

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN092925\
 Data File : VN087984.D
 Acq On : 29 Sep 2025 15:50
 Operator : JC\MD
 Sample : Q3188-01
 Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 4135

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\82N092325W.M
 Title : SW846 8260

Signal : TIC: VN087984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.194	1055	1061	1072	rVB2	1178822	2837913	3.74%	1.977%
2	8.300	1072	1079	1089	rVB2	331969	823742	1.08%	0.574%
3	8.418	1089	1099	1116	rBV	1355281	3247303	4.27%	2.262%
4	8.941	1179	1188	1203	rBV	1214204	2445778	3.22%	1.704%
5	9.077	1203	1211	1223	rVB	483990	1018474	1.34%	0.710%
6	10.547	1452	1461	1464	rBV	756903	1376102	1.81%	0.959%
7	10.612	1464	1472	1487	rVB2	41478060	75976673	100.00%	52.932%
8	11.847	1674	1682	1691	rBV	672370	1280638	1.69%	0.892%
9	11.941	1691	1698	1707	rBV	1021809	1765507	2.32%	1.230%
10	12.047	1707	1716	1728	rBV	4419510	8366468	11.01%	5.829%
11	12.376	1764	1772	1783	rBV	1584405	2804810	3.69%	1.954%
12	12.829	1844	1849	1861	rVB	483872	974459	1.28%	0.679%
13	13.135	1896	1901	1909	rVB	510841	874269	1.15%	0.609%
14	13.765	2004	2008	2016	rVV4	822792	1567031	2.06%	1.092%
15	14.082	2056	2062	2068	rBV	3158249	5078190	6.68%	3.538%
16	14.412	2113	2118	2123	rBV4	427555	854192	1.12%	0.595%
17	14.559	2138	2143	2146	rBV3	547140	1065411	1.40%	0.742%
18	14.600	2146	2150	2154	rVV2	1171580	1891051	2.49%	1.317%
19	14.706	2165	2168	2172	rBV3	721374	980584	1.29%	0.683%
20	14.935	2198	2207	2214	rBV3	3485223	6067341	7.99%	4.227%
21	15.029	2215	2223	2225	rBV4	944868	2530495	3.33%	1.763%
22	15.188	2246	2250	2256	rVB2	547350	1094067	1.44%	0.762%
23	15.294	2263	2268	2273	rBV2	602368	1043263	1.37%	0.727%
24	15.417	2282	2289	2295	rVB5	513567	1391875	1.83%	0.970%
25	15.482	2296	2300	2309	rVB7	559378	1508277	1.99%	1.051%
26	15.564	2309	2314	2324	rBV5	741616	1752561	2.31%	1.221%
27	15.800	2350	2354	2365	rVB	2182655	4452678	5.86%	3.102%
28	15.917	2365	2374	2382	rBV5	740505	2271310	2.99%	1.582%
29	16.135	2406	2411	2420	rVB	1297293	2724062	3.59%	1.898%
30	16.470	2463	2468	2473	rVB2	427028	808584	1.06%	0.563%
31	16.676	2496	2503	2509	rBV	873249	1855995	2.44%	1.293%
32	16.747	2510	2515	2519	rBV3	382593	807728	1.06%	0.563%

