

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
 Data File : VN087107.D
 Acq On : 19 Jun 2025 13:38
 Operator : JC\MD
 Sample : Q2333-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-08

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\82N060625W.M
 Title : SW846 8260

Signal : TIC: VN087107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.283	216	226	244	rBV	424084	1046030	2.37%	0.480%
2	3.671	281	292	313	rBV3	148921	453379	1.03%	0.208%
3	5.400	573	586	609	rVB5	137699	827651	1.87%	0.380%
4	5.830	642	659	676	rBV4	180753	693175	1.57%	0.318%
5	7.341	905	916	937	rVB	468342	1425053	3.22%	0.654%
6	8.177	1048	1058	1062	rBV	208155	504265	1.14%	0.231%
7	8.236	1062	1068	1080	rVV2	398817	1569856	3.55%	0.720%
8	8.612	1120	1132	1145	rBV2	1243096	3235983	7.32%	1.485%
9	9.106	1207	1216	1230	rBV	667612	1540710	3.49%	0.707%
10	9.606	1282	1301	1317	rBV2	270595	817074	1.85%	0.375%
11	10.565	1457	1464	1470	rBV	903746	1700611	3.85%	0.781%
12	10.630	1470	1475	1483	rVB	421927	782003	1.77%	0.359%
13	10.759	1488	1497	1503	rVV2	368838	689739	1.56%	0.317%
14	10.830	1503	1509	1517	rVB	351071	635604	1.44%	0.292%
15	11.865	1678	1685	1692	rBV	753496	1397031	3.16%	0.641%
16	11.965	1694	1702	1711	rVV	11872464	20576640	46.56%	9.444%
17	12.076	1711	1721	1733	rVB	22316266	44190943	100.00%	20.282%
18	12.394	1763	1775	1793	rVB	12145184	20726942	46.90%	9.513%
19	12.694	1820	1826	1833	rVB	799339	1300844	2.94%	0.597%
20	12.847	1845	1852	1863	rVB	538469	944209	2.14%	0.433%
21	13.035	1870	1884	1889	rBV	1704202	2881660	6.52%	1.323%
22	13.094	1889	1894	1896	rVV	2182226	3362981	7.61%	1.543%
23	13.129	1896	1900	1904	rVV	4274191	7065172	15.99%	3.243%
24	13.171	1904	1907	1915	rVB	1159987	1761199	3.99%	0.808%
25	13.335	1927	1935	1946	rBV	5134276	8455130	19.13%	3.881%
26	13.482	1951	1960	1973	rBV	18217449	29643401	67.08%	13.605%
27	13.818	2006	2017	2033	rVB	6115503	11250462	25.46%	5.163%
28	13.947	2033	2039	2041	rBV	687100	993828	2.25%	0.456%
29	13.994	2041	2047	2062	rVB	7493527	13736386	31.08%	6.304%
30	14.176	2072	2078	2084	rVV2	946184	1678720	3.80%	0.770%
31	14.241	2084	2089	2092	rVV	797347	1382048	3.13%	0.634%
32	14.270	2092	2094	2099	rVV	693007	902766	2.04%	0.414%
33	14.329	2099	2104	2110	rVV	1778543	2737747	6.20%	1.257%
34	14.394	2110	2115	2118	rVV	315975	508087	1.15%	0.233%
35	14.441	2118	2123	2132	rVB2	1394257	2383888	5.39%	1.094%
36	14.570	2139	2145	2151	rBV	417346	654499	1.48%	0.300%

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Instrument :
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ClientSampleId :
MW-08

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\82N060625W.M
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37	14.653	2151	2159	2162	rBV	1017073	1728992	3.91%	0.794%
38	14.688	2162	2165	2171	rVB	1057892	1556303	3.52%	0.714%
39	14.923	2199	2205	2211	rBV	1139158	1867284	4.23%	0.857%
40	15.047	2217	2226	2233	rBV2	2306881	4947547	11.20%	2.271%
41	15.117	2233	2238	2246	rVB2	249591	473794	1.07%	0.217%
42	15.206	2246	2253	2260	rBV2	481891	903844	2.05%	0.415%
43	15.312	2261	2271	2277	rBV4	251028	653105	1.48%	0.300%
44	15.435	2284	2292	2299	rVB3	218399	539737	1.22%	0.248%
45	15.635	2318	2326	2337	rVB	5263617	10147602	22.96%	4.657%
46	15.741	2337	2344	2350	rBV	316249	611488	1.38%	0.281%

