

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032625\
 Data File : VN086124.D
 Acq On : 26 Mar 2025 14:23
 Operator : JC\MD
 Sample : Q1634-01
 Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 HR-01-032425

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\82N031825W.M
 Title : SW846 8260

Signal : TIC: VN086124.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	52	58	66	rVB	9322	14975	1.84%	0.179%
2	2.859	137	154	156	rBV6	19483	78510	9.63%	0.940%
3	8.159	1045	1055	1060	rBV	131741	322582	39.58%	3.863%
4	8.218	1060	1065	1075	rVB	208405	440692	54.07%	5.277%
5	8.571	1116	1125	1134	rBV	130927	300991	36.93%	3.604%
6	8.653	1134	1139	1147	rBV3	4276	11651	1.43%	0.140%
7	8.782	1156	1161	1179	rVB5	10610	38791	4.76%	0.465%
8	9.094	1205	1214	1227	rBV	295742	604519	74.17%	7.239%
9	10.565	1454	1464	1472	rBV	447167	815003	100.00%	9.760%
10	10.623	1472	1474	1483	rVB2	7017	10028	1.23%	0.120%
11	11.865	1677	1685	1697	rBV	398505	694677	85.24%	8.319%
12	12.070	1715	1720	1724	rBV4	4199	8234	1.01%	0.099%
13	12.770	1835	1839	1840	rVV4	6456	8694	1.07%	0.104%
14	12.847	1846	1852	1863	rBV	290160	493344	60.53%	5.908%
15	13.012	1877	1880	1887	rVB6	5512	10889	1.34%	0.130%
16	13.088	1887	1893	1897	rBV4	5833	11460	1.41%	0.137%
17	13.159	1897	1905	1912	rBV2	67291	128636	15.78%	1.540%
18	13.223	1912	1916	1921	rVB6	9511	15706	1.93%	0.188%
19	13.306	1925	1930	1933	rBV4	8455	15373	1.89%	0.184%
20	13.394	1940	1945	1950	rVB	22470	34419	4.22%	0.412%
21	13.453	1952	1955	1959	rVB4	6730	9814	1.20%	0.118%
22	13.517	1959	1966	1970	rBV6	10932	18667	2.29%	0.224%
23	13.570	1972	1975	1979	rBV4	8902	11393	1.40%	0.136%
24	13.670	1986	1992	1997	rBV6	26687	62576	7.68%	0.749%
25	13.711	1997	1999	2003	rVV3	24679	38212	4.69%	0.458%
26	13.788	2006	2012	2020	rVV	418160	720175	88.36%	8.624%
27	13.853	2020	2023	2029	rVB2	30311	47088	5.78%	0.564%
28	13.941	2031	2038	2041	rBV9	12387	24811	3.04%	0.297%
29	13.982	2041	2045	2048	rBV3	15834	23244	2.85%	0.278%
30	14.017	2048	2051	2057	rVB3	18979	33128	4.06%	0.397%
31	14.100	2060	2065	2072	rBV	202377	350320	42.98%	4.195%
32	14.258	2087	2092	2098	rBV5	24159	49010	6.01%	0.587%
33	14.323	2098	2103	2107	rVV3	32477	53953	6.62%	0.646%
34	14.364	2107	2110	2116	rVB6	26358	40966	5.03%	0.491%
35	14.435	2116	2122	2127	rBV6	35969	70502	8.65%	0.844%
36	14.494	2129	2132	2140	rBV8	12969	24488	3.00%	0.293%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

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Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	14.582	2141	2147	2149	rBV4	40482	70864	8.69%	0.849%
38	14.623	2150	2154	2157	rVV3	91593	136224	16.71%	1.631%
39	14.658	2157	2160	2163	rVV2	39558	54649	6.71%	0.654%
40	14.688	2163	2165	2168	rVB2	21916	25794	3.16%	0.309%
41	14.729	2168	2172	2176	rVB4	53895	70738	8.68%	0.847%
42	14.788	2176	2182	2187	rVB6	31853	69447	8.52%	0.832%
43	14.841	2187	2191	2194	rBV5	21741	39712	4.87%	0.476%
44	14.958	2202	2211	2218	rBV2	225222	392296	48.13%	4.698%
45	15.041	2218	2225	2229	rBV5	77776	211282	25.92%	2.530%
46	15.217	2250	2255	2260	rVB3	45210	91536	11.23%	1.096%
47	15.311	2267	2271	2276	rBV5	44055	75140	9.22%	0.900%
48	15.429	2287	2291	2299	rVB5	33940	95549	11.72%	1.144%
49	15.505	2299	2304	2313	rVB8	43327	116027	14.24%	1.389%
50	15.588	2313	2318	2328	rVB7	59320	129987	15.95%	1.557%
51	15.670	2329	2332	2333	rBV3	13887	15562	1.91%	0.186%
52	15.694	2333	2336	2340	rBV3	23237	39076	4.79%	0.468%
53	15.829	2354	2359	2369	rVB	172986	355473	43.62%	4.257%
54	15.941	2370	2378	2386	rBV7	50651	152834	18.75%	1.830%
55	16.123	2402	2409	2411	rBV6	25085	57197	7.02%	0.685%
56	16.164	2411	2416	2426	rVB2	77976	165365	20.29%	1.980%
57	16.494	2462	2472	2477	rBV7	58836	171687	21.07%	2.056%
58	16.705	2501	2508	2516	rBV4	74319	176708	21.68%	2.116%