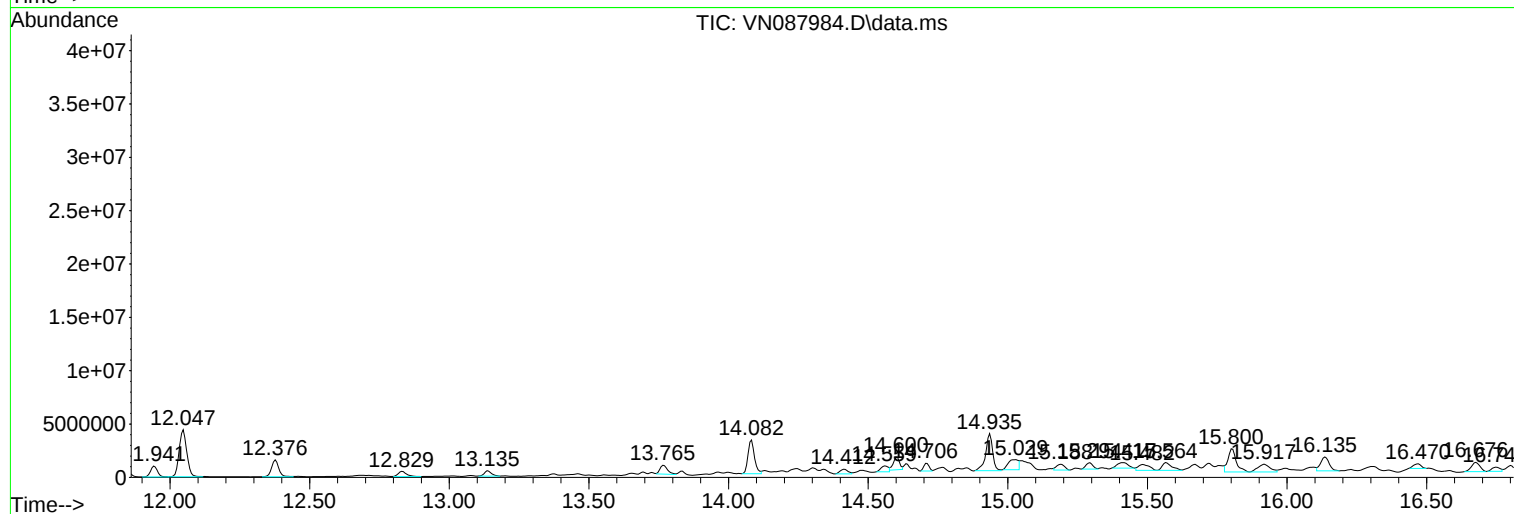
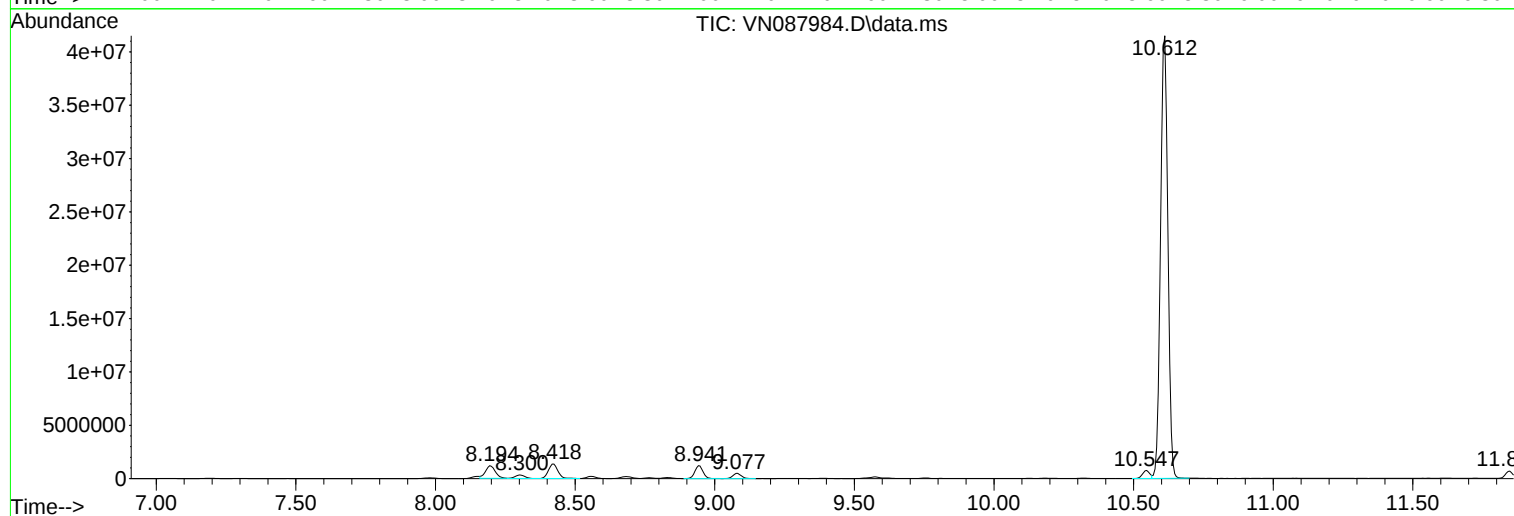
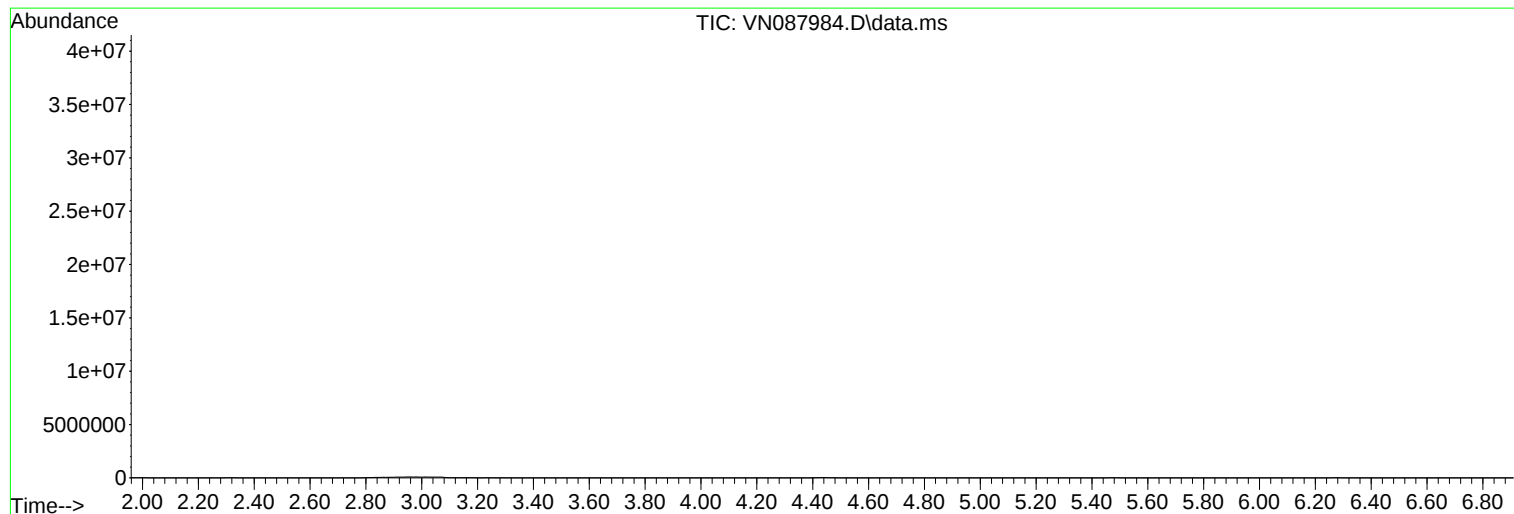
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Quant Title : SW846 8260

