

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
 Data File : VN086306.D
 Acq On : 16 Apr 2025 18:51
 Operator : JC\MD
 Sample : Q1791-09 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VB16193

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\82N041525W.M
 Title : SW846 8260

Signal : TIC: VN086306.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.812	140	146	153	rVB2	8006	21243	1.81%	0.195%
2	5.565	605	614	624	rBV2	4598	13197	1.13%	0.121%
3	8.165	1045	1056	1060	rBV	125471	294285	25.10%	2.703%
4	8.218	1060	1065	1078	rVB	255348	569709	48.58%	5.232%
5	8.577	1115	1126	1135	rBV	160445	360858	30.77%	3.314%
6	9.094	1206	1214	1225	rBV	400335	822968	70.18%	7.558%
7	10.565	1454	1464	1473	rBV	626449	1172615	100.00%	10.769%
8	11.865	1677	1685	1694	rBV	549483	994416	84.80%	9.133%
9	12.847	1841	1852	1859	rVV2	433653	872697	74.42%	8.015%
10	12.918	1859	1864	1870	rVV5	11053	26160	2.23%	0.240%
11	12.988	1870	1876	1885	rVB	37683	86608	7.39%	0.795%
12	13.194	1901	1911	1915	rBV	37855	86589	7.38%	0.795%
13	13.241	1915	1919	1925	rVB3	11982	22502	1.92%	0.207%
14	13.359	1928	1939	1941	rBV5	12876	31012	2.64%	0.285%
15	13.417	1941	1949	1958	rVB	212133	394714	33.66%	3.625%
16	13.529	1962	1968	1975	rBV	97409	151831	12.95%	1.394%
17	13.641	1975	1987	1993	rBV	317460	621581	53.01%	5.709%
18	13.706	1994	1998	2001	rVV2	31947	55432	4.73%	0.509%
19	13.753	2001	2006	2007	rVV2	79324	124581	10.62%	1.144%
20	13.788	2007	2012	2016	rVV	578615	1006911	85.87%	9.247%
21	13.835	2016	2020	2030	rVV	530669	1068355	91.11%	9.812%
22	13.935	2030	2037	2041	rVV2	32624	87850	7.49%	0.807%
23	13.994	2041	2047	2055	rVV2	237397	519547	44.31%	4.771%
24	14.065	2055	2059	2064	rVV	58912	126305	10.77%	1.160%
25	14.135	2066	2071	2073	rVV3	70456	135179	11.53%	1.241%
26	14.176	2074	2078	2089	rVV2	93312	240742	20.53%	2.211%
27	14.270	2091	2094	2095	rVV2	18728	23755	2.03%	0.218%
28	14.306	2095	2100	2102	rVV2	47069	90469	7.72%	0.831%
29	14.341	2102	2106	2115	rVB2	77859	160825	13.72%	1.477%
30	14.488	2123	2131	2133	rBV2	24139	49126	4.19%	0.451%
31	14.653	2156	2159	2164	rVB3	10197	14613	1.25%	0.134%
32	14.735	2167	2173	2182	rVB3	111023	242613	20.69%	2.228%
33	14.870	2192	2196	2200	rBV2	24708	38084	3.25%	0.350%
34	14.912	2200	2203	2208	rVB2	15297	19937	1.70%	0.183%
35	15.064	2225	2229	2243	rVB8	16807	52754	4.50%	0.484%
36	15.170	2243	2247	2250	rBV2	10611	14694	1.25%	0.135%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

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\82N041525W.M

Title : SW846 8260

37	15.511	2299	2305	2313	rBV10	10160	28373	2.42%	0.261%
38	15.594	2313	2319	2326	rVB3	25879	58578	5.00%	0.538%
39	15.829	2354	2359	2369	rVB	36661	75248	6.42%	0.691%
40	16.182	2414	2419	2428	rBV	4960	18491	1.58%	0.170%
41	16.400	2452	2456	2460	rVB4	6795	11750	1.00%	0.108%
42	16.453	2461	2465	2469	rBV6	8388	15454	1.32%	0.142%
43	16.541	2476	2480	2485	rVB5	12421	21131	1.80%	0.194%
44	16.611	2486	2492	2500	rVB	23071	44806	3.82%	0.411%