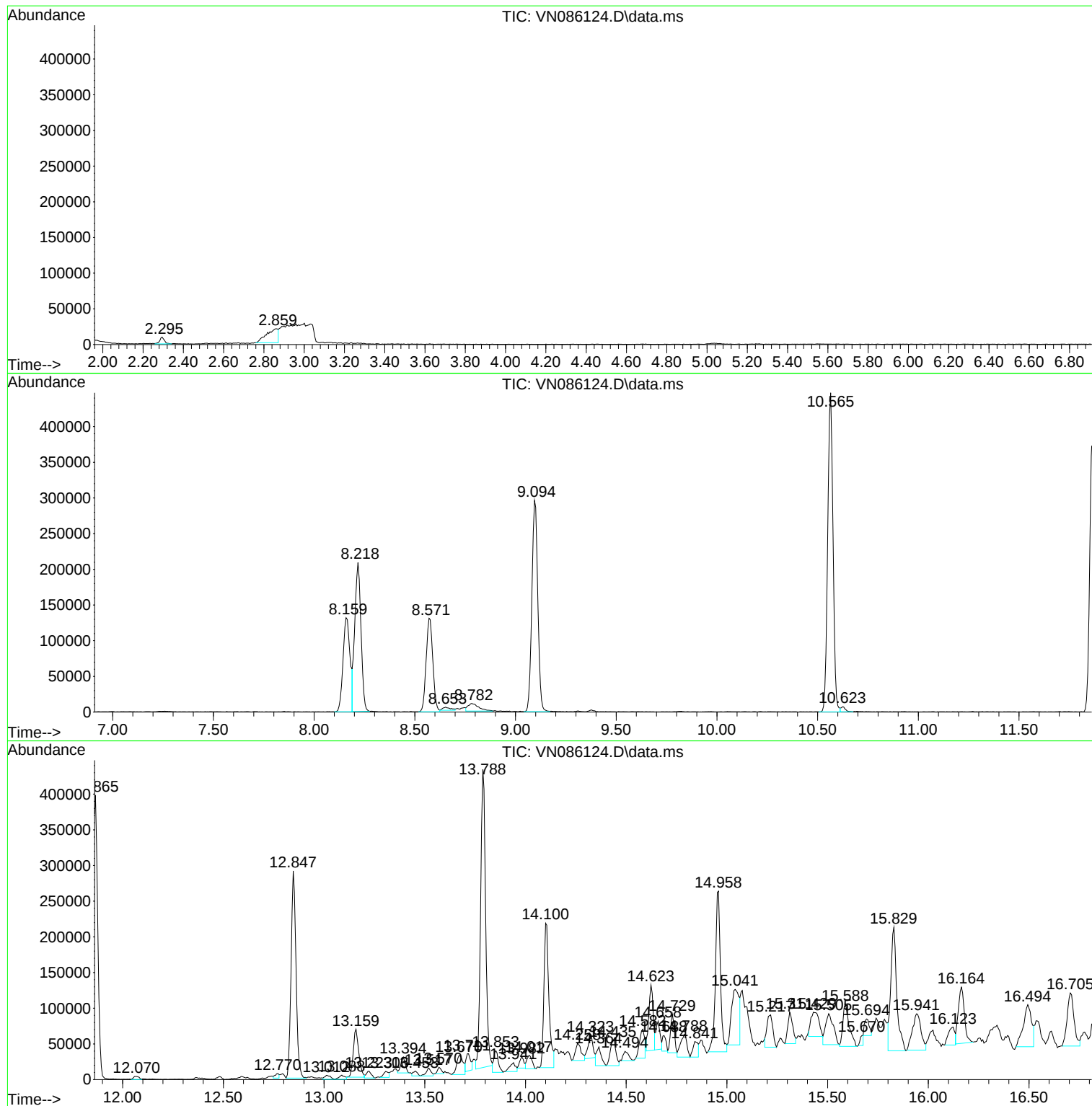
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_N
ClientSampleId :
HR-01-032425

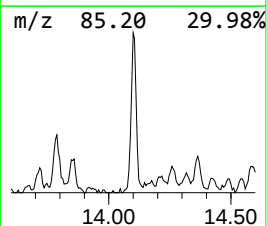
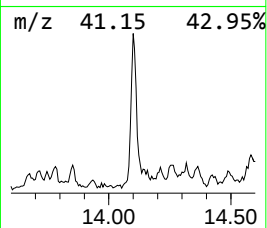
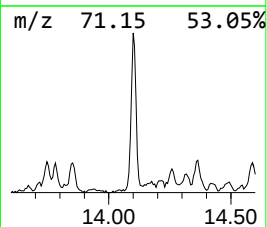
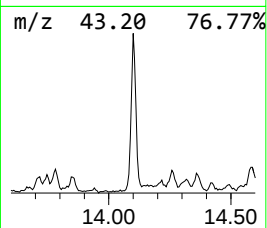
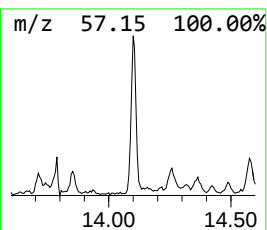
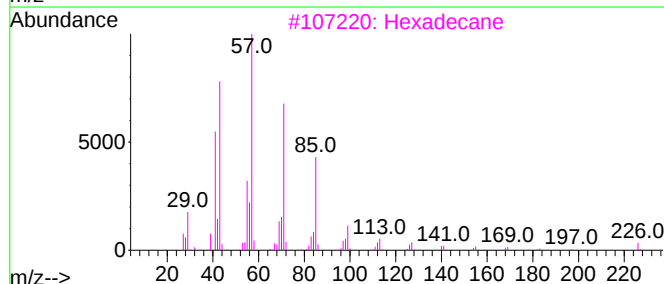
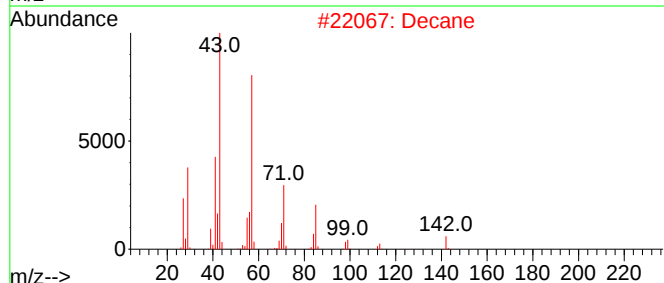
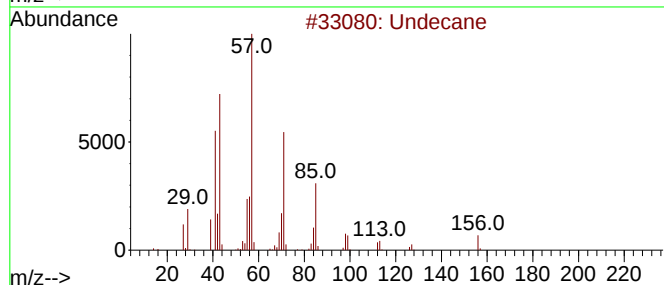
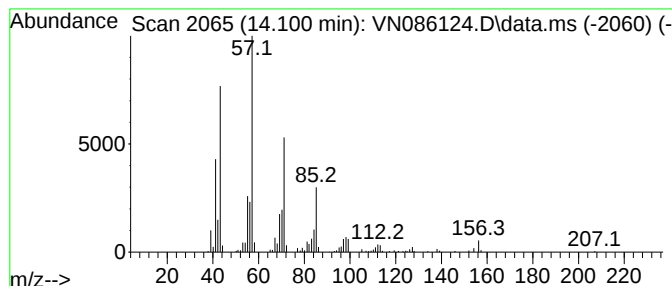
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.100	24.32 ug/l	350320	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Decane			142	C10H22	000124-18-5	90
3	Hexadecane			226	C16H34	000544-76-3	80
4	Carbonic acid, dodecyl vinyl ester			256	C15H28O3	1000382-54-8	78
5	Tridecane			184	C13H28	000629-50-5	64