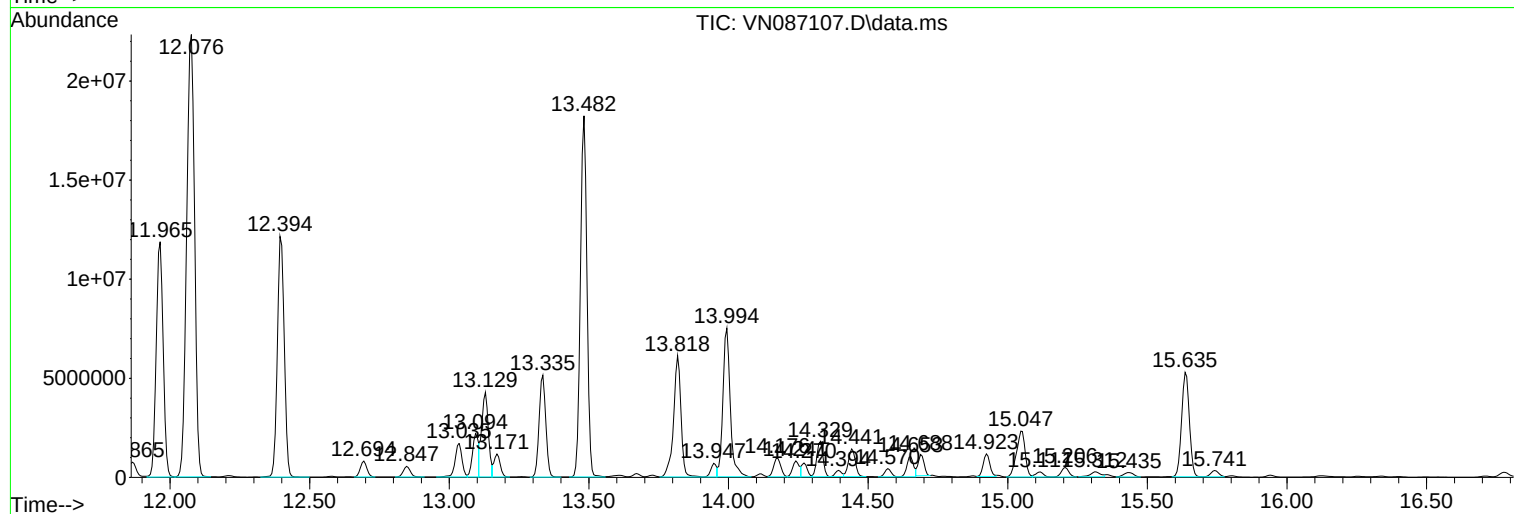
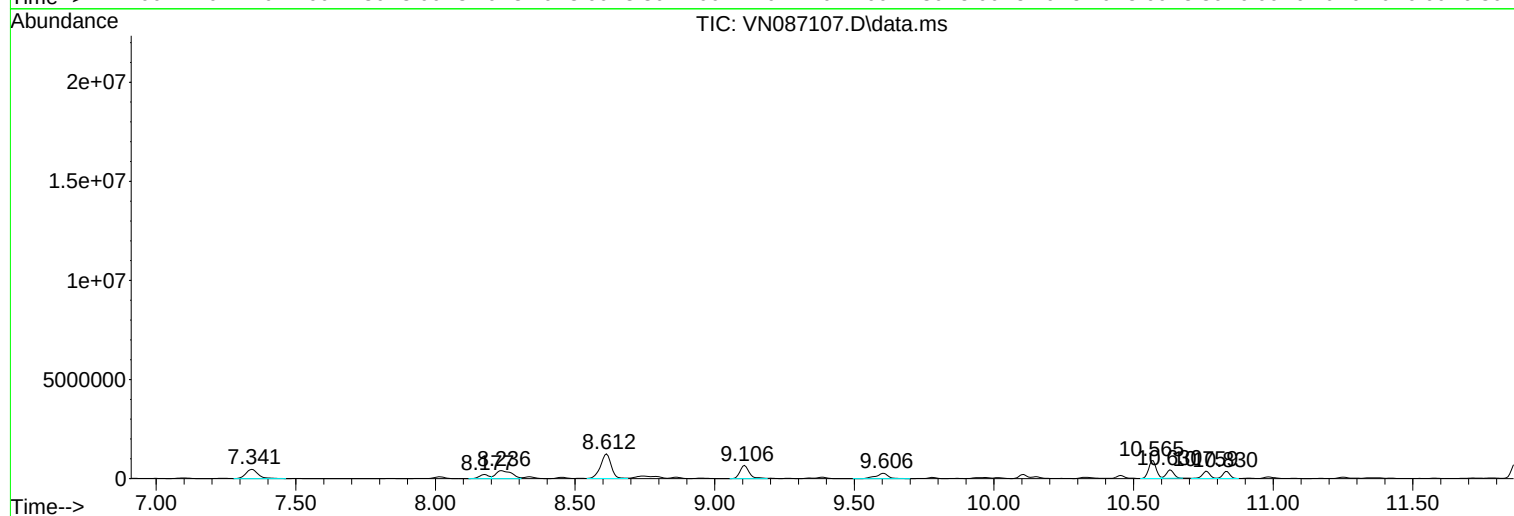
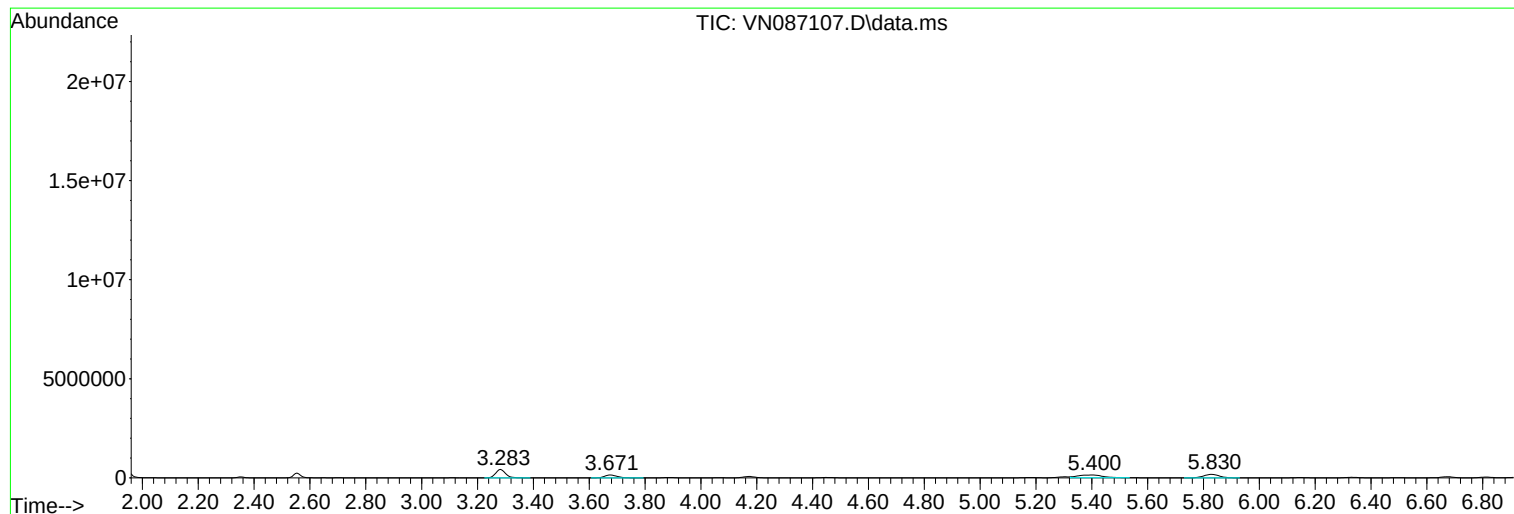
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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