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



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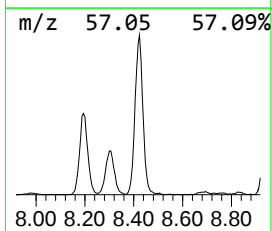
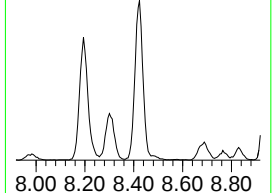
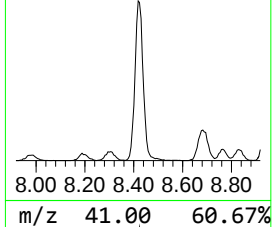
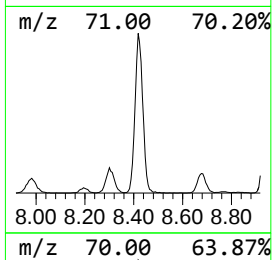
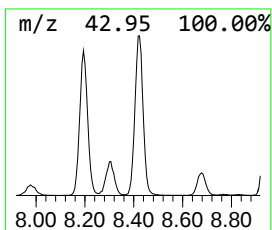
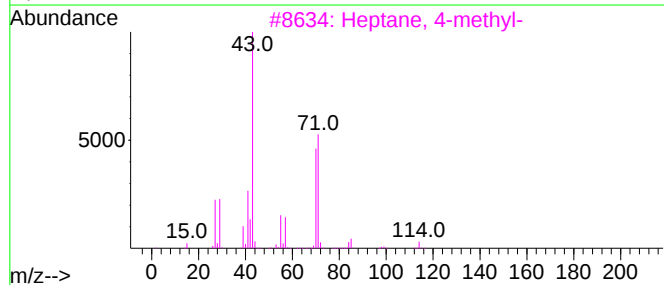
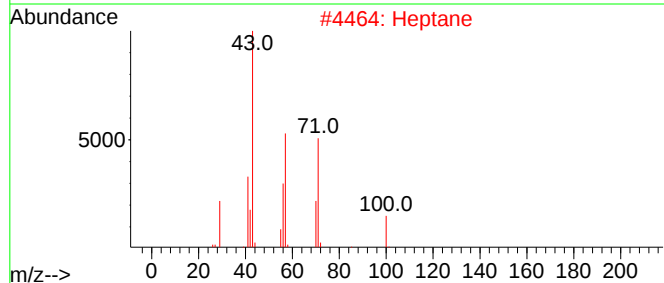
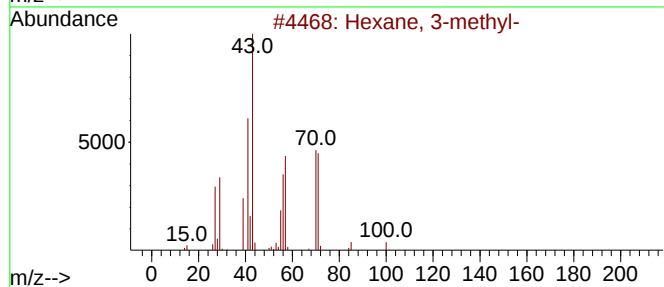
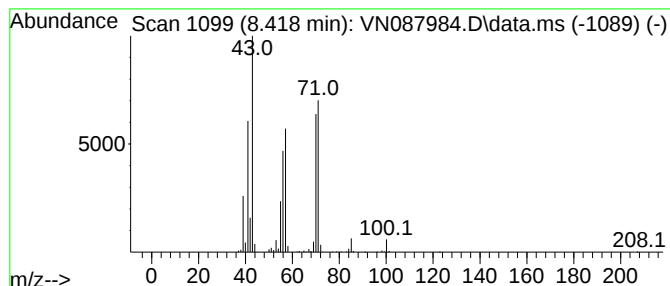
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092325W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.418	57.21 ug/l	3247300	Pentafluorobenzene	8.200

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5			Diisooamyl ether	158	C10H22O	000544-01-4	53