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Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-01-032425

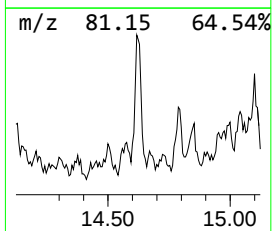
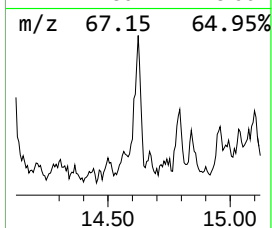
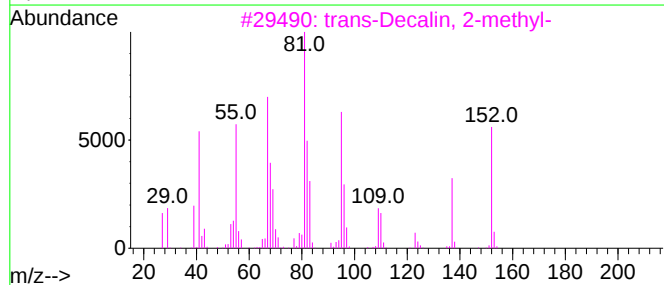
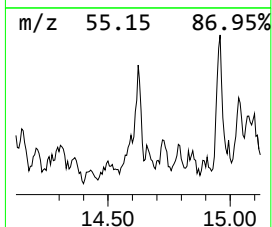
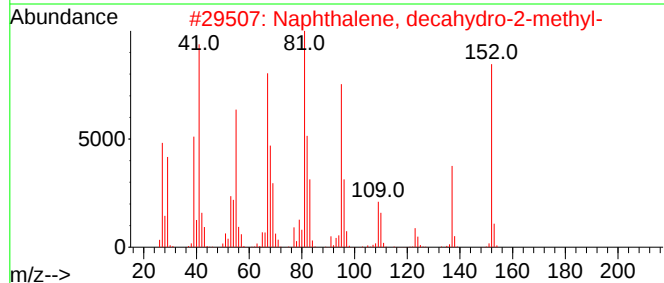
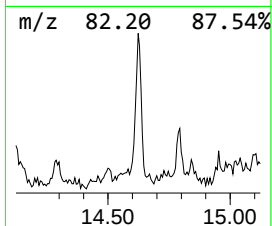
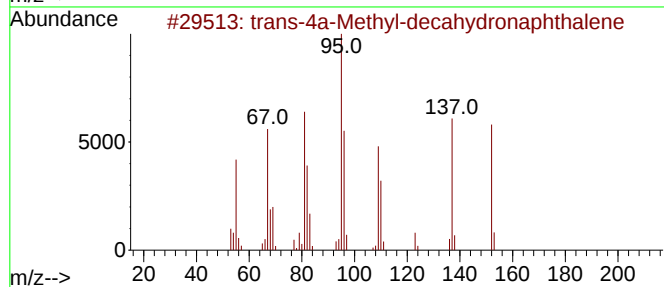
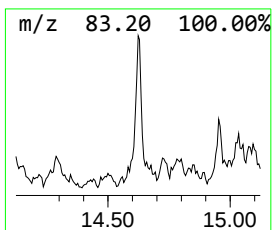
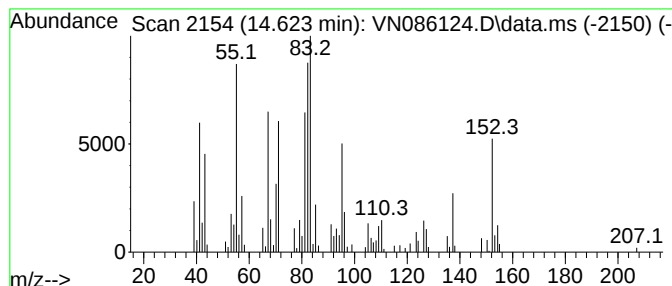
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 2 trans-4a-Methyl-decahydrona... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.623	9.46 ug/l	136224	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	81
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	66
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	53
4			Vinylcyclohexyl ether	126	C8H14O	002182-55-0	43
5			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	38