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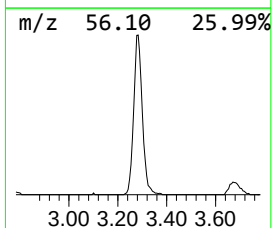
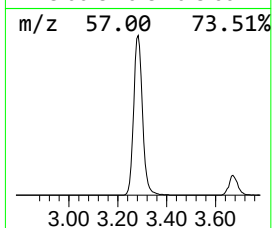
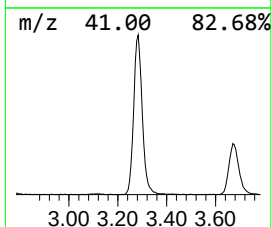
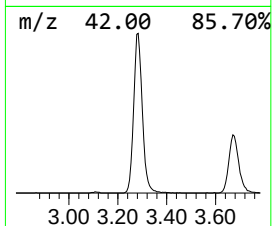
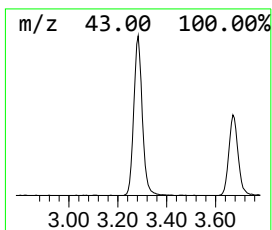
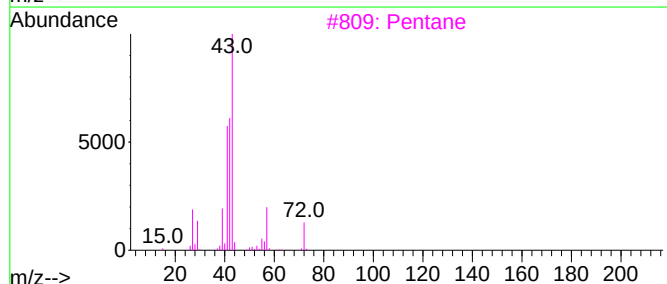
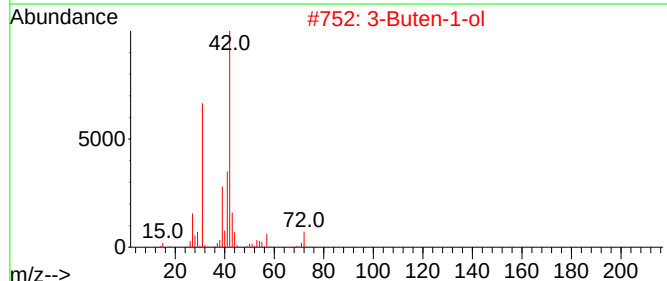
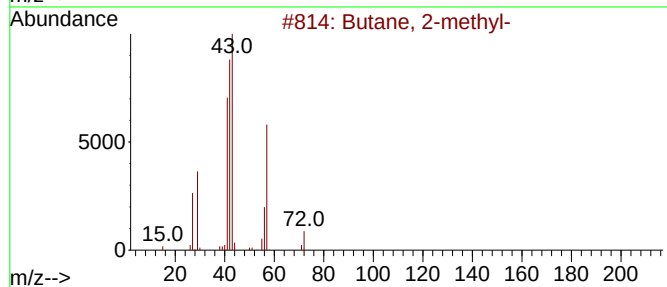
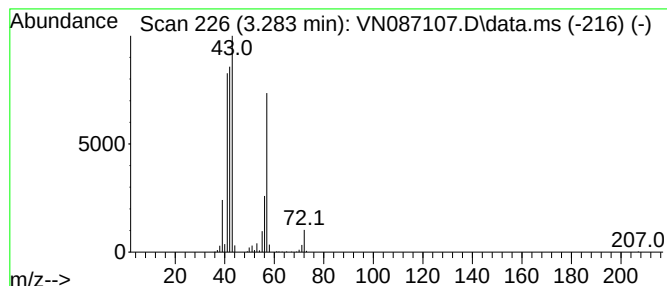
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.283	33.32 ug/l	1046030	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			3-Buten-1-ol	72	C4H8O	000627-27-0	37
3			Pentane	72	C5H12	000109-66-0	32
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	28
5			1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	16



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-08

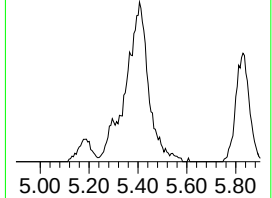
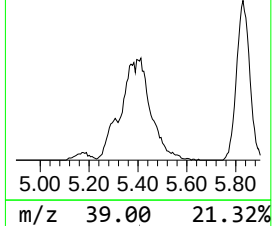
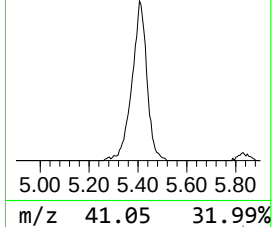
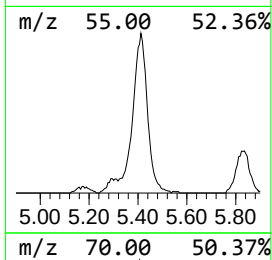
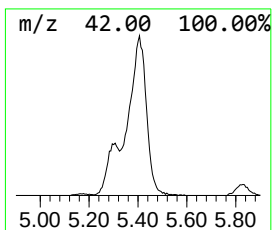
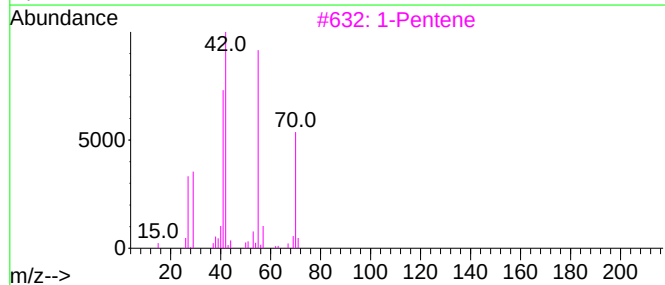
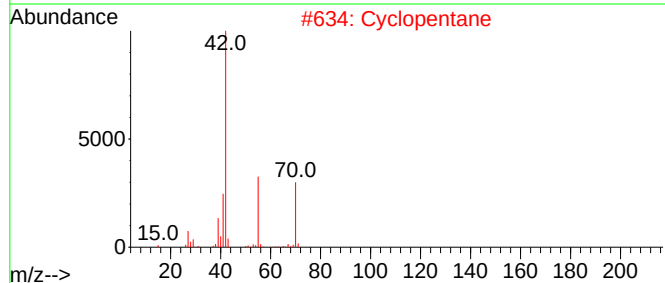
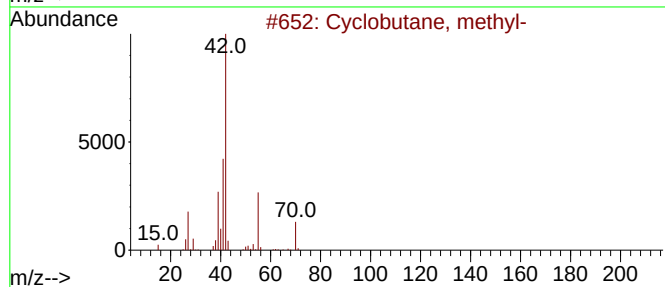
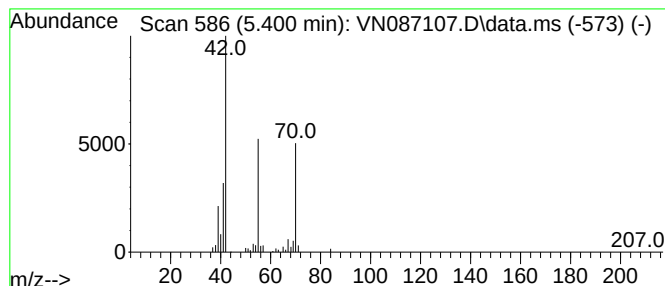
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclobutane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.400	26.36 ug/l	827651	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2			Cyclopentane	70	C5H10	000287-92-3	78
3			1-Pentene	70	C5H10	000109-67-1	64
4			1-Butanol, 3-methyl-, formate	116	C6H12O2	000110-45-2	47
5			2-Pentene	70	C5H10	000109-68-2	43