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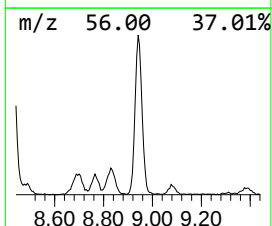
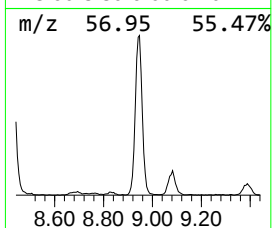
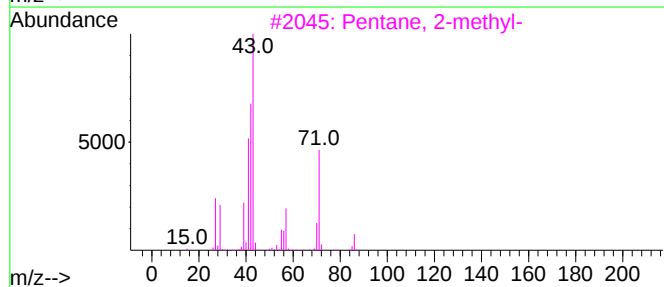
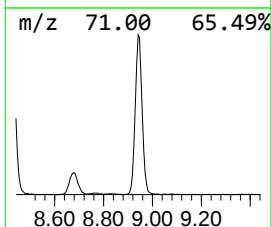
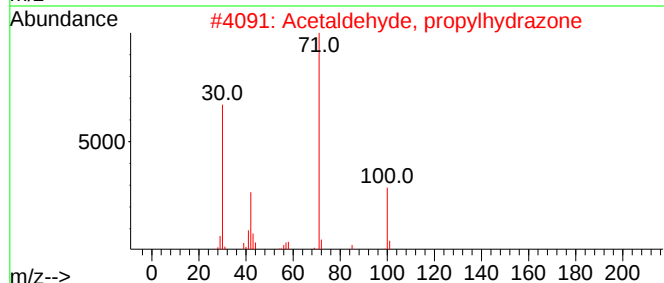
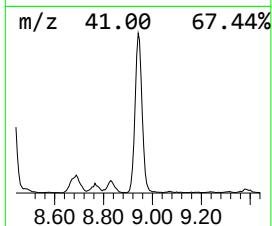
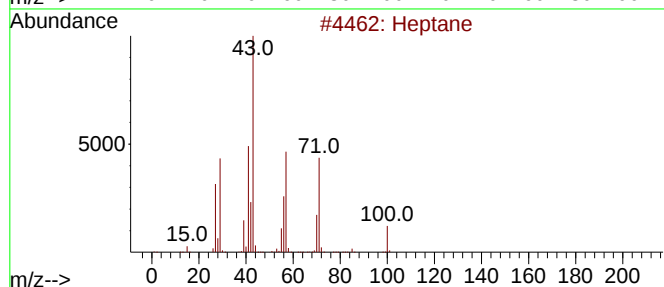
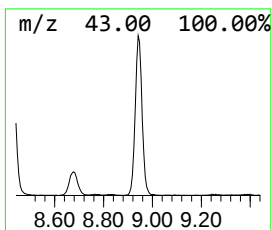
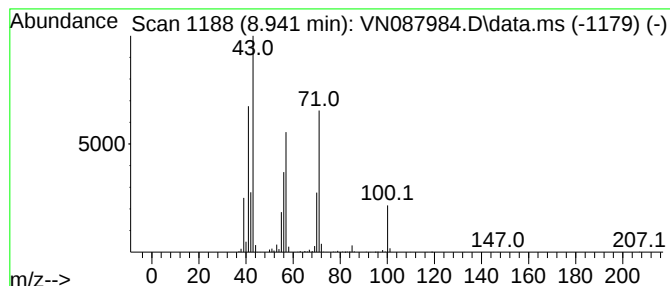
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.941	120.07 ug/l	2445780	1,4-Difluorobenzene	9.082

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	87
2			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	43
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	43
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38



