LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

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: VN087111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.554	91	102	113	rBV	390970	708118	3.40%	0.613%
2	3.283	215	226	246	rBV	571783	1418171	6.81%	1.227%
3	3.677	284	293	313	rVB3	263687	835129	4.01%	0.723%
4	3.883	318	328	344	rVB	189791	502482	2.41%	0.435%
5	4.071	346	360	369	rBV	109671	312711	1.50%	0.271%
6	4.171	369	377	393	rVB2	116132	339826	1.63%	0.294%
7	5.183	533	549	560	rBV2	63912	239369	1.15%	0.207%
8	5.406	573	587	610	rVB4	241627	1253029	6.02%	1.084%
9	5.836	646	660	678	rVB4	107542	389065	1.87%	0.337%
10	6.906	833	842	852	rBV3	58536	212405	1.02%	0.184%
11	7.342	905	916	935	rVB	398525	1168124	5.61%	1.011%
12	8.177	1048	1058	1062	rBV	148669	356352	1.71%	0.308%
13	8.236	1062	1068	1081	rVV2	286120	1226236	5.89%	1.061%
14	8.612	1120	1132	1145	rBV	1945090	4769818	22.90%	4.128%
15	8.747	1146	1155	1161	rBV3	125106	341243	1.64%	0.295%
16	9.106	1207	1216	1230	rBV	438328	960208	4.61%	0.831%
17	9.606	1282	1301	1317	rBV2	182487	533352	2.56%	0.462%
18	10.565	1457	1464	1470	rBV	645374	1202030	5.77%	1.040%
19	10.630	1470	1475	1490	rVV	816134	1557659	7.48%	1.348%
20	10.759	1490	1497	1503	rVV	242311	433672	2.08%	0.375%
21	10.830	1503	1509	1516	rVV	245615	416798	2.00%	0.361%
22	11.865	1677	1685	1693	rBV	542802	995084	4.78%	0.861%
23	11.965	1693	1702	1711	rVV	12263266	20828229	100.00%	18.025%
24	12.077	1712	1721	1735	rVB	5743867	9900657	47.53%	8.568%
25	12.394	1764	1775	1790	rVB	2696127	4717447	22.65%	4.082%
26	12.694	1819	1826	1833	rBV	370689	621697	2.98%	0.538%
27	12.847	1845	1852	1862	rBV	399903	687297	3.30%	0.595%
28	13.035	1875	1884	1889	rBV	778175	1292106	6.20%	1.118%
29	13.129	1889	1900	1905	rBV	1093116	1959909	9.41%	1.696%
30	13.335	1927	1935	1947	rBV	4846611	7942348	38.13%	6.873%
31	13.482	1947	1960	1973	rBV	7214891	11970386	57.47%	10.359%
32	13.818	2006	2017	2033	rVB	5608211	10192744	48.94%	8.821%
33	13.947	2033	2039	2041	rBV	365727	536495	2.58%	0.464%
34	13.994	2041	2047	2062	rVB	5363535	9584714	46.02%	8.295%
35	14.176	2071	2078	2084	rBV2	631554	1105703	5.31%	0.957%
36	14.241	2084	2089	2092	rBV	524236	835417	4.01%	0.723%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

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

37	14.329	2098	2104	2110	rVB	862356	1351826	6.49%	1.170%
38	14.394	2110	2115	2118	rVV	220854	355832	1.71%	0.308%
39	14.441	2118	2123	2132	rVB2	824414	1393995	6.69%	1.206%
40	14.570	2139	2145	2152	rBV	306601	489990	2.35%	0.424%
41	14.653	2152	2159	2162	rBV	497734	821783	3.95%	0.711%
42	14.688	2162	2165	2171	rVB	420153	614244	2.95%	0.532%
43	14.923	2199	2205	2211	rBV	503506	822978	3.95%	0.712%
44	15.047	2217	2226	2233	rBV2	1268670	2622864	12.59%	2.270%
45	15.206	2246	2253	2261	rBV2	193570	363093	1.74%	0.314%
46	15.312	2261	2271	2276	rBV3	103432	268085	1.29%	0.232%
47	15.435	2284	2292	2302	rVB4	107137	281978	1.35%	0.244%
48	15.635	2318	2326	2337	rBV	1609835	3125572	15.01%	2.705%
49	15.741	2337	2344	2351	rVB	356006	695065	3.34%	0.602%