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Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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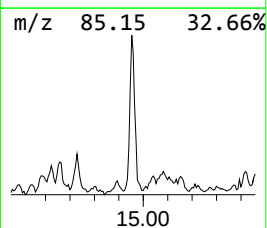
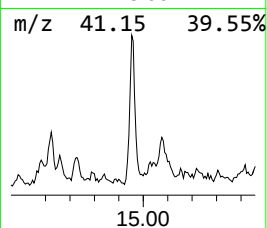
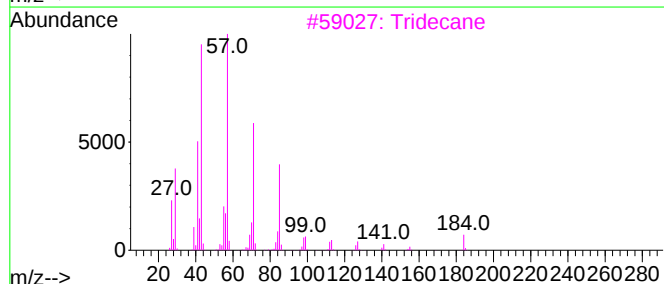
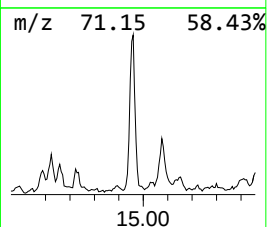
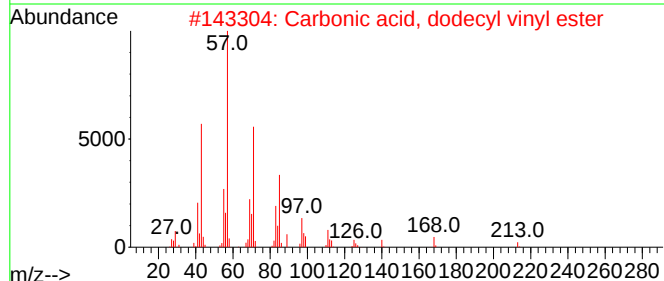
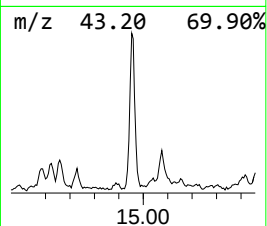
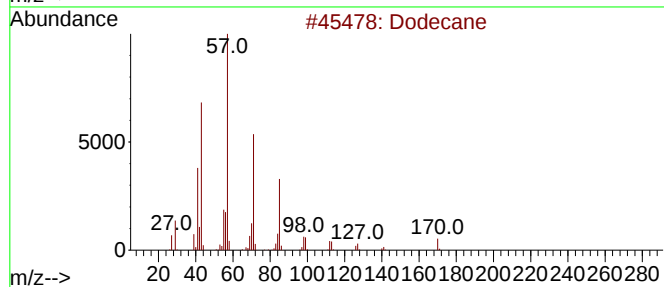
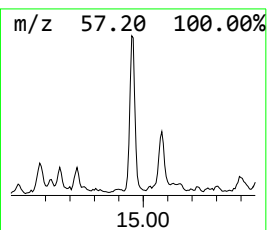
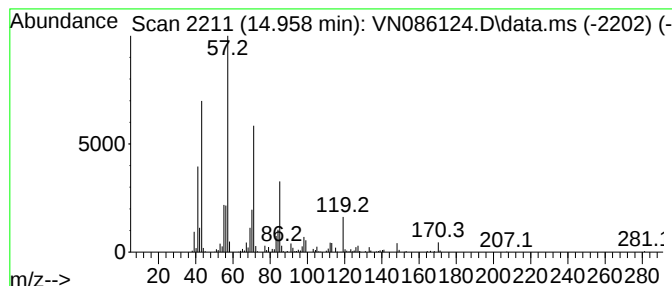
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.958	27.24 ug/l	392296	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	72
3			Tridecane	184	C13H28	000629-50-5	64
4			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	53
5			Pentadecane	212	C15H32	000629-62-9	53



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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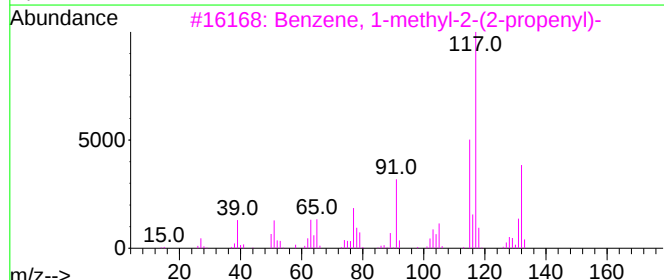
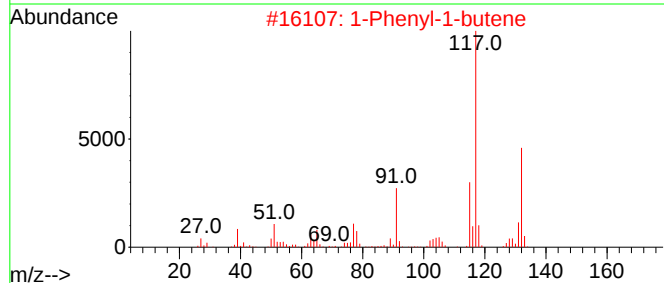
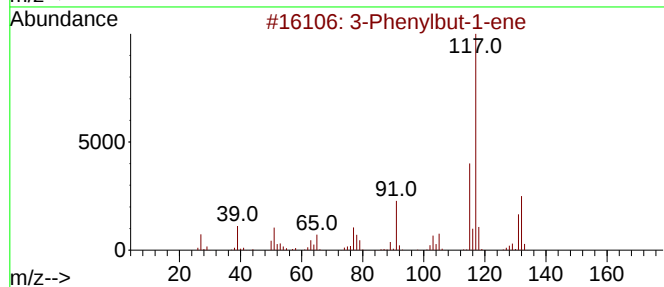
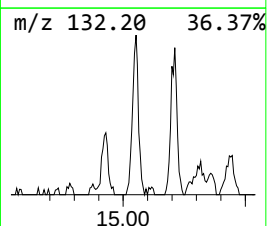
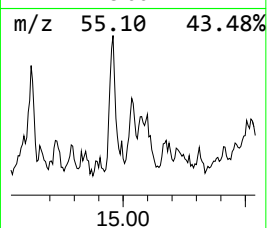
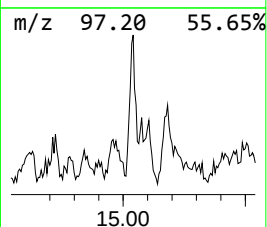
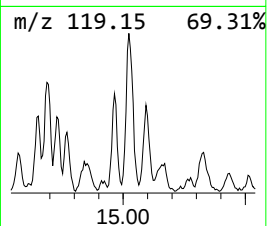
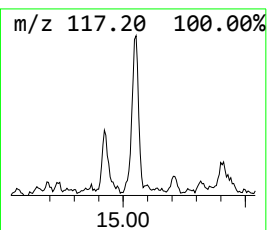
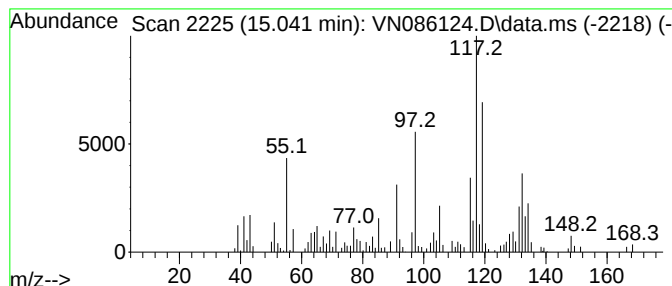
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 4 3-Phenylbut-1-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	14.67 ug/l	211282	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	55
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	50
3			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	50
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	50
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	50