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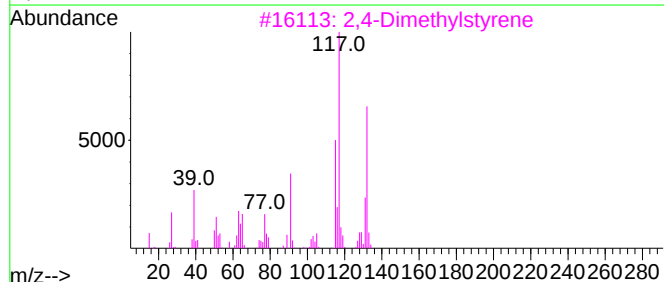
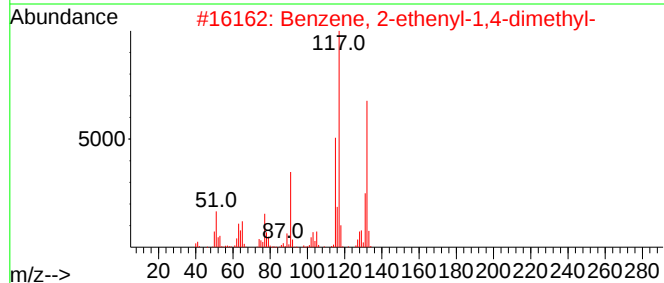
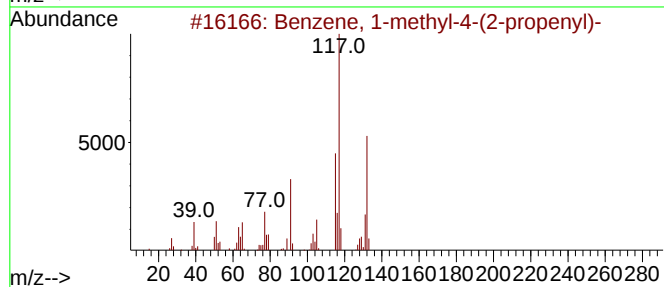
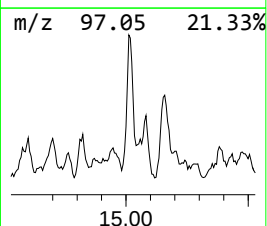
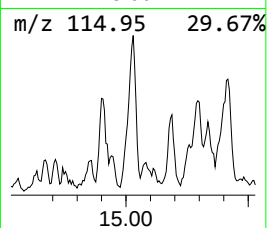
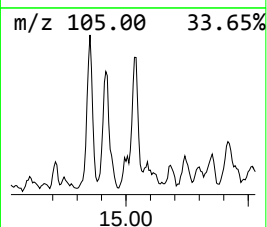
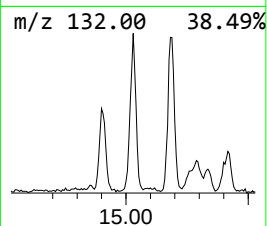
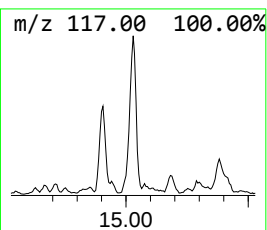
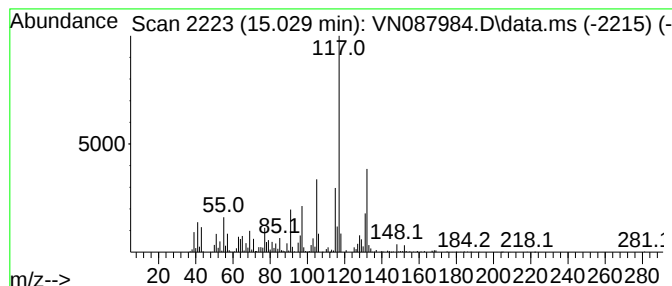
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzene, 1-methyl-4-(2-prop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.029	80.74 ug/l	2530500	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	90
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	87
3			2,4-Dimethylstyrene	132	C10H12	002234-20-0	87
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	76
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	76



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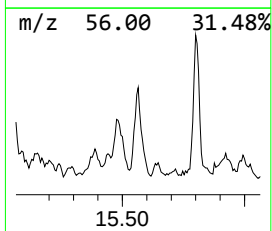
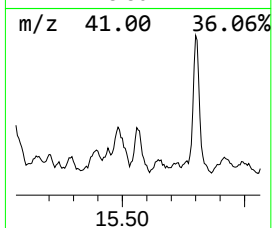
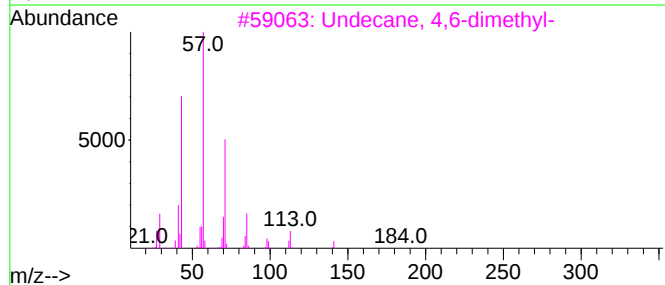
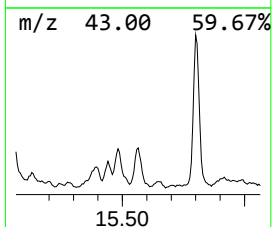
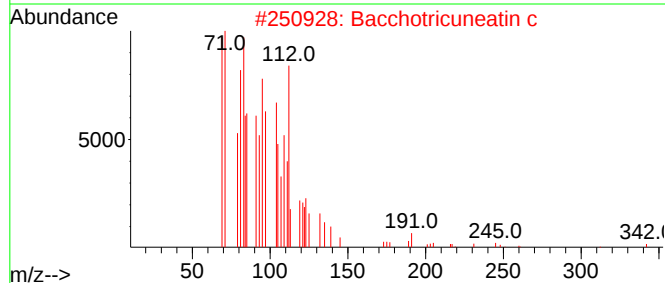
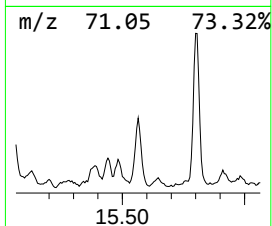
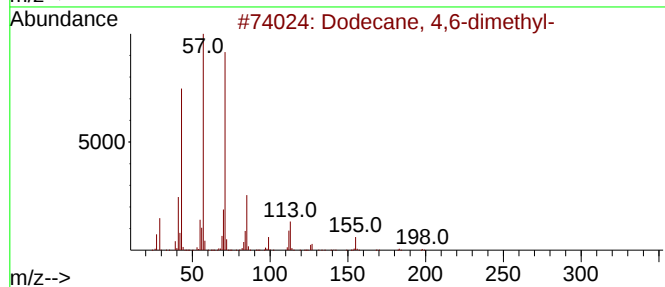
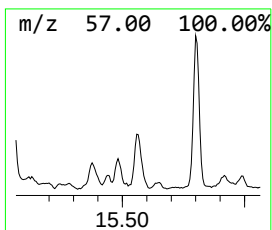
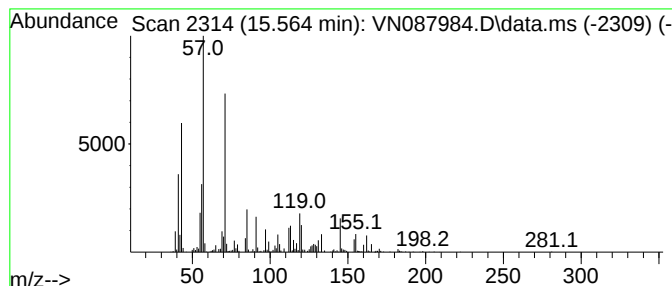
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dodecane, 4,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.564	55.92 ug/l	1752560	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	86
2			Bacchotricuneatin c	342	C20H22O5	066563-30-2	74
3			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	70
4			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	64
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	58