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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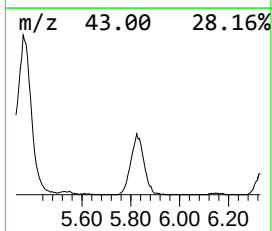
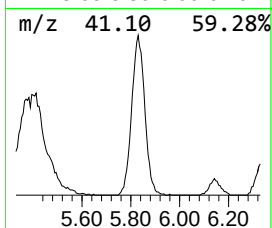
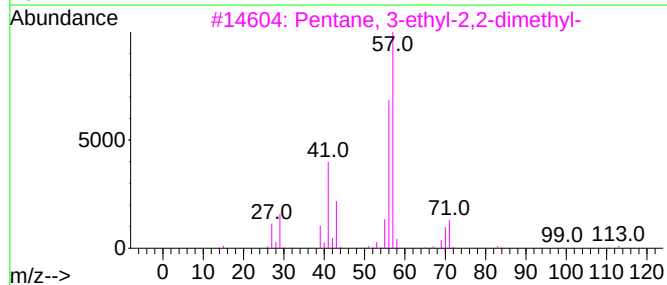
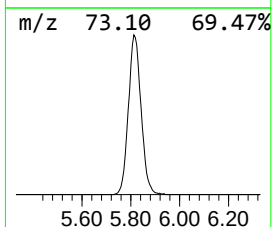
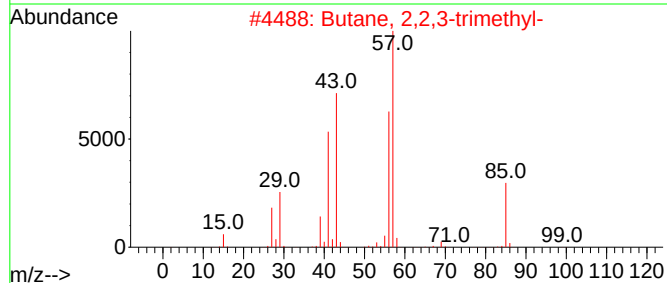
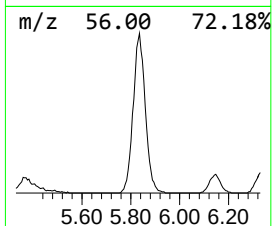
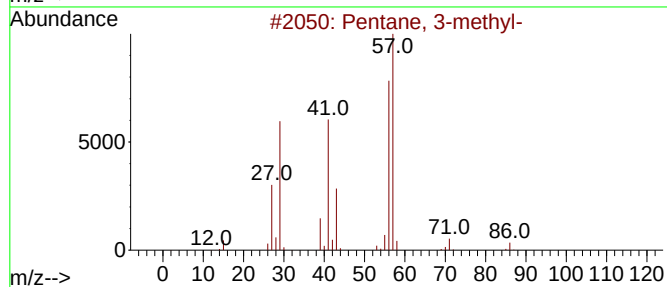
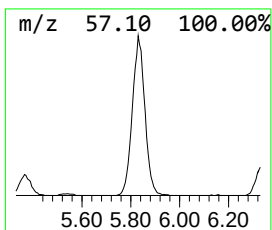
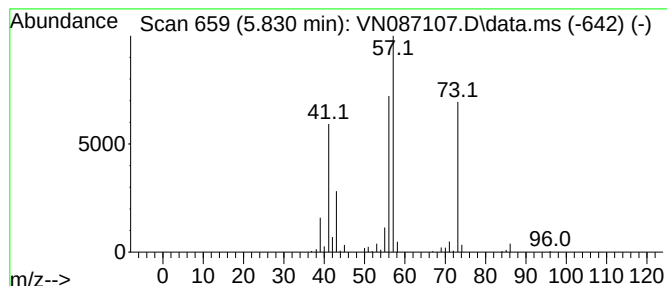
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.830	22.08 ug/l	693175	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	74
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	59
4			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	56
5			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	53



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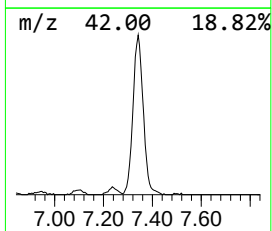
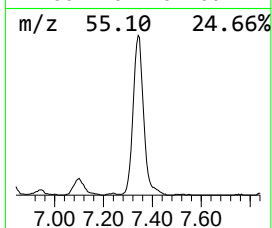
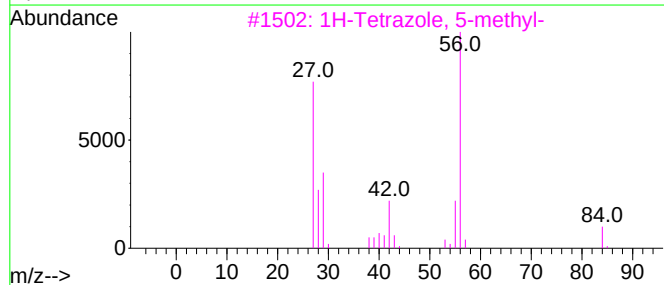
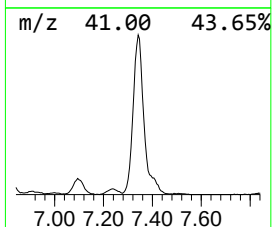
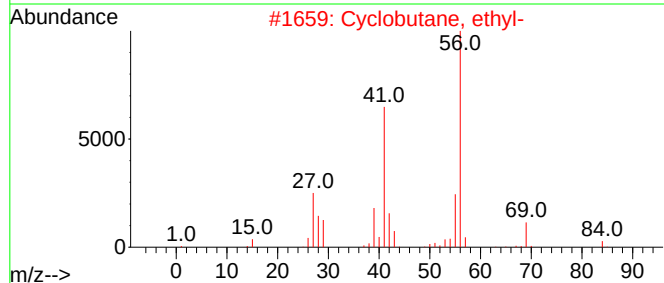
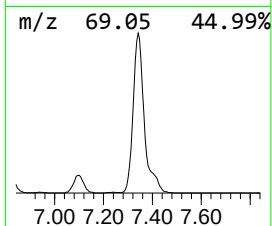
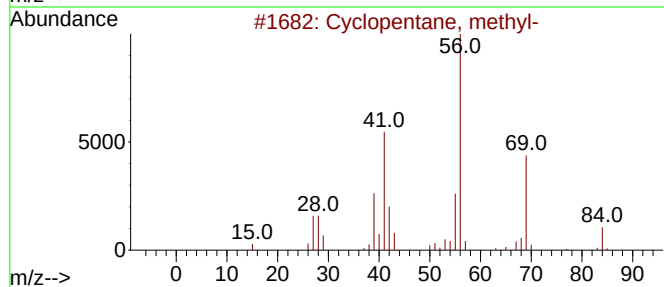
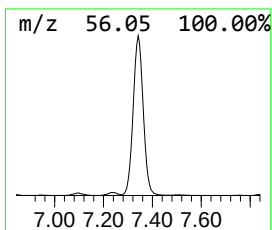
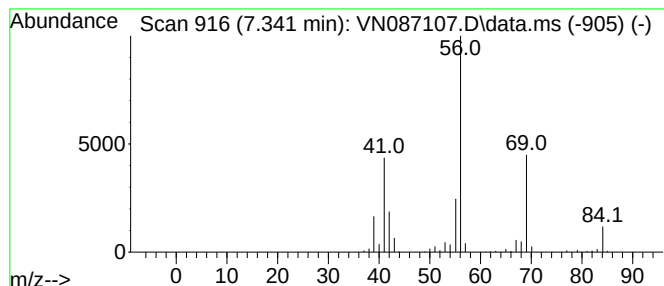
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.341	45.39 ug/l	1425050	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4		Cyclohexane	84	C6H12	000110-82-7	64
5		Cyclobutane, butyl-	112	C8H16	013152-44-8	56