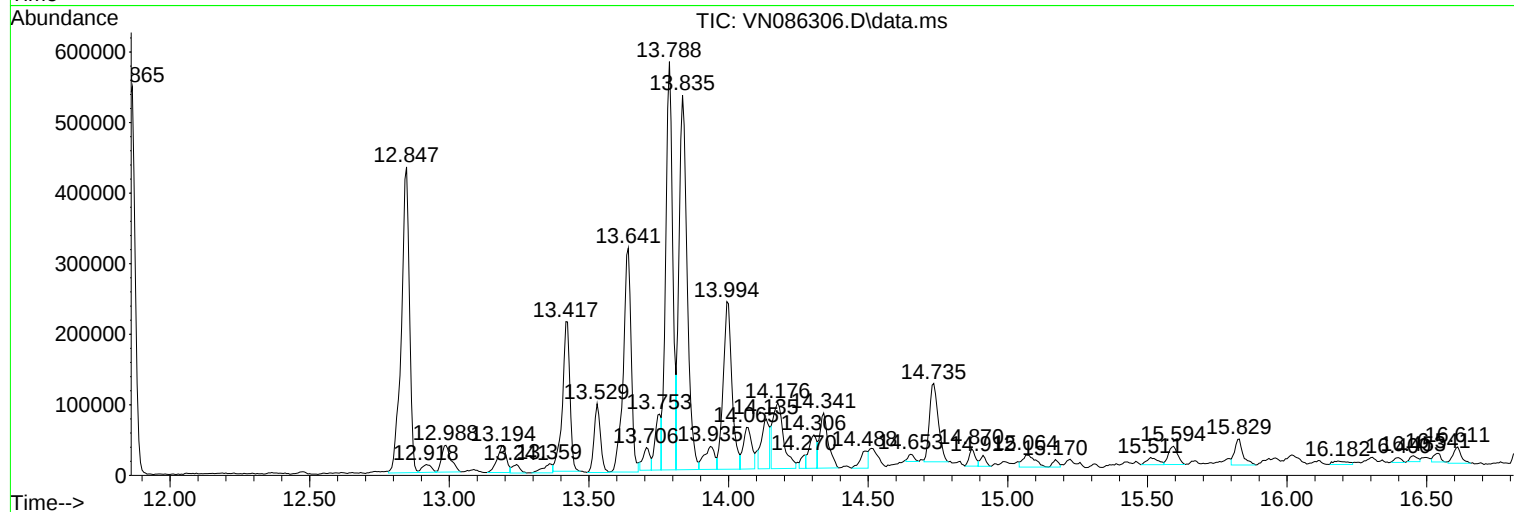
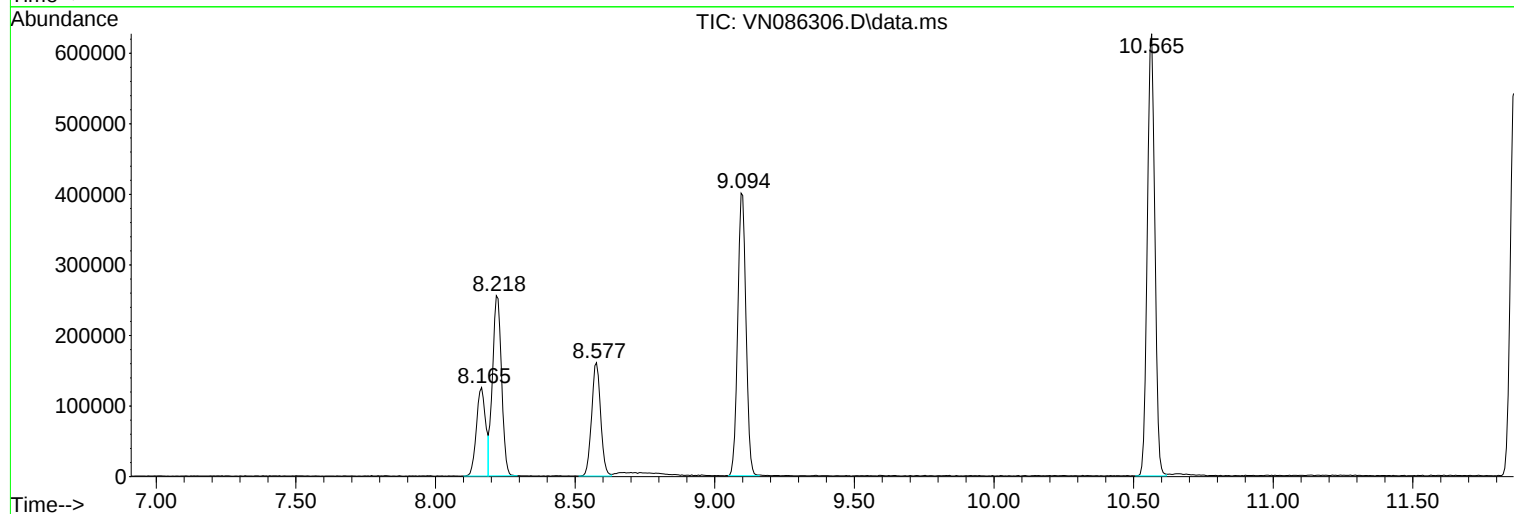
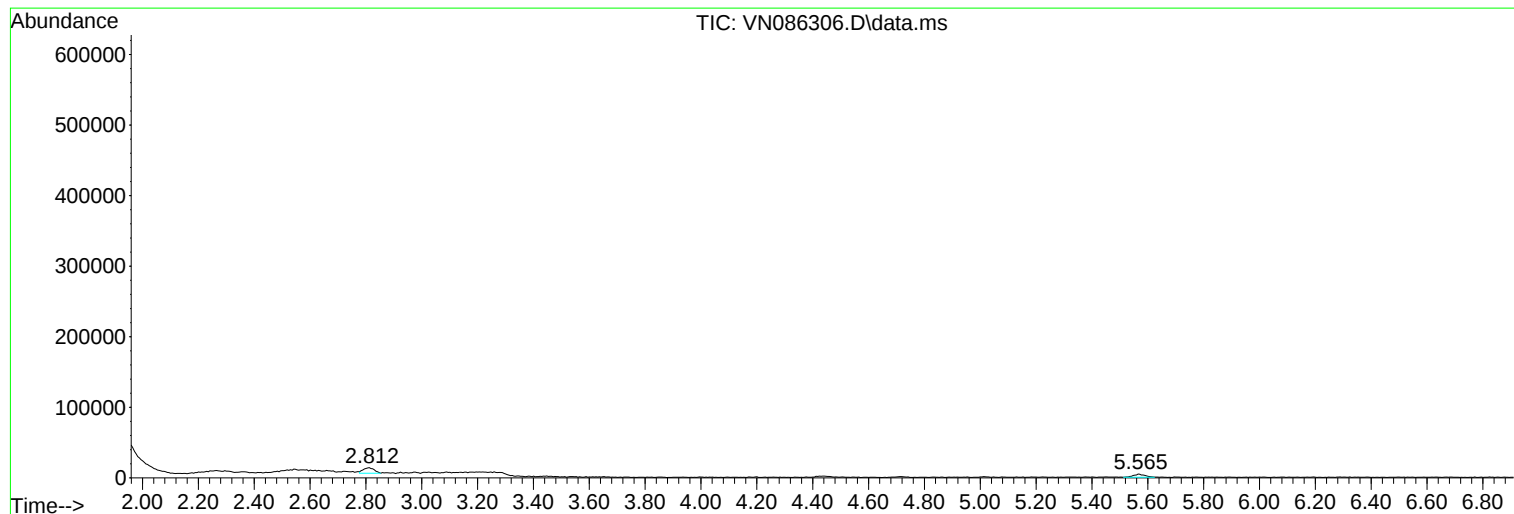
Sum of corrected areas: 10888588