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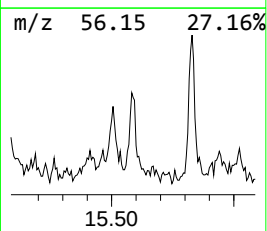
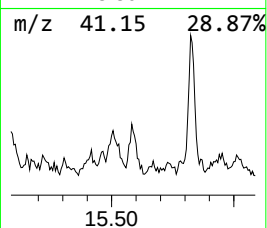
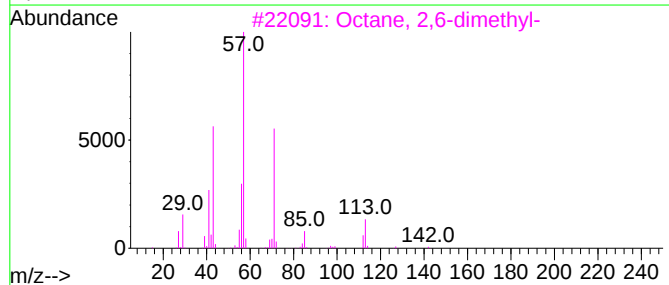
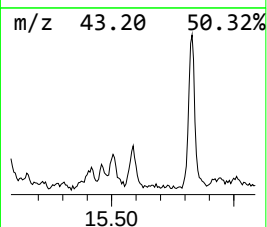
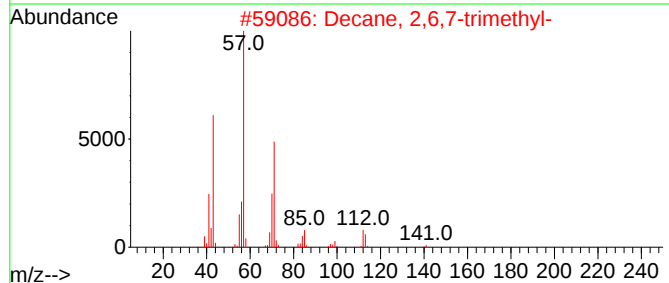
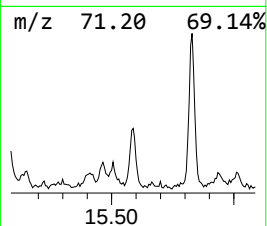
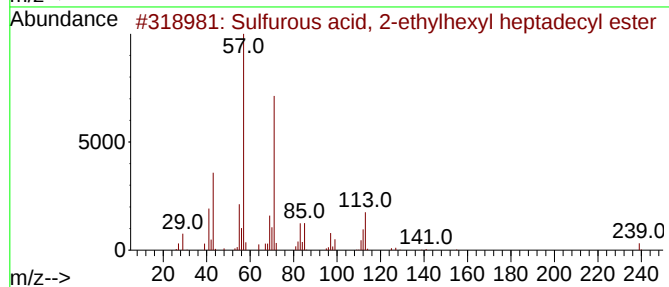
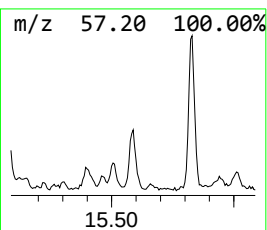
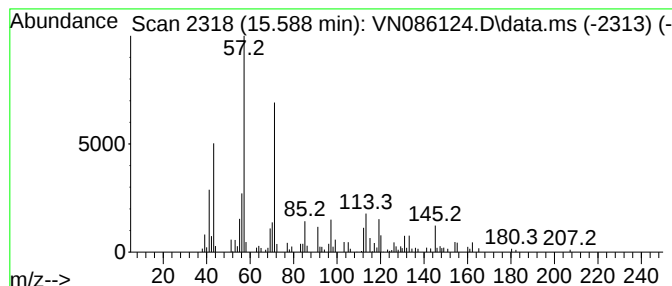
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Quant Title : SW846 8260

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

Peak Number 5 Sulfurous acid, 2-ethylhexy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.588	9.02 ug/l	129987	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	64
2			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	59
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
4			Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	58
5			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032625\
Data File : VN086124.D
Acq On : 26 Mar 2025 14:23
Operator : JC\MD
Sample : Q1634-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-01-032425

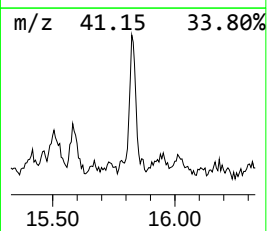
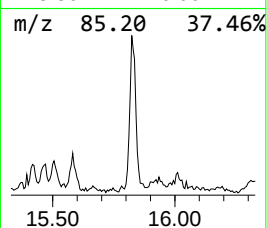
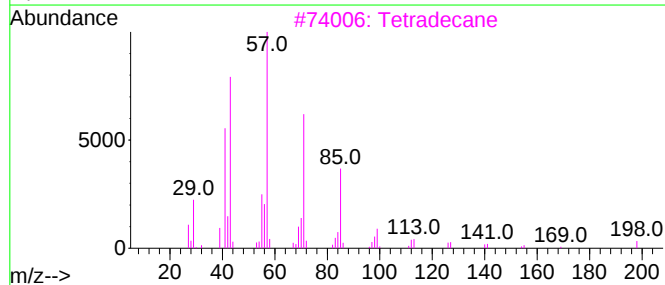
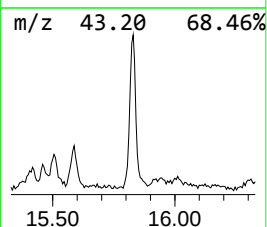
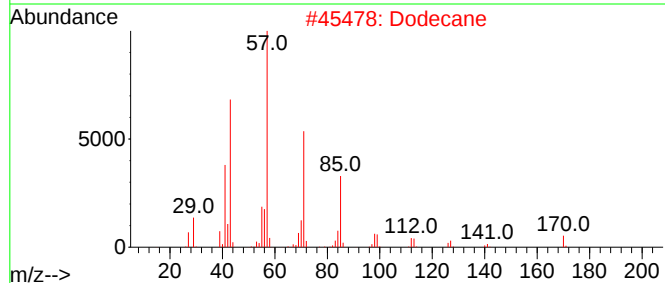
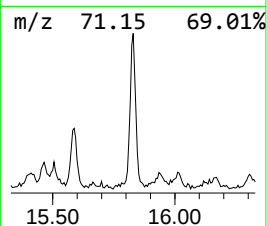
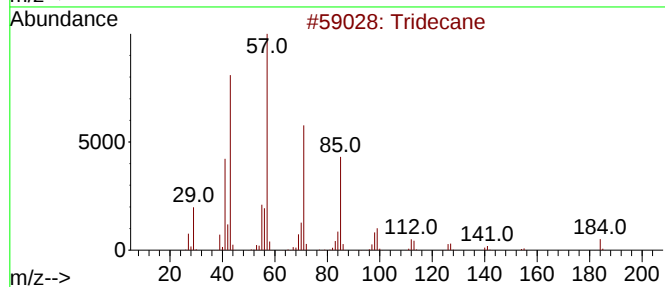
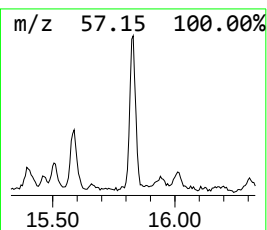
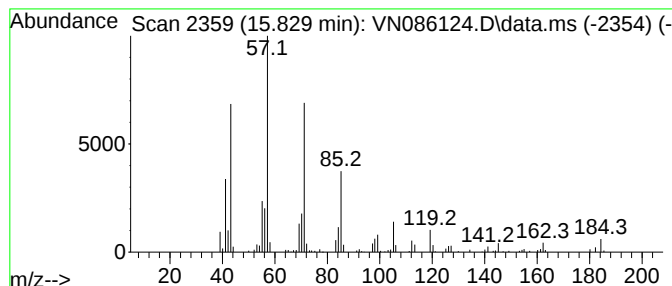
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Quant Title : SW846 8260