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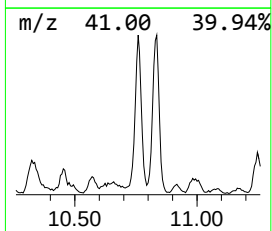
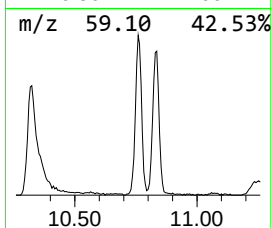
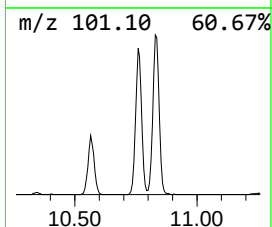
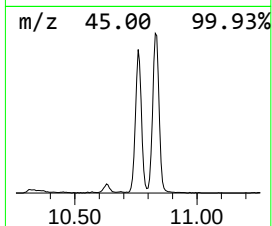
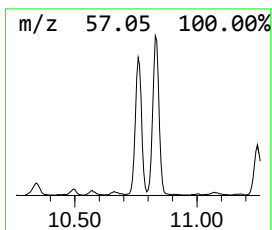
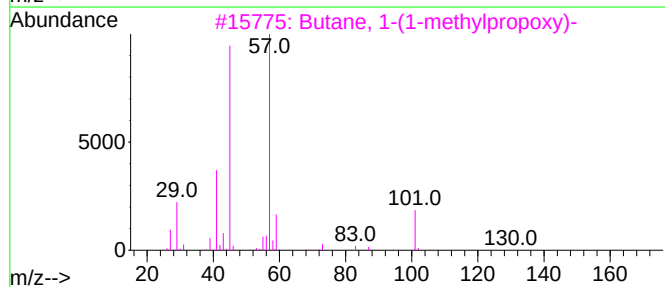
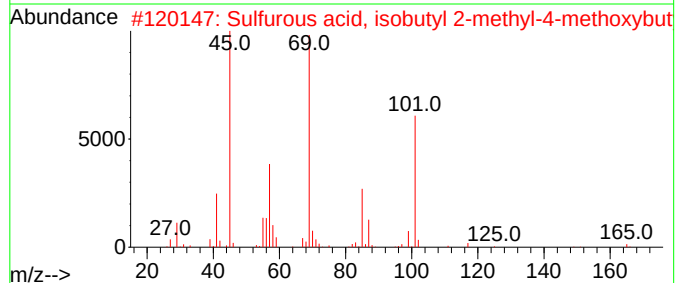
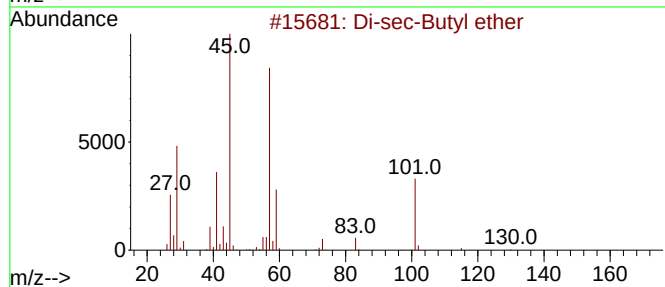
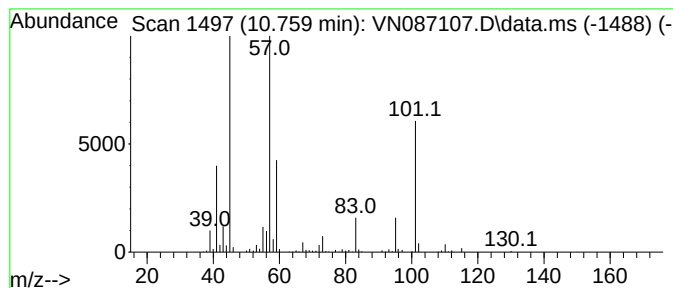
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Quant Title : SW846 8260

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

Peak Number 5 Di-sec-Butyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.759	24.69 ug/l	689739	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	90
2			Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	50
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	47
4			2-t-Butyl-5-methyl[1,3]dioxolan...	158	C8H14O3	130930-47-1	40
5			Trichloroacetic acid, 2-methoxye...	220	C5H7Cl3O3	1000330-88-6	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087107.D
Acq On : 19 Jun 2025 13:38
Operator : JC\MD
Sample : Q2333-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-08