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

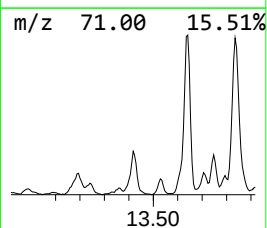
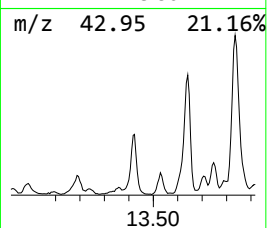
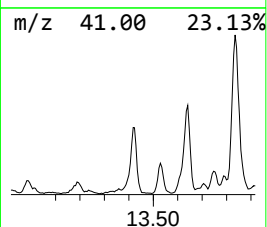
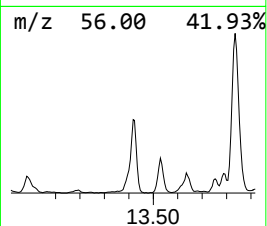
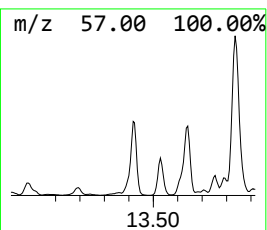
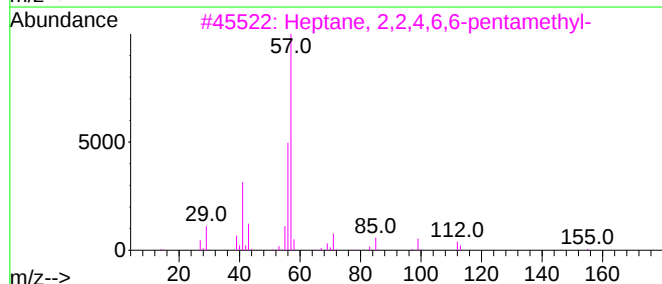
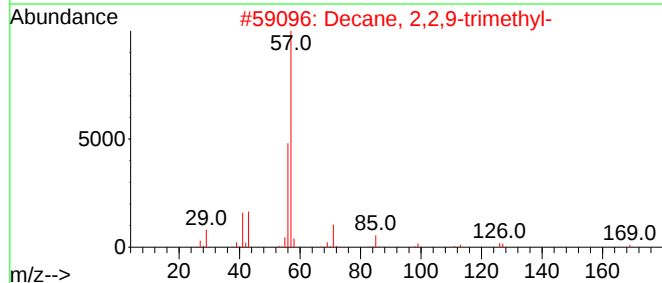
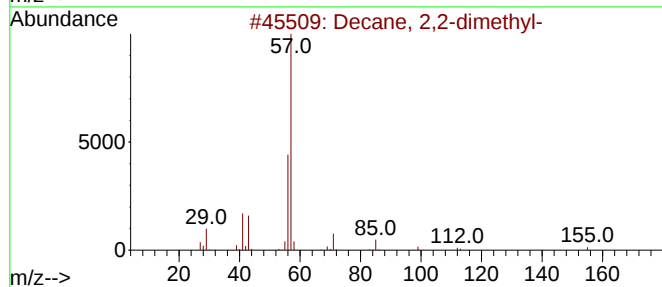
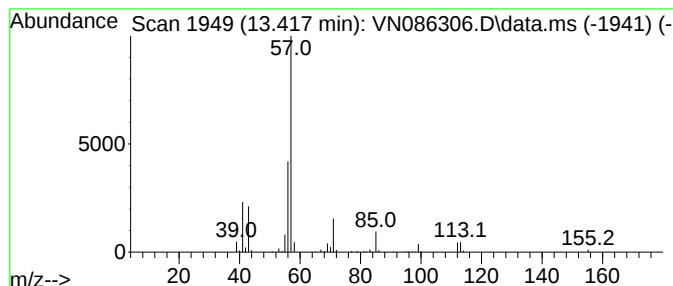
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 1 Decane, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.418	19.60 ug/l	394714	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	78
2			Decane, 2,2,9-trimethyl-	184	C13H28	062238-00-0	72
3			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72
4			Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	64
5			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

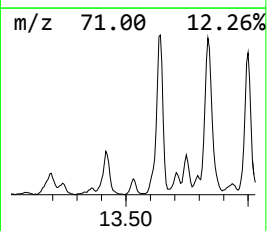
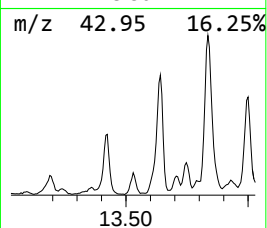
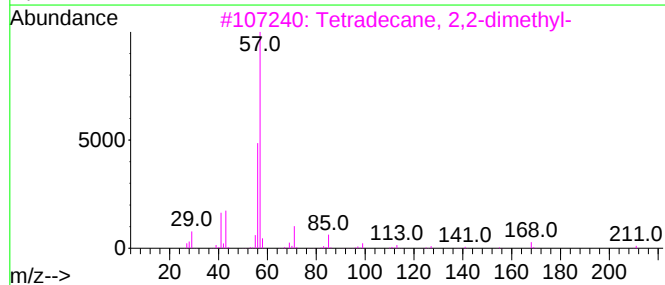
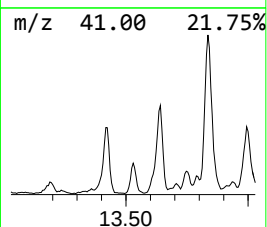
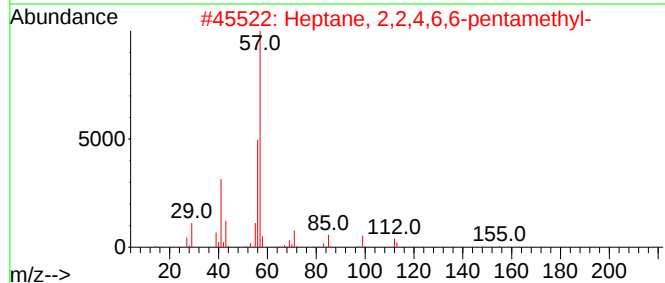
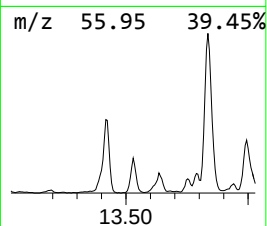
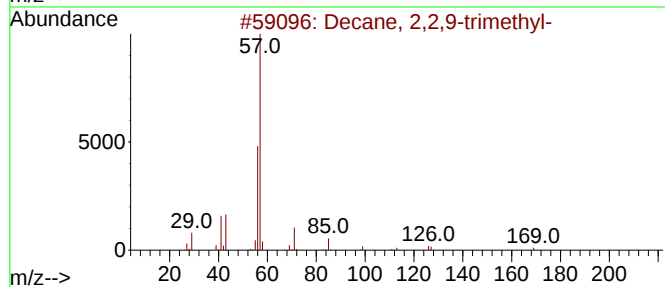
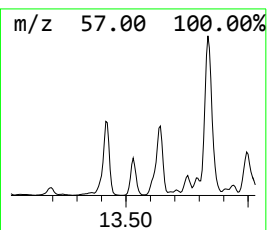
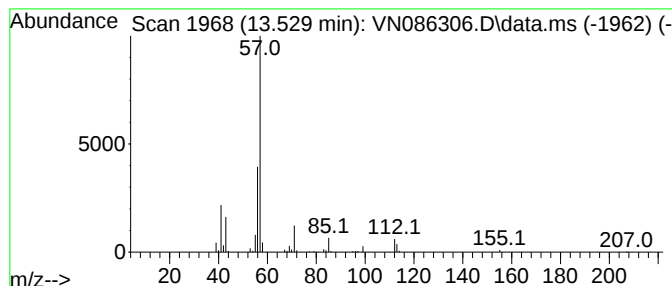
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 2 Decane, 2,2,9-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.529	7.54 ug/l	151831	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,2,9-trimethyl-	184	C13H28	062238-00-0	78
2			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	78
3			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	78
4			Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	72
5			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