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

Peak Number 6 Tridecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.829	24.68 ug/l	355473	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Dodecane	170	C12H26	000112-40-3	72
3			Tetradecane	198	C14H30	000629-59-4	72
4			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	72
5			Hexadecane	226	C16H34	000544-76-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032625\
Data File : VN086124.D
Acq On : 26 Mar 2025 14:23
Operator : JC\MD
Sample : Q1634-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-01-032425

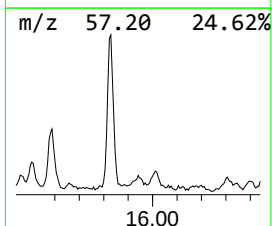
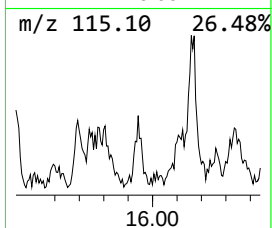
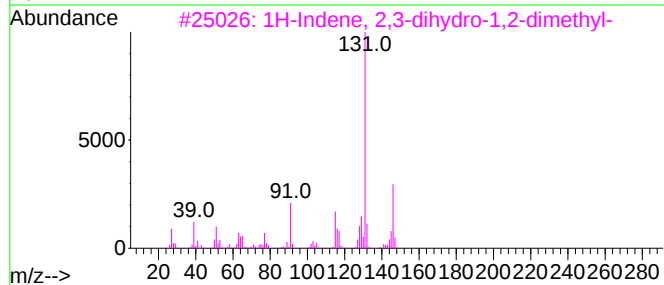
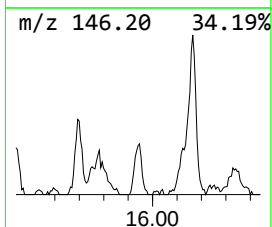
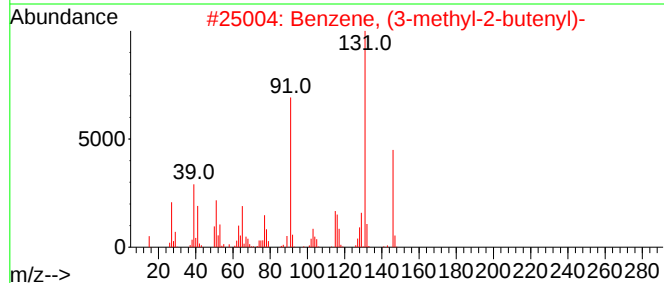
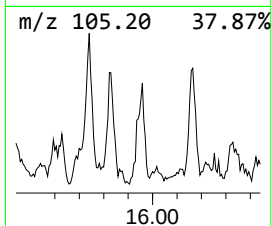
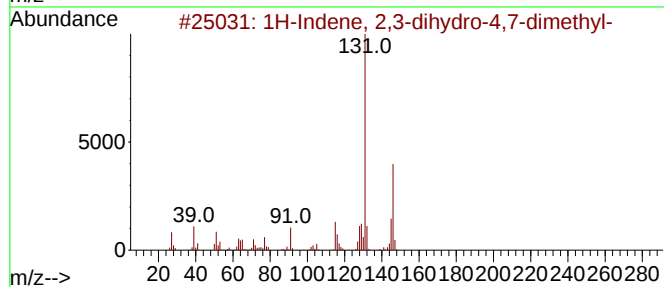
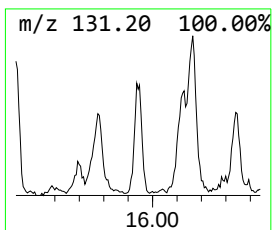
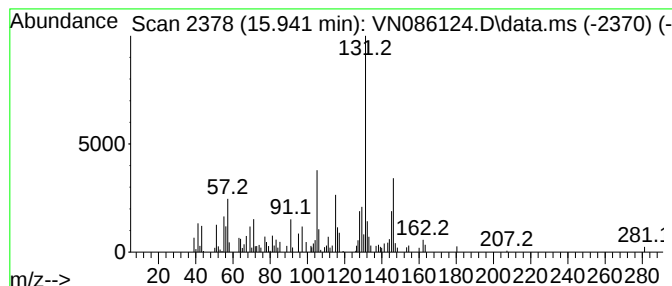
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.941	10.61 ug/l	152834	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	76
2			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	76
3			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	76
4			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	76
5			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032625\
Data File : VN086124.D
Acq On : 26 Mar 2025 14:23
Operator : JC\MD
Sample : Q1634-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-01-032425