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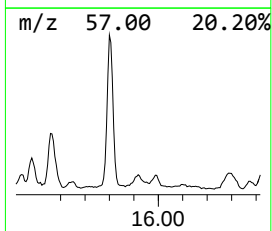
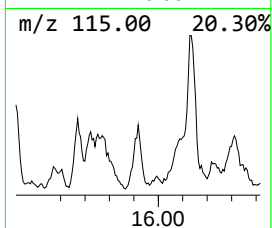
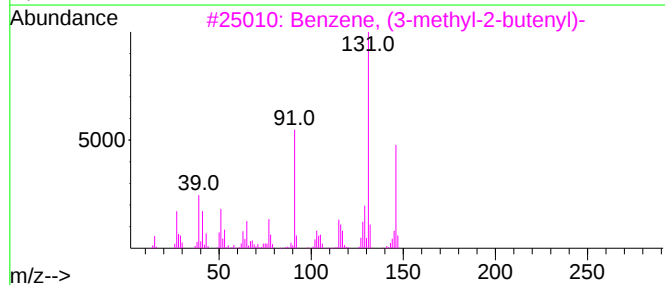
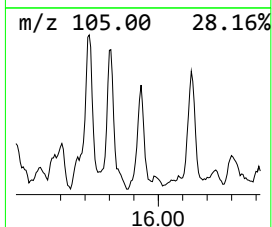
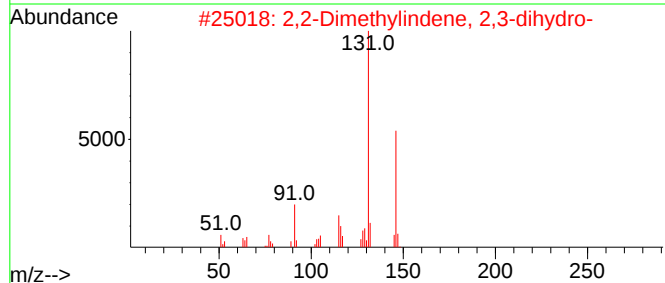
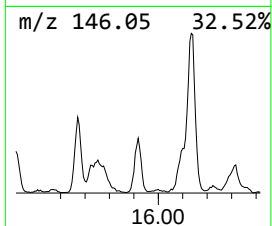
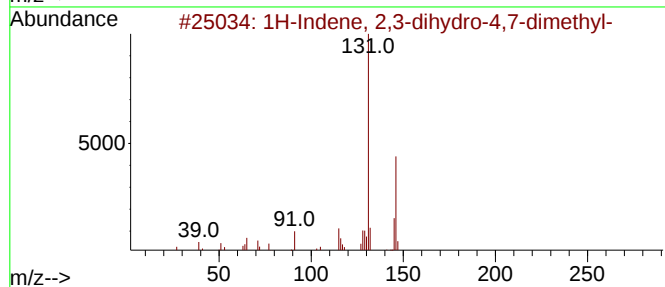
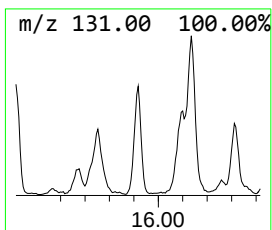
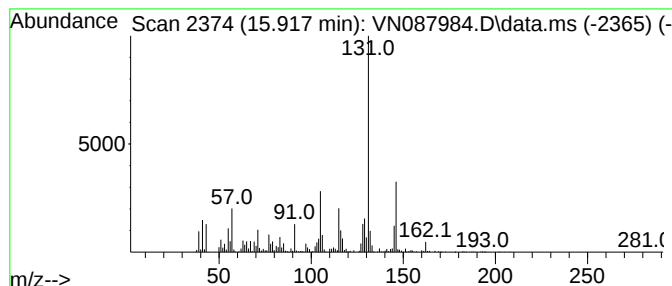
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TIC Integration Parameters: LSCINT.P