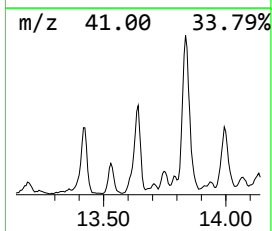
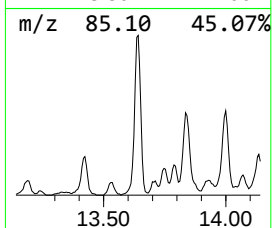
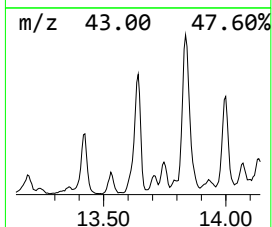
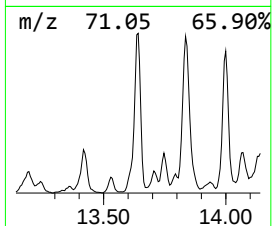
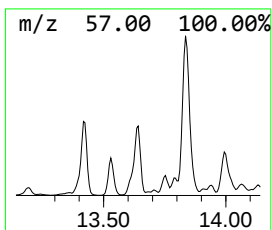
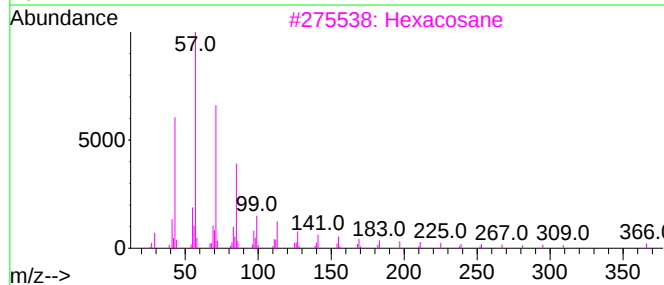
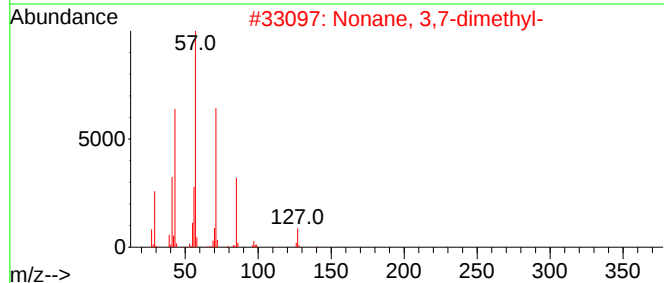
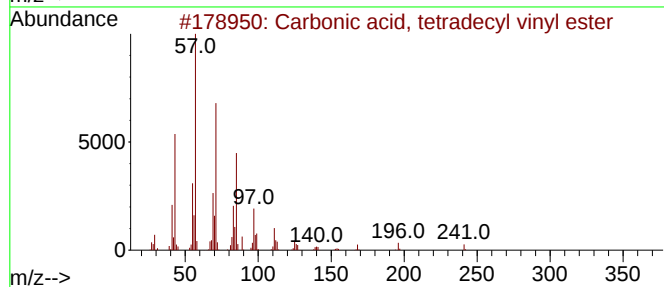
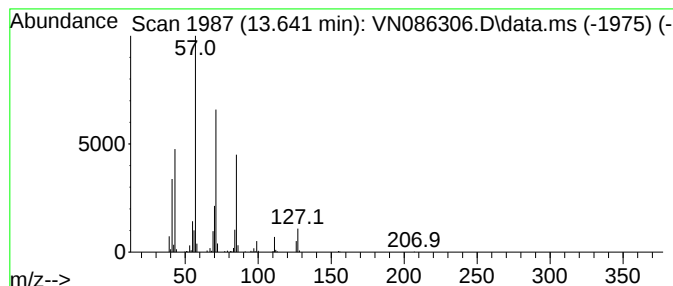
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 3 Carbonic acid, tetradecyl v... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	30.87 ug/l	621581	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	78
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	72
3			Hexacosane	366	C26H54	000630-01-3	64
4			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
5			Bacchotricuneatin c	342	C20H22O5	066563-30-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