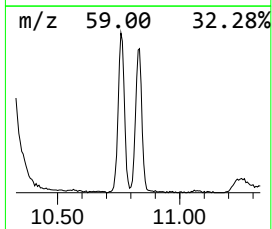
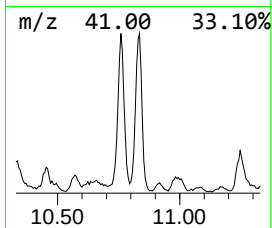
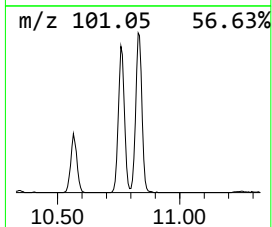
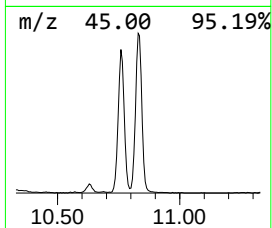
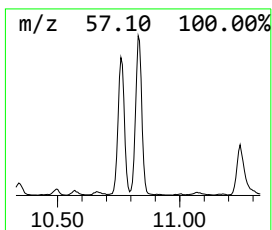
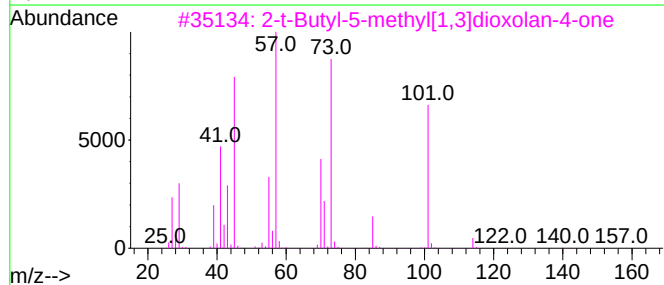
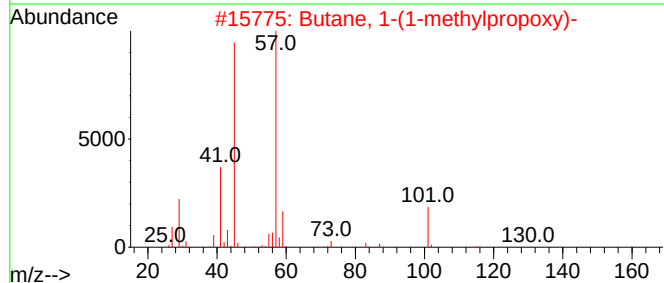
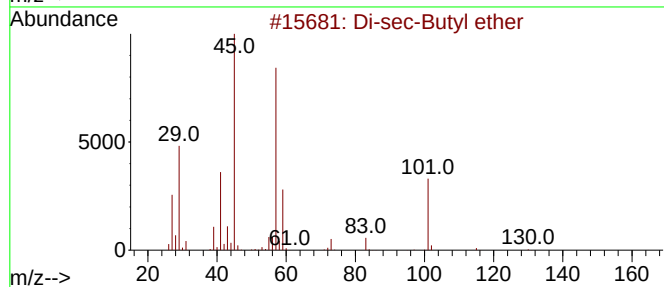
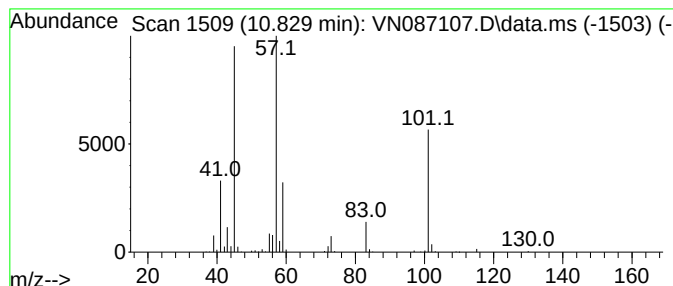
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Quant Title : SW846 8260

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

Peak Number 6 Butane, 1-(1-methylpropoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.829	22.75 ug/l	635604	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3			2-t-Butyl-5-methyl[1,3]dioxolan-...	158	C8H14O3	130930-47-1	45
4			Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	45
5			Sulfurous acid, di(2-methyl-4-me...	282	C12H26O5S	1000309-20-7	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087107.D
Acq On : 19 Jun 2025 13:38
Operator : JC\MD
Sample : Q2333-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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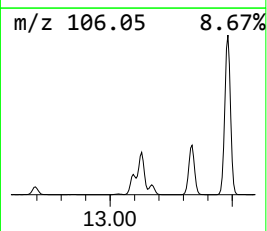
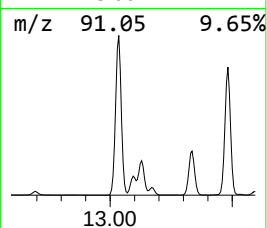
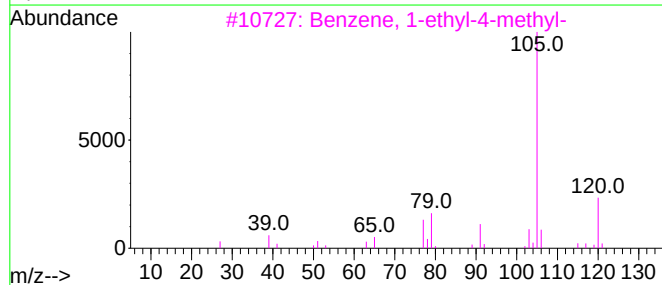
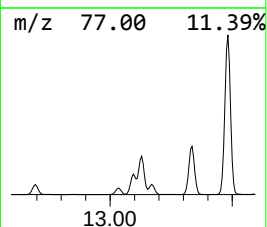
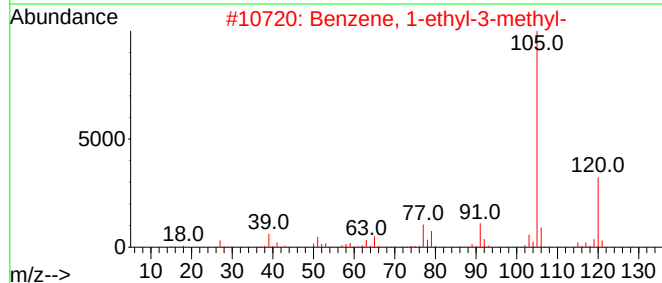
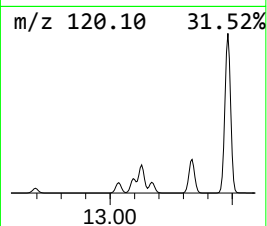
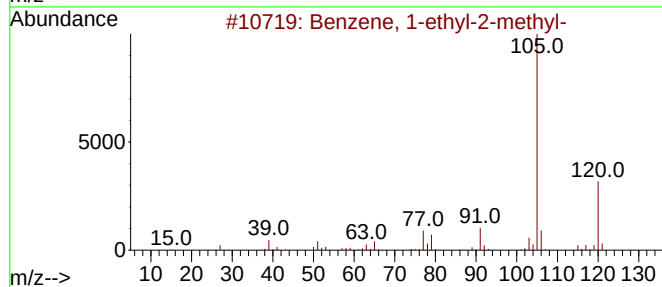
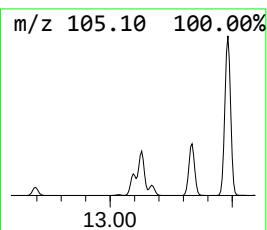
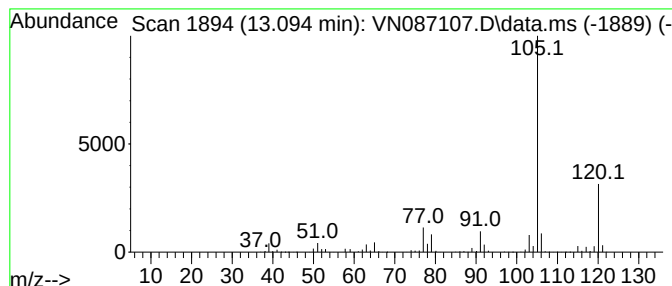
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	14.95 ug/l	3362980	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087107.D
Acq On : 19 Jun 2025 13:38
Operator : JC\MD
Sample : Q2333-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-08