Peak Number 8 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.917	72.47 ug/l	2271310	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
2			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	81
3			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	81
4			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	81
5			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN092925\
Data File : VN087984.D
Acq On : 29 Sep 2025 15:50
Operator : JC\MD
Sample : Q3188-01
Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
4135

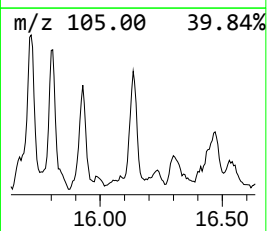
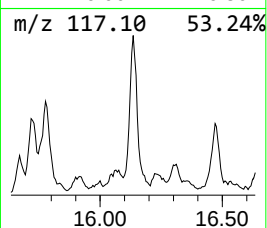
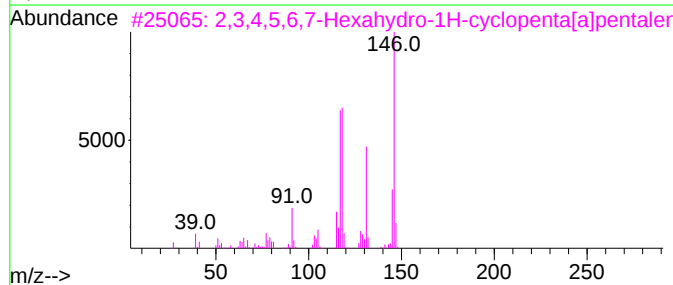
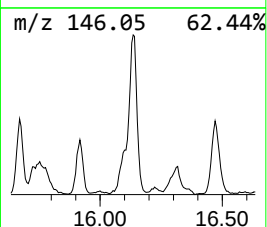
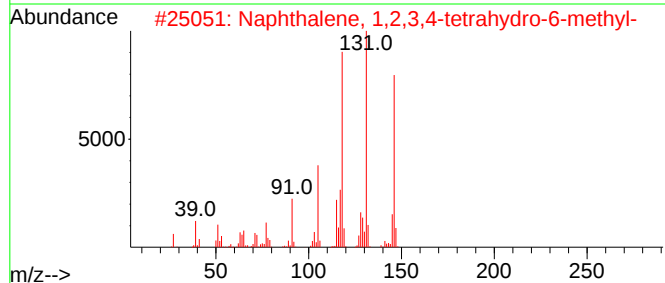
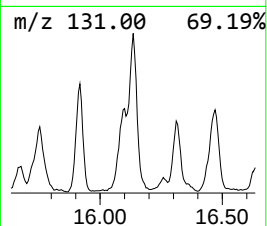
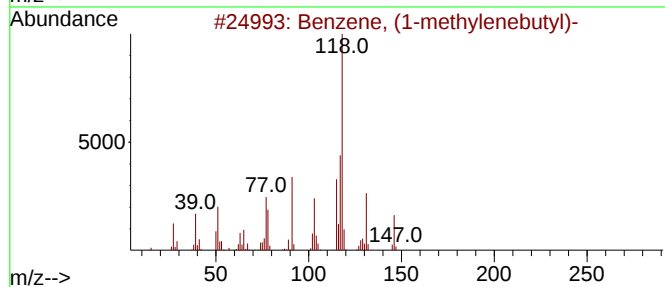
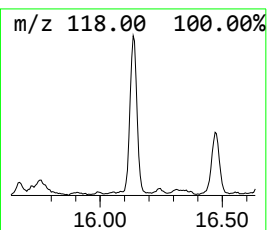
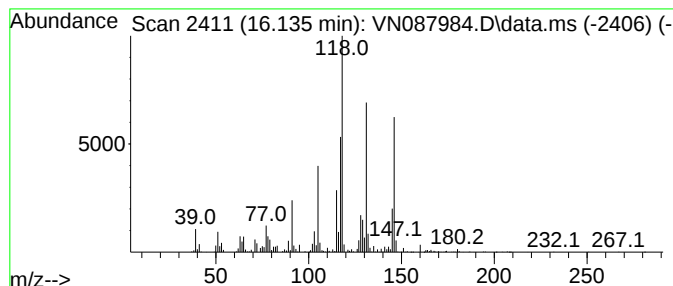
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, (1-methylenebutyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.135	86.92 ug/l	2724060	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	87
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	81
3			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	76
4			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	68
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	62