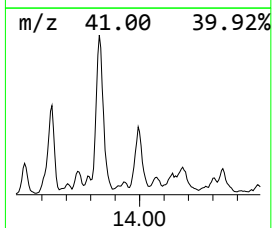
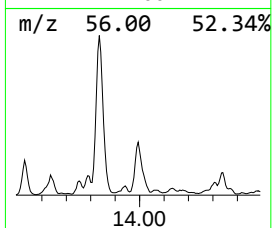
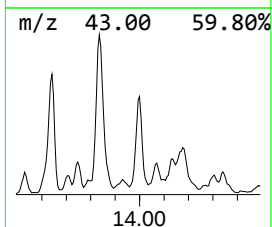
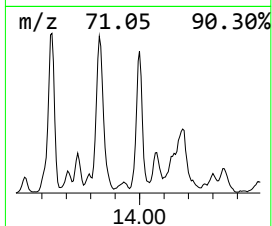
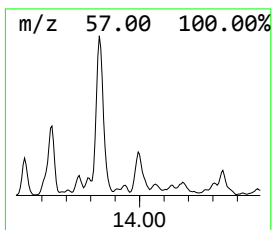
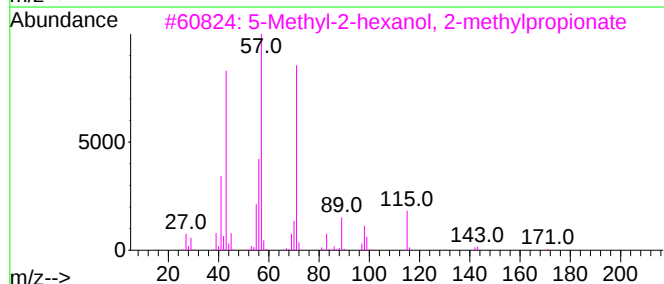
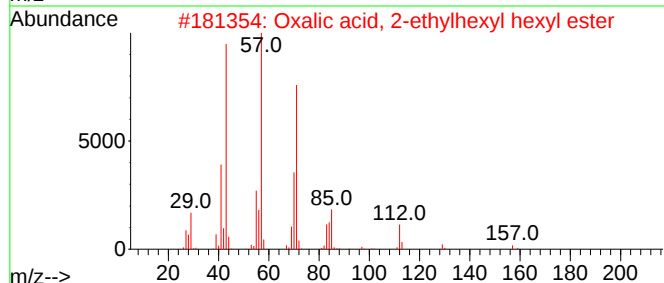
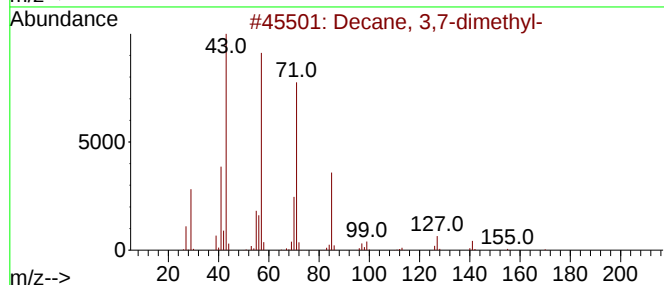
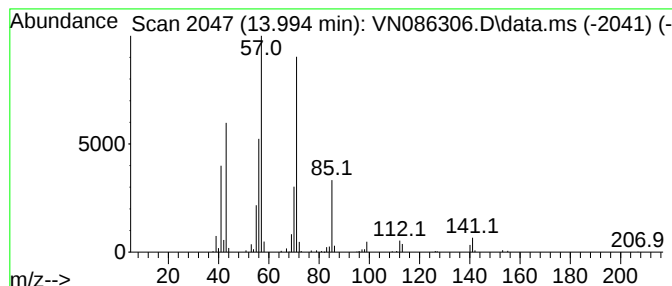
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 4 Decane, 3,7-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	25.80 ug/l	519547	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	59
2			Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	59
3			5-Methyl-2-hexanol, 2-methylprop...	186	C11H22O2	1000447-34-4	59
4			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	53
5			Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

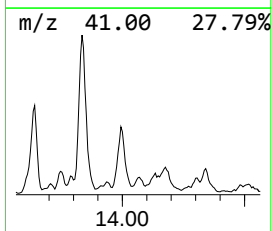
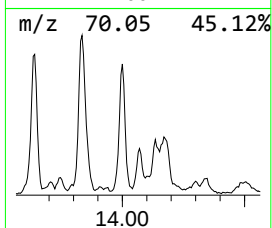
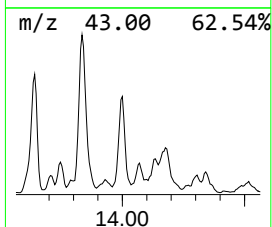
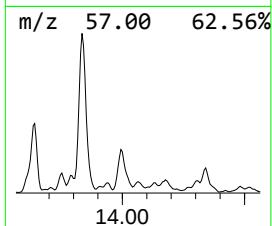
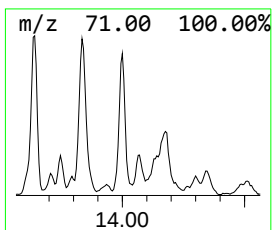
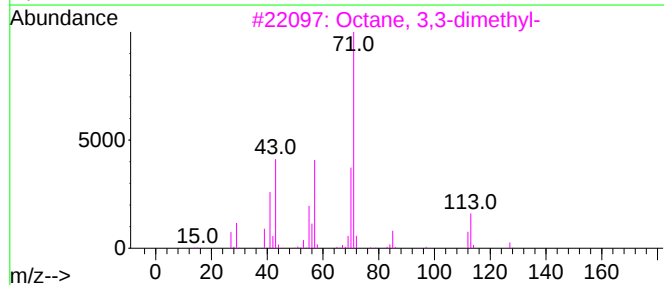
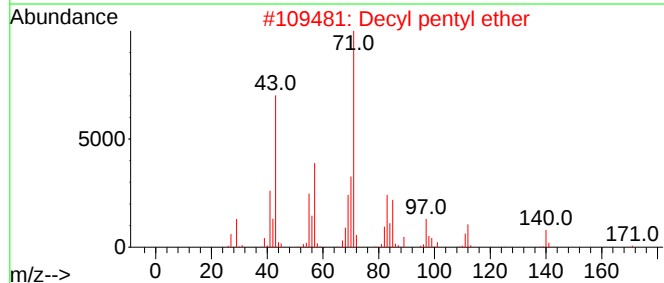
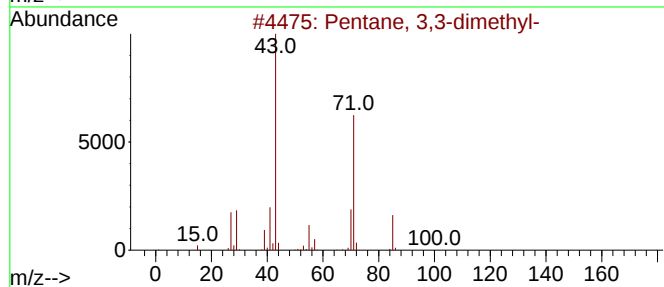
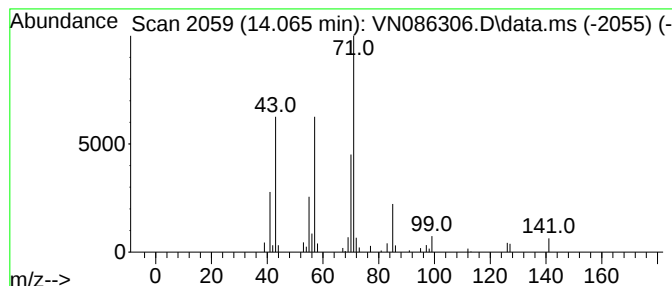
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 5 Pentane, 3,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.065	6.27 ug/l	126305	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	72
2			Decyl pentyl ether	228	C15H32O	1000406-41-5	64
3			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	64
4			1,1-Dimethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-99-2	64
5			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