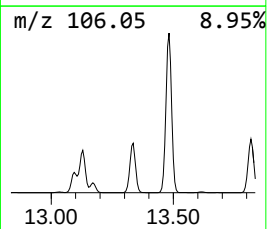
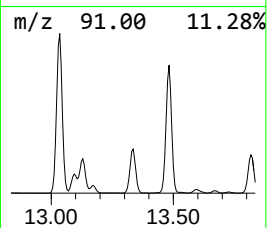
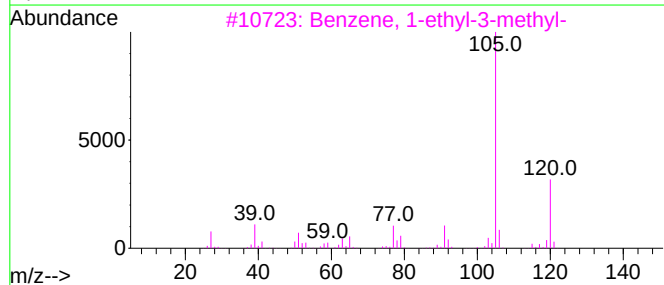
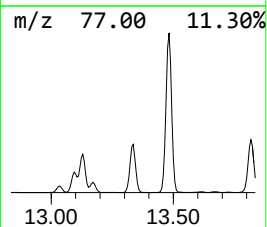
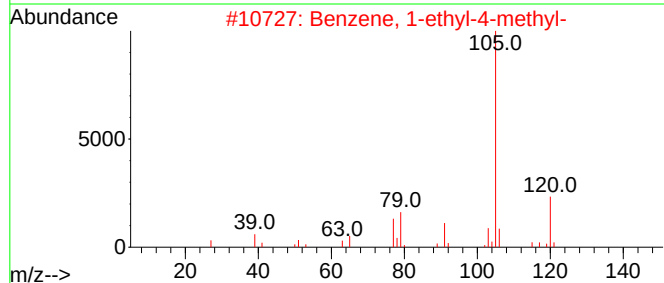
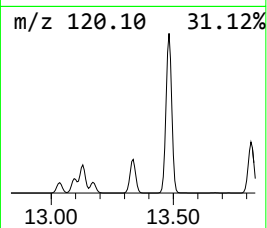
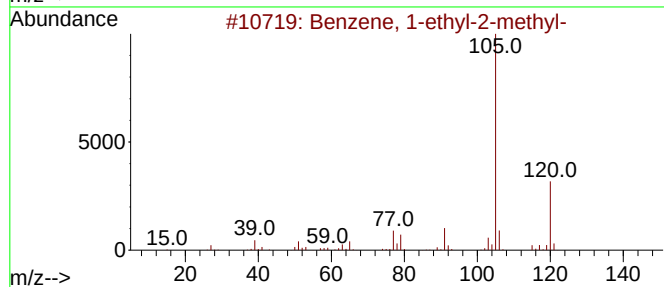
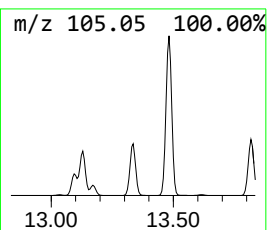
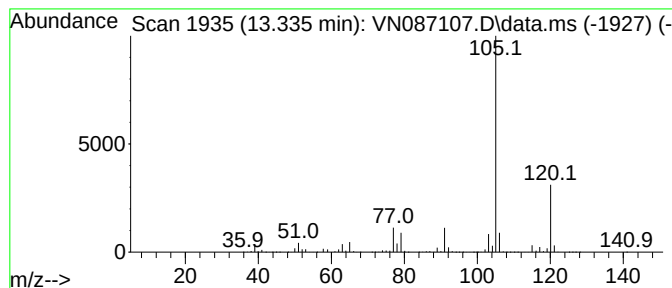
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	37.58 ug/l	8455130	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087107.D
Acq On : 19 Jun 2025 13:38
Operator : JC\MD
Sample : Q2333-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-08

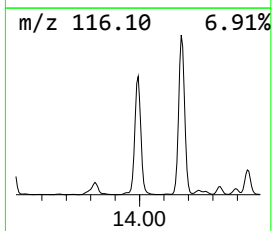
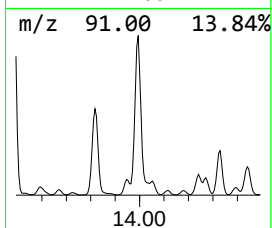
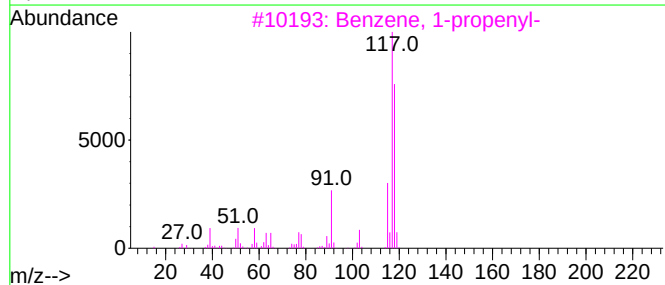
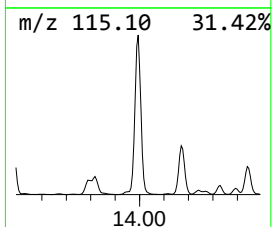
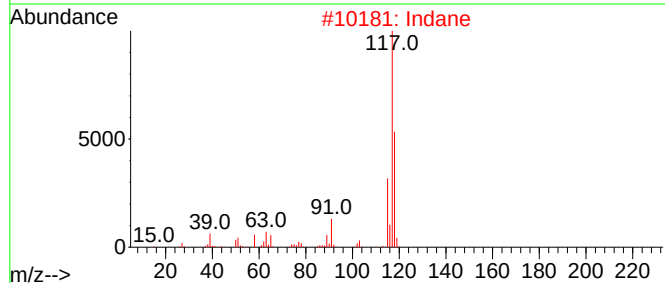
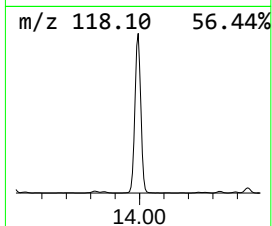
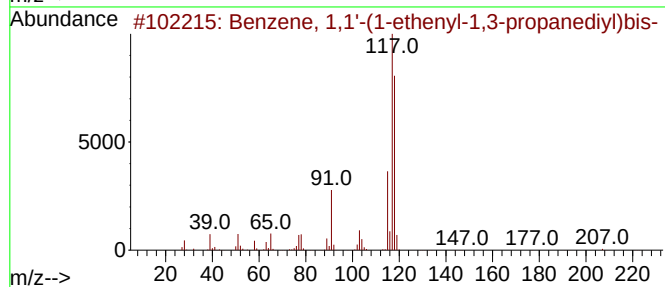
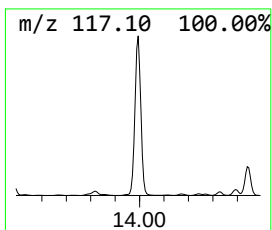
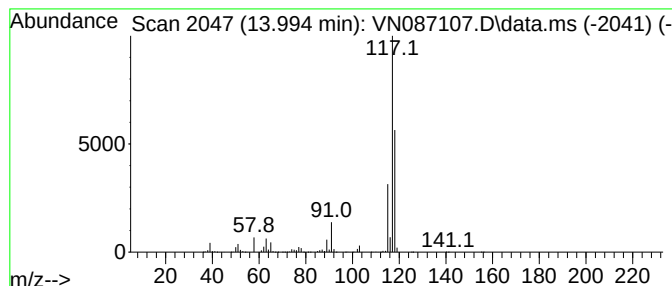
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,1'-(1-ethenyl-1,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	61.05 ug/l	13736400	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	83
2			Indane	118	C9H10	000496-11-7	81
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64
4			Delta-cyclene	118	C9H10	007785-10-6	64
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087107.D
Acq On : 19 Jun 2025 13:38
Operator : JC\MD
Sample : Q2333-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-08