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Acq On : 29 Sep 2025 15:50
Operator : JC\MD
Sample : Q3188-01
Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
4135

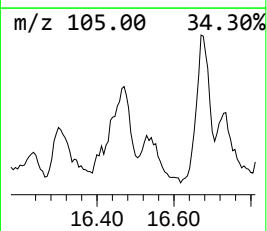
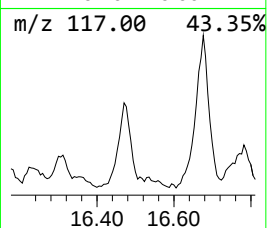
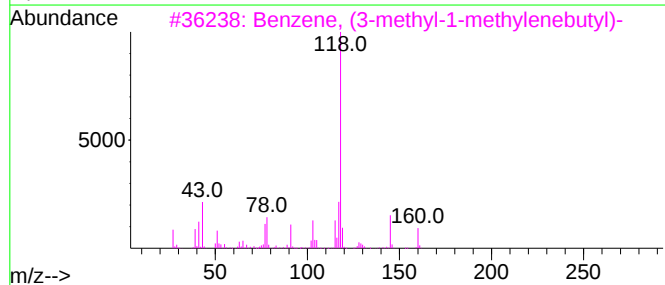
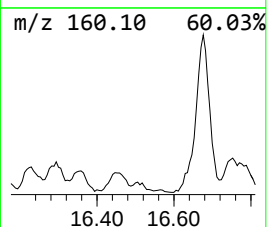
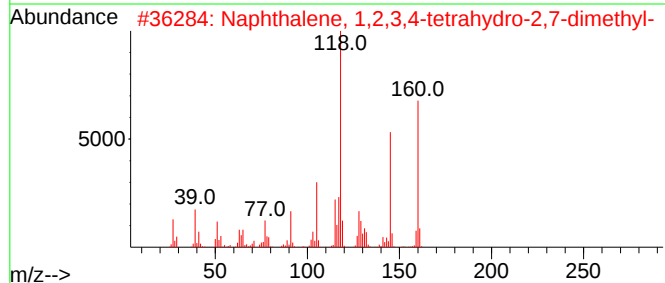
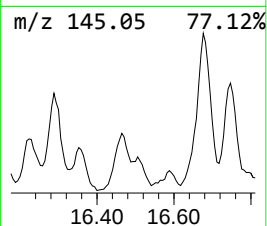
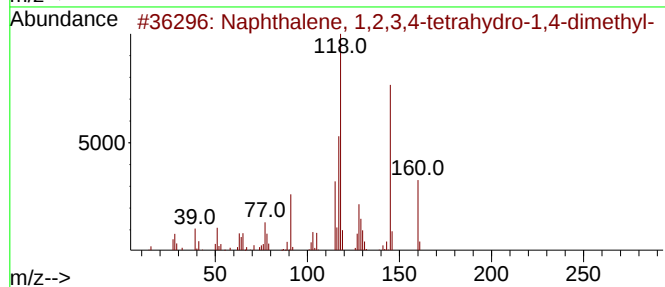
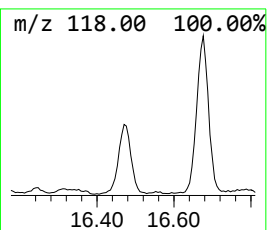
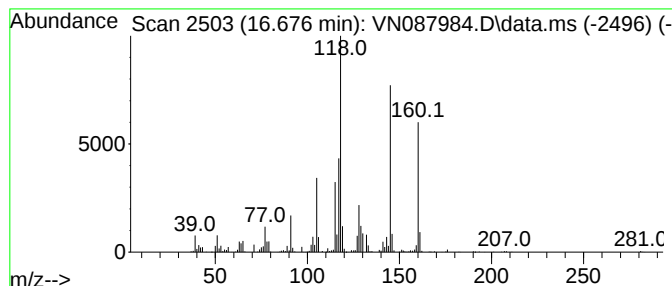
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092325W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.676	59.22 ug/l	1856000	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	96
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	70
3			Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	68
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	64
5			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	64



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Acq On : 29 Sep 2025 15:50
Operator : JC\MD
Sample : Q3188-01
Misc : 1.14g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
4135

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092325W.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
Hexane, 3-methyl-	8.418	57.2	ug/l	3247300	1	8.200	2837910	50.0
Heptane	8.941	120.1	ug/l	2445780	2	9.082	1018470	50.0
Benzene, 1-meth...	15.029	80.7	ug/l	2530500	4	13.770	1567030	50.0
Dodecane, 4,6-d...	15.564	55.9	ug/l	1752560	4	13.770	1567030	50.0
1H-Indene, 2,3-...	15.917	72.5	ug/l	2271310	4	13.770	1567030	50.0
Benzene, (1-met...	16.135	86.9	ug/l	2724060	4	13.770	1567030	50.0
Naphthalene, 1,...	16.676	59.2	ug/l	1856000	4	13.770	1567030	50.0