Sum of corrected areas: 115553335

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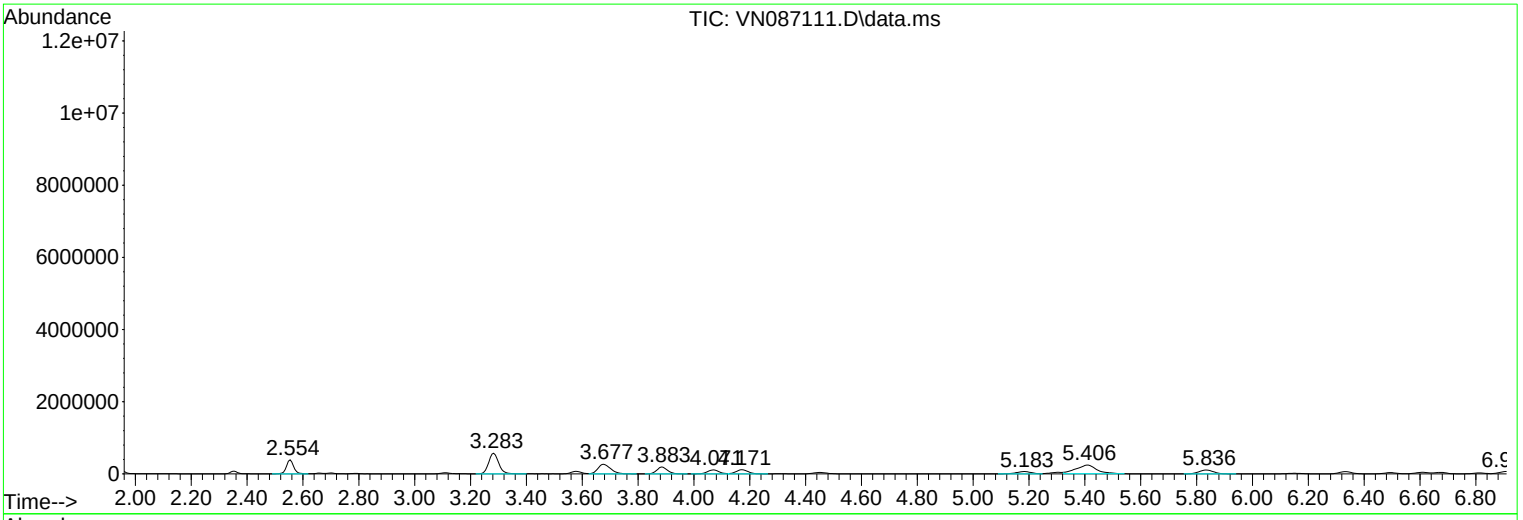
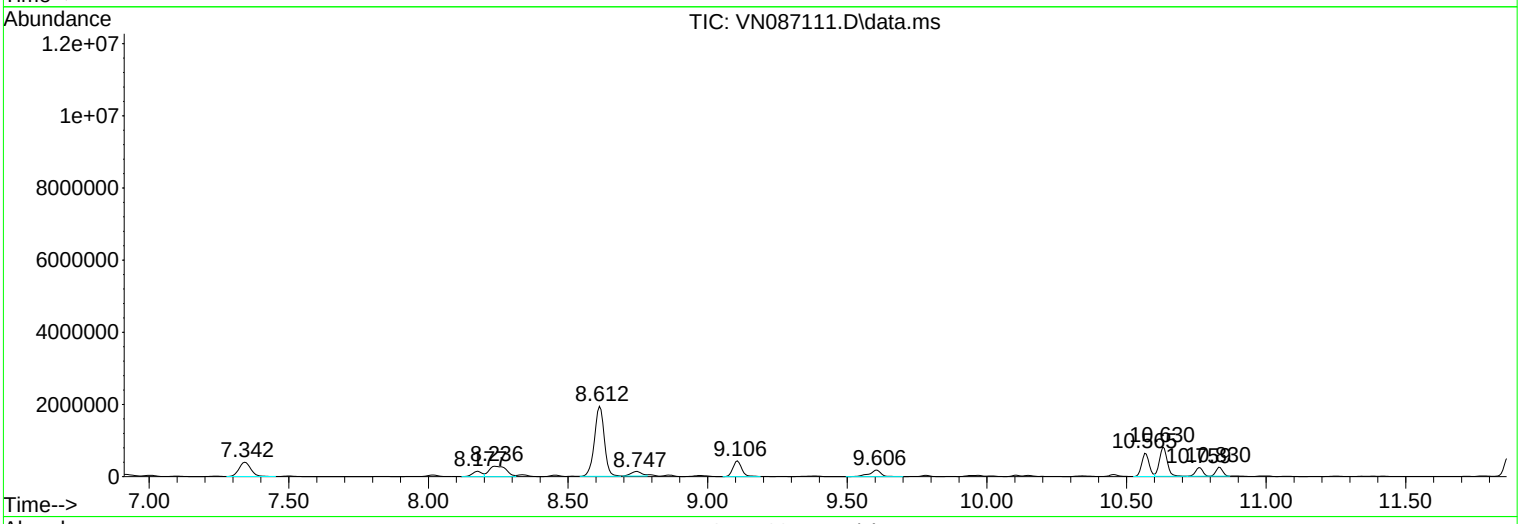
ALS Vial : 13 Sample Multiplier: 1