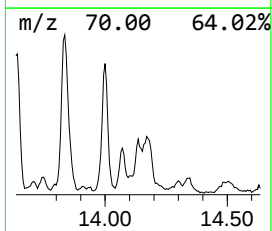
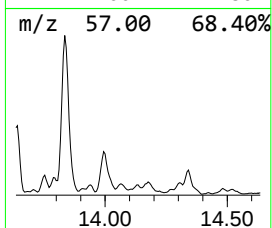
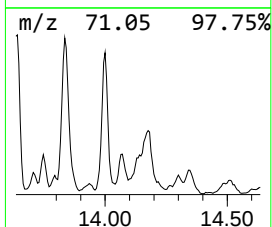
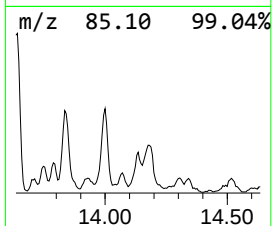
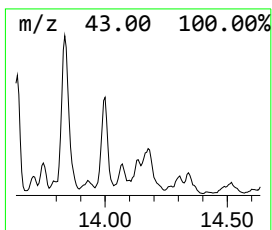
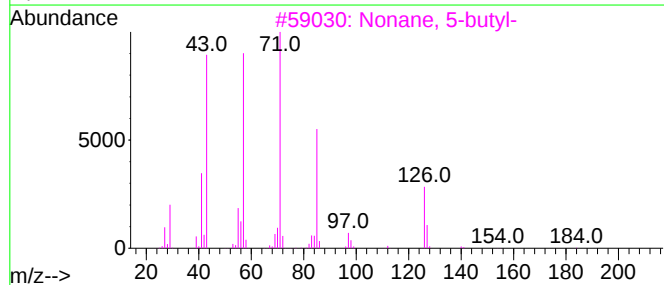
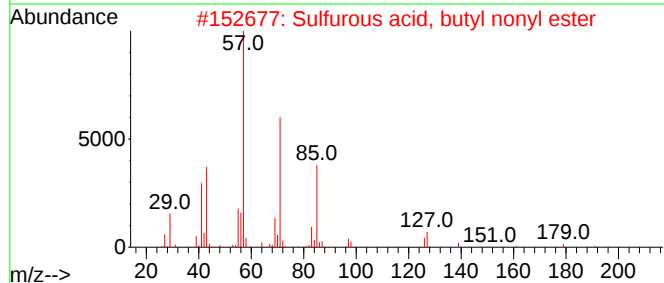
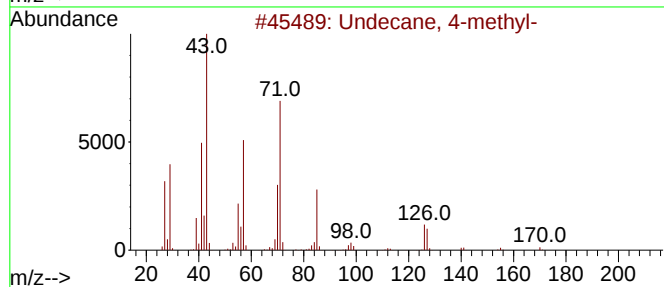
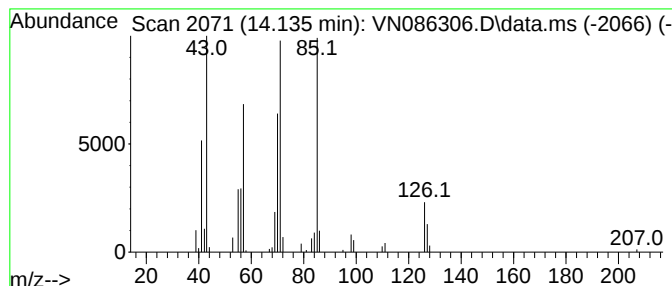
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 6 Undecane, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.135	6.71 ug/l	135179	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 4-methyl-	170	C12H26	002980-69-0	53
2			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	53
3			Nonane, 5-butyl-	184	C13H28	017312-63-9	47
4			Decan-2-yl 2-methylbutanoate	242	C15H30O2	1000372-72-7	38
5			Isobutyl isopentyl carbonate	188	C10H20O3	1000372-76-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