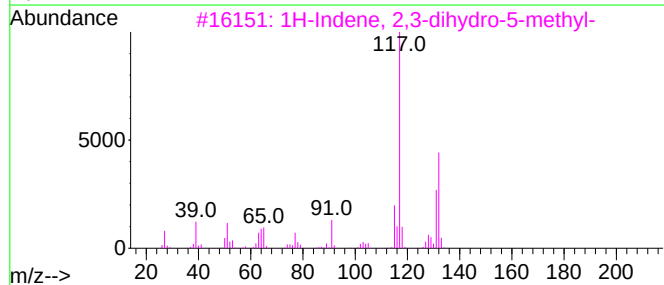
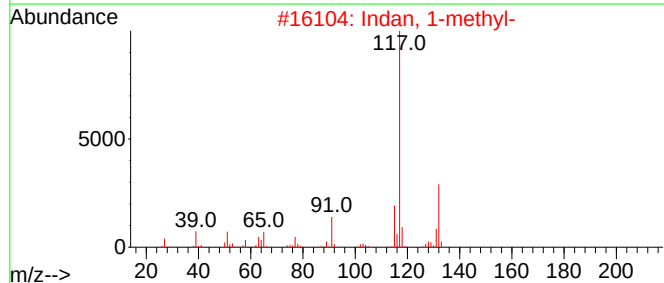
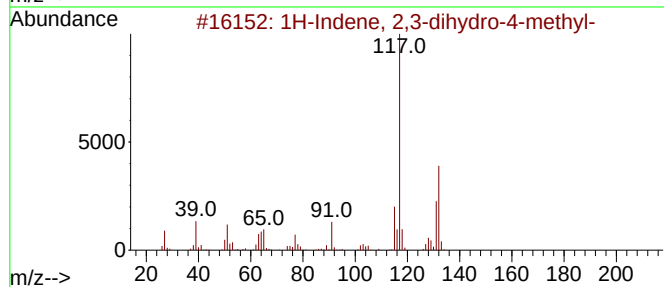
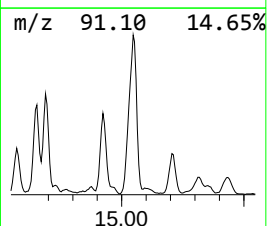
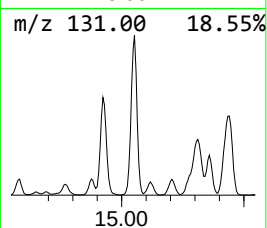
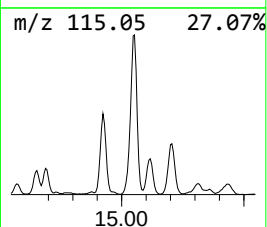
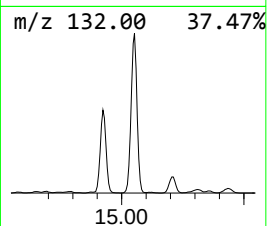
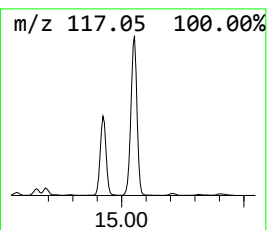
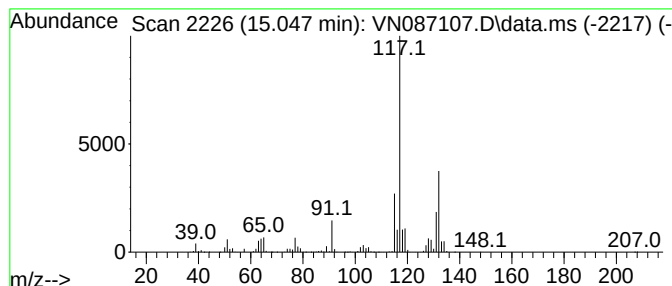
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.047	21.99 ug/l	4947550	1,4-Dichlorobenzene-d4	13.788

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
2		Indan, 1-methyl-	132	C10H12	000767-58-8	93
3		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
5		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087107.D
Acq On : 19 Jun 2025 13:38
Operator : JC\MD
Sample : Q2333-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-08

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.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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Cyclobutane, me...	5.400	26.4	ug/l	827651	1	8.230	1569860	50.0
Pentane, 3-methyl-	5.830	22.1	ug/l	693175	1	8.230	1569860	50.0
Cyclopentane, m...	7.341	45.4	ug/l	1425050	1	8.230	1569860	50.0
Di-sec-Butyl ether	10.759	24.7	ug/l	689739	3	11.865	1397030	50.0
Butane, 1-(1-me...	10.829	22.8	ug/l	635604	3	11.865	1397030	50.0
Benzene, 1-ethy...	13.094	14.9	ug/l	3362980	4	13.788	11250500	50.0
Benzene, 1-ethy...	13.335	37.6	ug/l	8455130	4	13.788	11250500	50.0
Benzene, 1,1'-(...	13.994	61.0	ug/l	13736400	4	13.788	11250500	50.0
1H-Indene, 2,3-...	15.047	22.0	ug/l	4947550	4	13.788	11250500	50.0