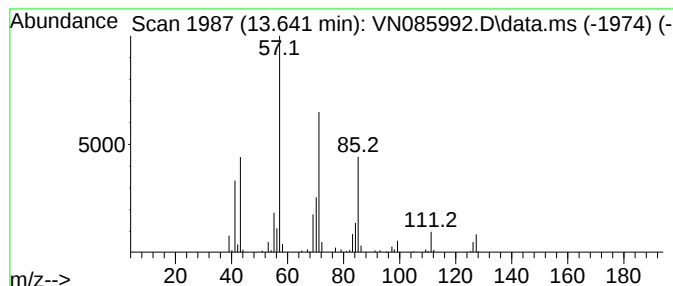
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Quant Title : SW846 8260

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

Peak Number 9 Nonane, 3,7-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	16.19 ug/l	239855	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	59
2			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	59
3			3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	50
4			Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	50
5			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031425\
Data File : VN085992.D
Acq On : 14 Mar 2025 16:21
Operator : JC\MD
Sample : Q1575-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3

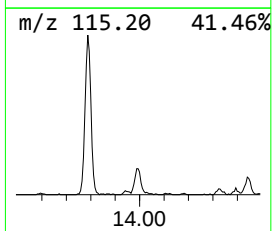
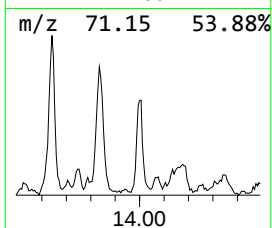
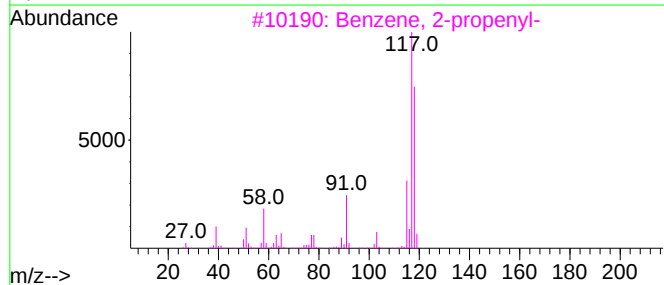
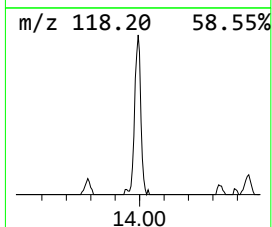
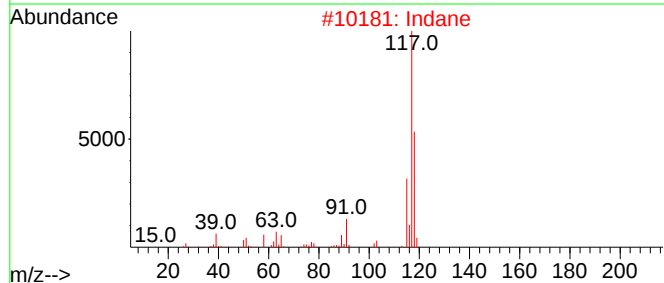
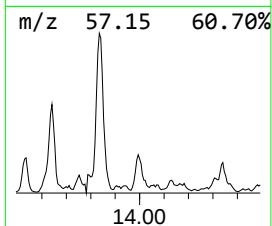
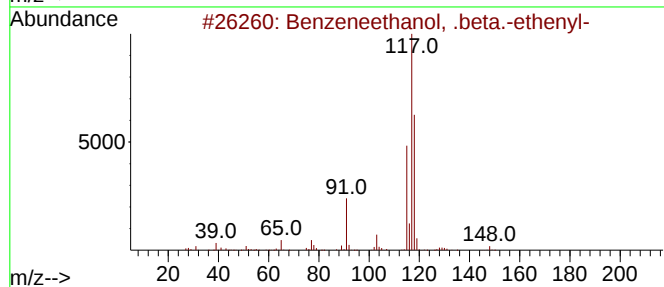
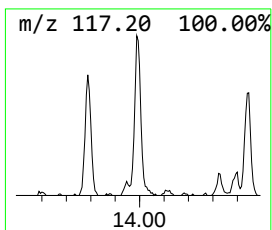
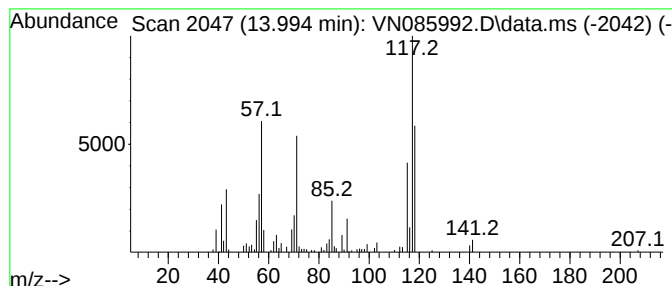
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzeneethanol, .beta.-ethe... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	16.03 ug/l	237543	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	50
2			Indane	118	C9H10	000496-11-7	50
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	43
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	38
5			Indane-5-carboxylic acid	162	C10H10O2	065898-38-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031425\
Data File : VN085992.D
Acq On : 14 Mar 2025 16:21
Operator : JC\MD
Sample : Q1575-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.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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Pentane, 2,3-di...	8.324	67.0	ug/l	689710	1	8.224	514514	50.0
Butane, 2,2,3,3...	8.759	235.6	ug/l	3208180	2	9.100	680986	50.0
Dodecane, 2,2,1...	9.723	16.2	ug/l	220766	2	9.100	680986	50.0
Pentane, 2,3,4-...	10.012	126.5	ug/l	1722380	2	9.100	680986	50.0
Pentane, 2,3,3-...	10.141	208.9	ug/l	2845630	2	9.100	680986	50.0
Hexane, 2,2,4-t...	10.494	19.9	ug/l	331971	3	11.865	832715	50.0
3-Pentanone, 2,...	11.241	16.6	ug/l	276240	3	11.865	832715	50.0
Nonane, 3,7-dim...	13.641	16.2	ug/l	239855	4	13.788	740729	50.0
Benzeneethanol,...	13.994	16.0	ug/l	237543	4	13.788	740729	50.0