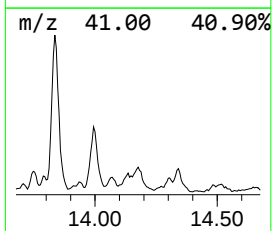
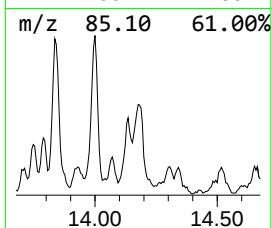
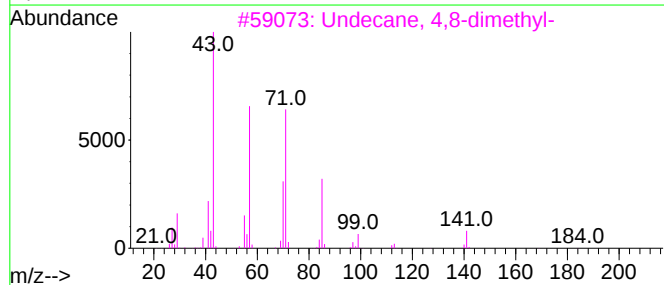
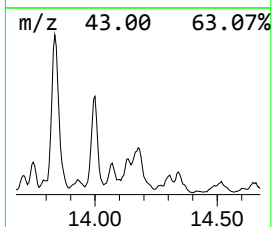
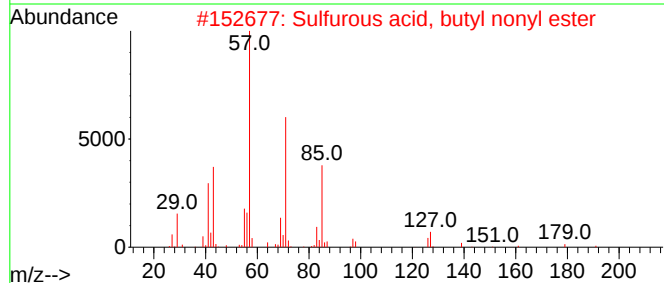
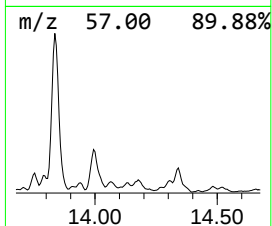
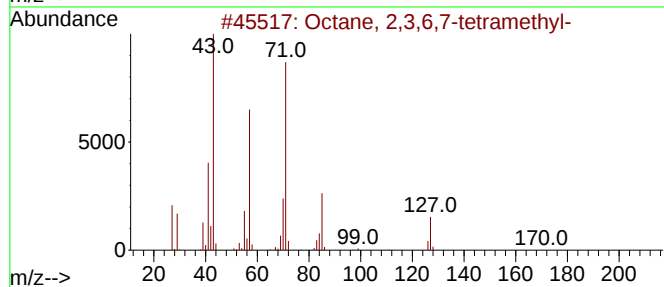
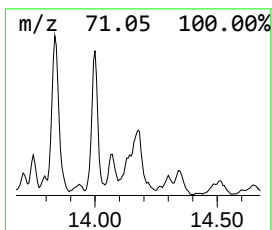
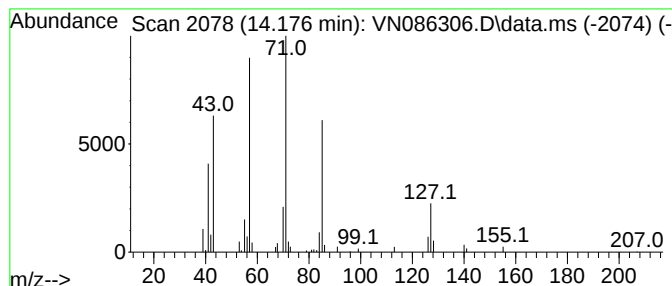
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 7 Octane, 2,3,6,7-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	11.95 ug/l	240742	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,3,6,7-tetramethyl-	170	C12H26	052670-34-5	64
2			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	64
3			Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	59
4			Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	53
5			Dodecane, 4-methyl-	184	C13H28	006117-97-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

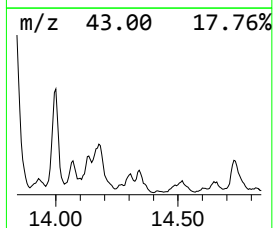
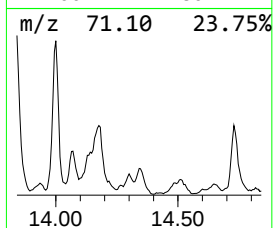
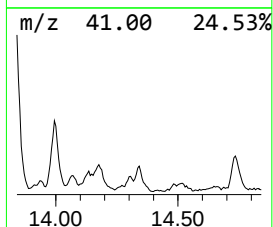
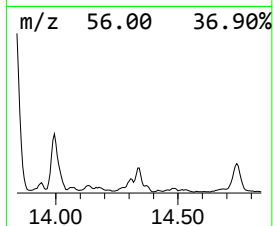
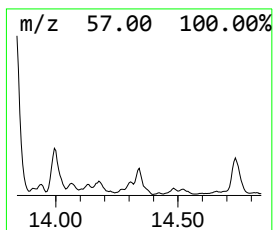
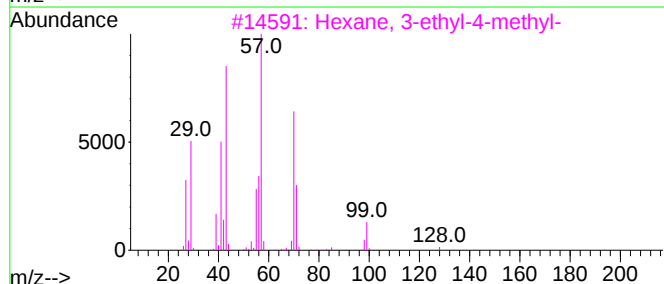
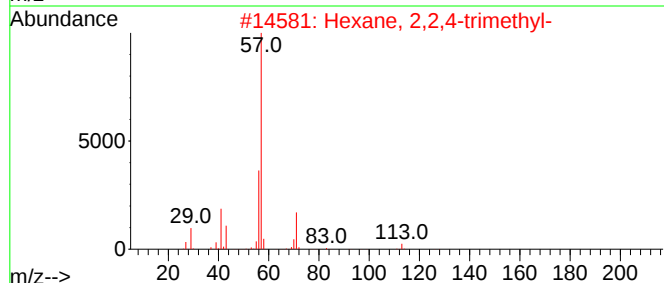
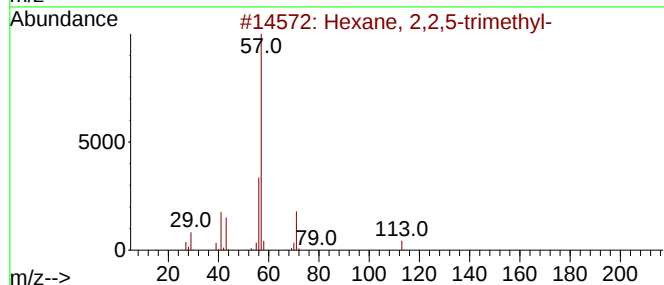
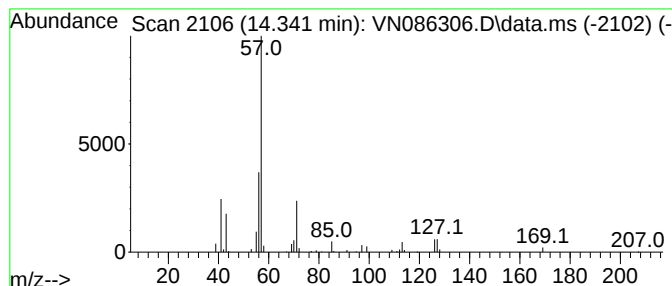
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 8 Hexane, 2,2,5-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.341	7.99 ug/l	160825	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
3			Hexane, 3-ethyl-4-methyl-	128	C9H20	003074-77-9	53
4			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	45
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