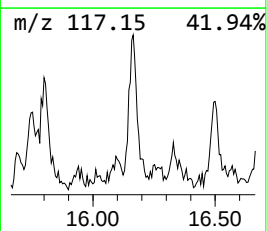
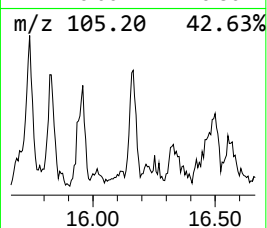
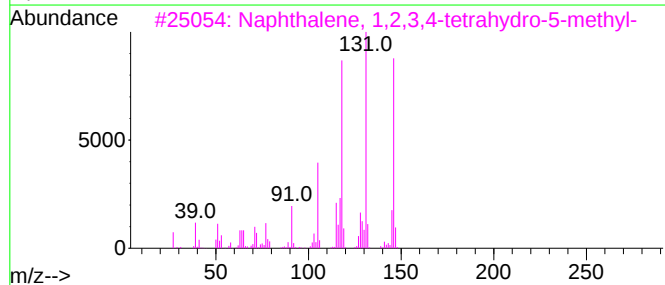
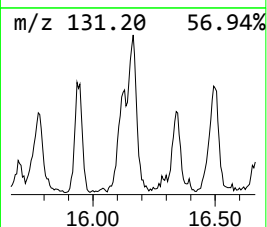
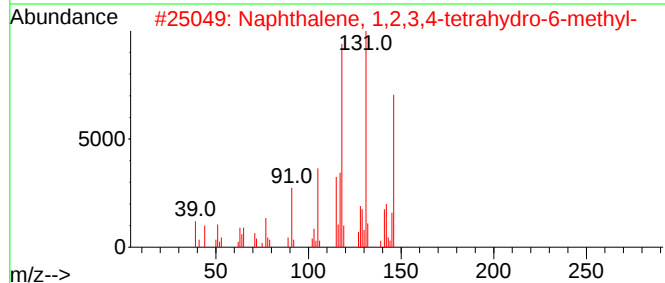
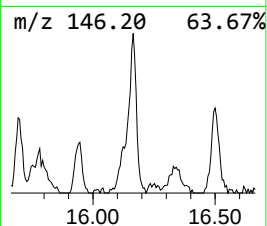
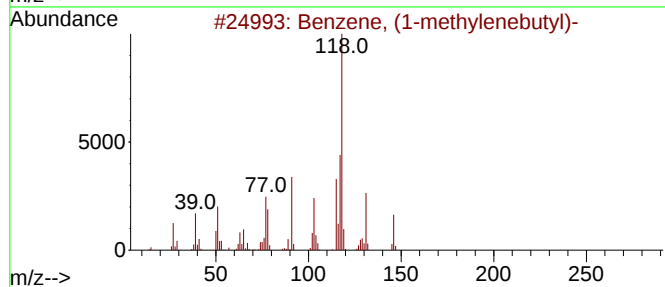
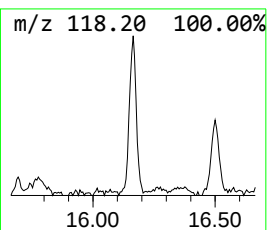
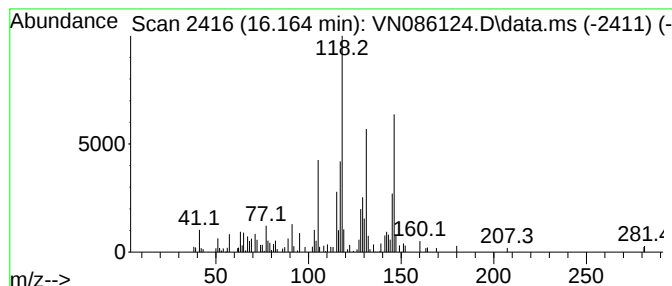
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, (1-methylenebutyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.164	11.48 ug/l	165365	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	76
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	76
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	70
4			Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	68
5			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032625\
Data File : VN086124.D
Acq On : 26 Mar 2025 14:23
Operator : JC\MD
Sample : Q1634-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-01-032425

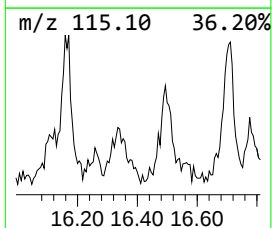
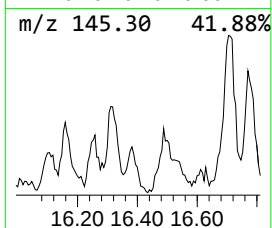
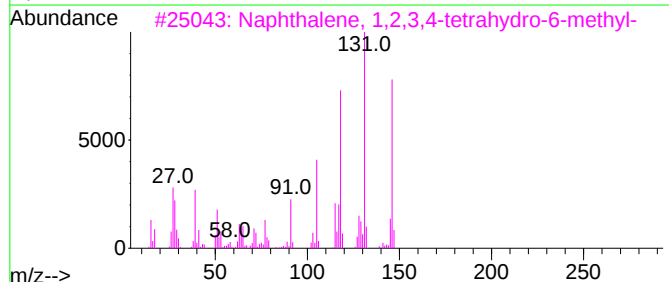
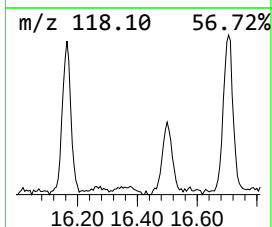
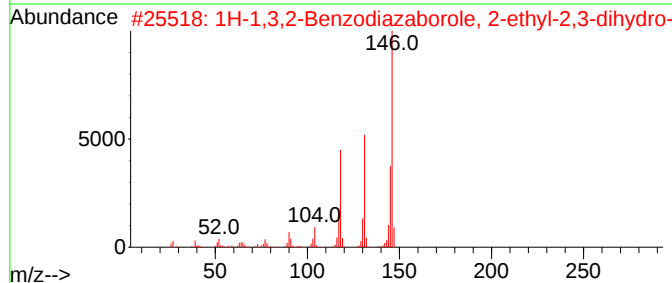
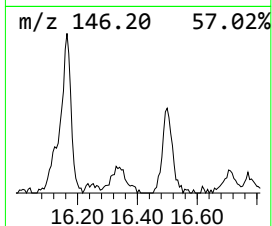
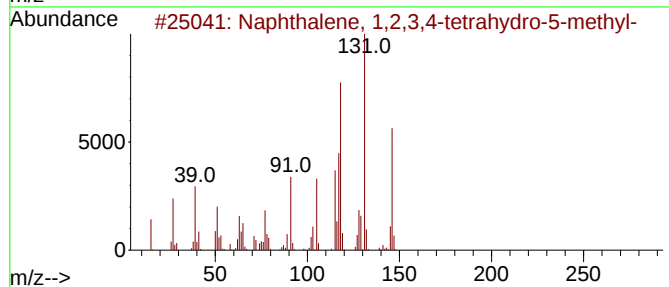
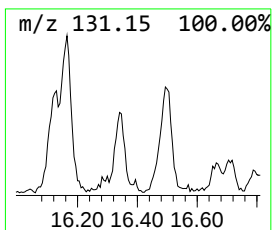
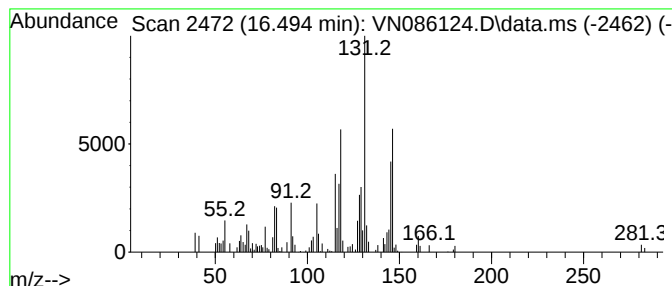
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.494	11.92 ug/l	171687	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	76
2			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	68
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	58
4			2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	58
5			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032625\
Data File : VN086124.D
Acq On : 26 Mar 2025 14:23
Operator : JC\MD
Sample : Q1634-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

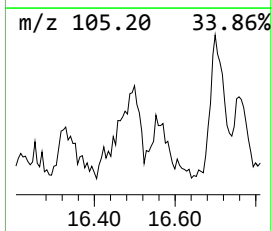
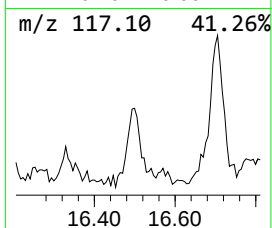
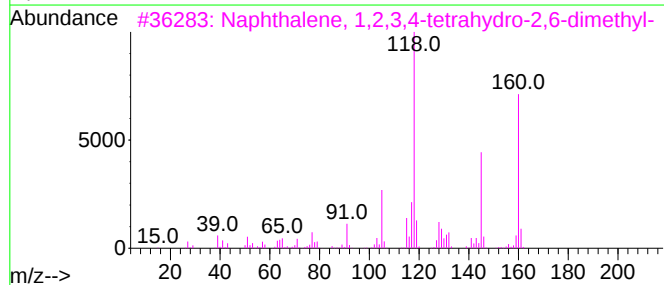
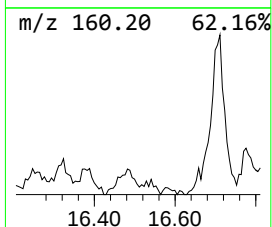
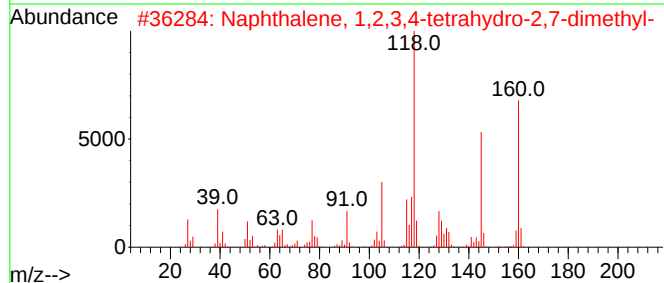
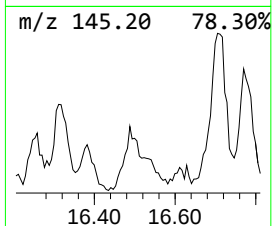
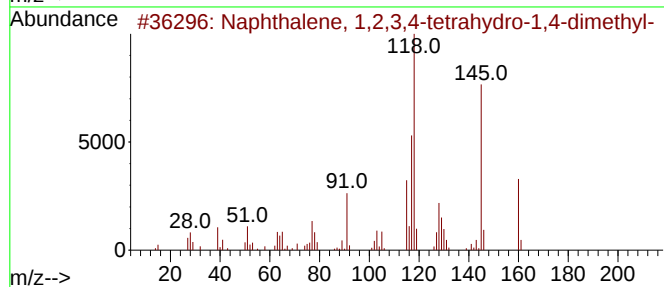
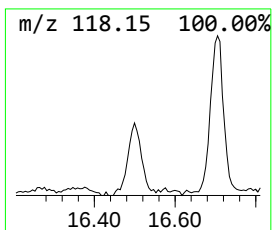
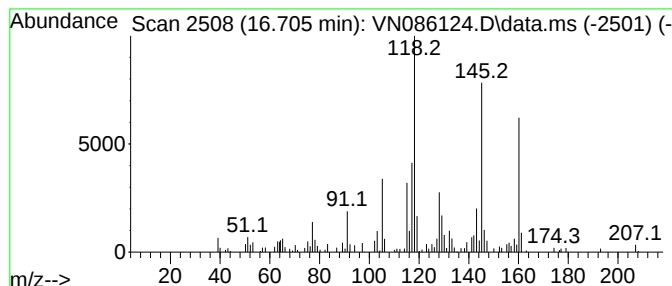
Instrument :
MSVOA_N
ClientSampleId :
HR-01-032425

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
16.705	12.27 ug/l	176708	1,4-Dichlorobenzene-d4			13.794
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	004175-54-6	91
2	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	013065-07-1	87
3	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	007524-63-2	74
4	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	021564-91-0	58
5	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	001076-61-5	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032625\
Data File : VN086124.D
Acq On : 26 Mar 2025 14:23
Operator : JC\MD
Sample : Q1634-01
Misc : 5.08g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
HR-01-032425

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.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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trans-4a-Methyl...	14.623	9.5	ug/l	136224	4	13.794	720175	50.0
Dodecane	14.958	27.2	ug/l	392296	4	13.794	720175	50.0
3-Phenylbut-1-ene	15.041	14.7	ug/l	211282	4	13.794	720175	50.0
Sulfurous acid,...	15.588	9.0	ug/l	129987	4	13.794	720175	50.0
Tridecane	15.829	24.7	ug/l	355473	4	13.794	720175	50.0
1H-Indene, 2,3-...	15.941	10.6	ug/l	152834	4	13.794	720175	50.0
Benzene, (1-met...	16.164	11.5	ug/l	165365	4	13.794	720175	50.0
Naphthalene, 1,...	16.494	11.9	ug/l	171687	4	13.794	720175	50.0
Naphthalene, 1,...	16.705	12.3	ug/l	176708	4	13.794	720175	50.0