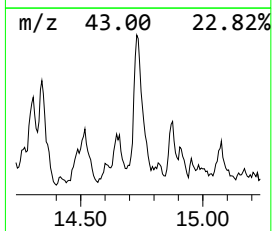
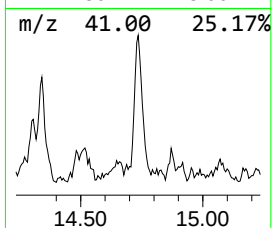
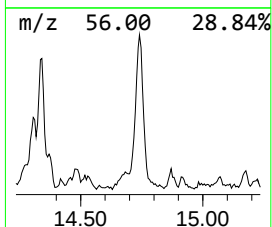
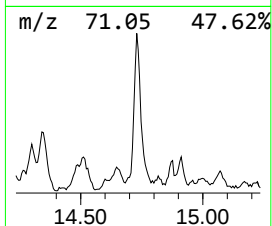
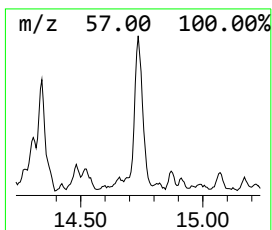
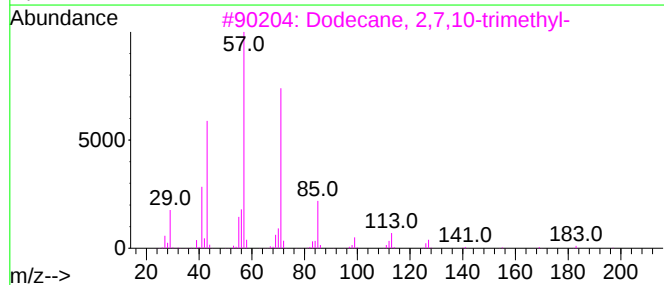
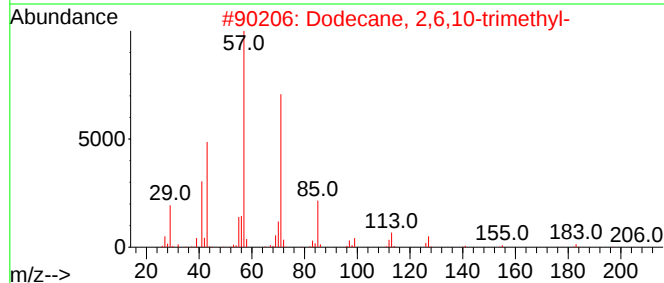
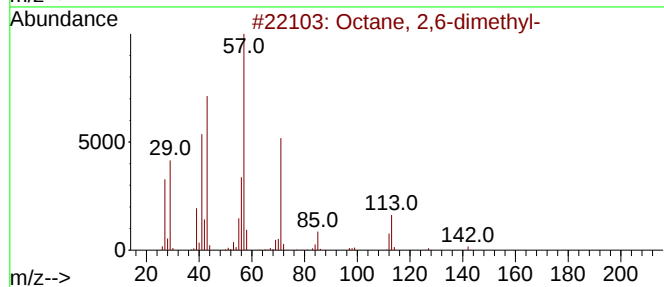
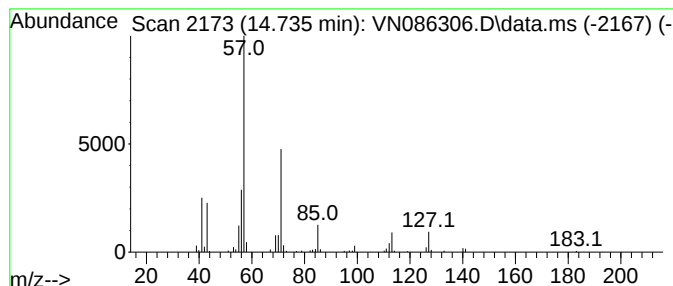
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 9 Octane, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	12.05 ug/l	242613	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
2			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	72
3			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
4			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	53
5			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086306.D
Acq On : 16 Apr 2025 18:51
Operator : JC\MD
Sample : Q1791-09 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16193

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.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
Decane, 2,2-dim...	13.418	19.6	ug/l	394714	4	13.788	1006910	50.0
Decane, 2,2,9-t...	13.529	7.5	ug/l	151831	4	13.788	1006910	50.0
Carbonic acid, ...	13.641	30.9	ug/l	621581	4	13.788	1006910	50.0
Decane, 3,7-dim...	13.994	25.8	ug/l	519547	4	13.788	1006910	50.0
Pentane, 3,3-di...	14.065	6.3	ug/l	126305	4	13.788	1006910	50.0
Undecane, 4-met...	14.135	6.7	ug/l	135179	4	13.788	1006910	50.0
Octane, 2,3,6,7...	14.176	11.9	ug/l	240742	4	13.788	1006910	50.0
Hexane, 2,2,5-t...	14.341	8.0	ug/l	160825	4	13.788	1006910	50.0
Octane, 2,6-dim...	14.735	12.1	ug/l	242613	4	13.788	1006910	50.0