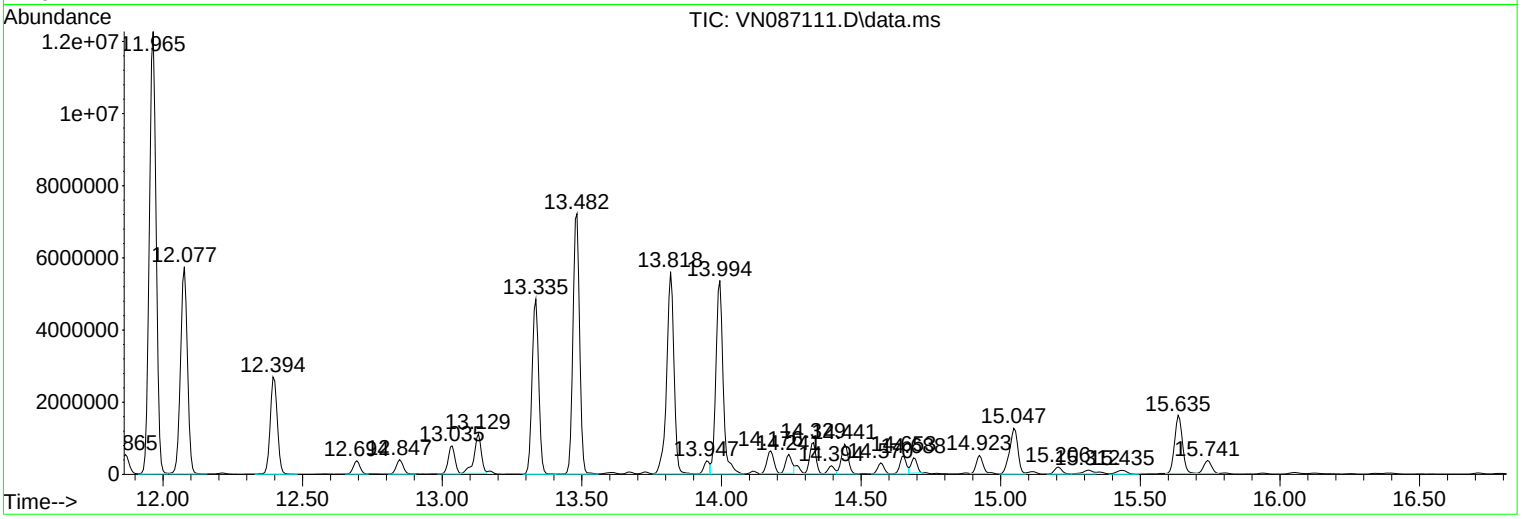
Instrument :
MSVOA_N
ClientSampleId :
MW-12

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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Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

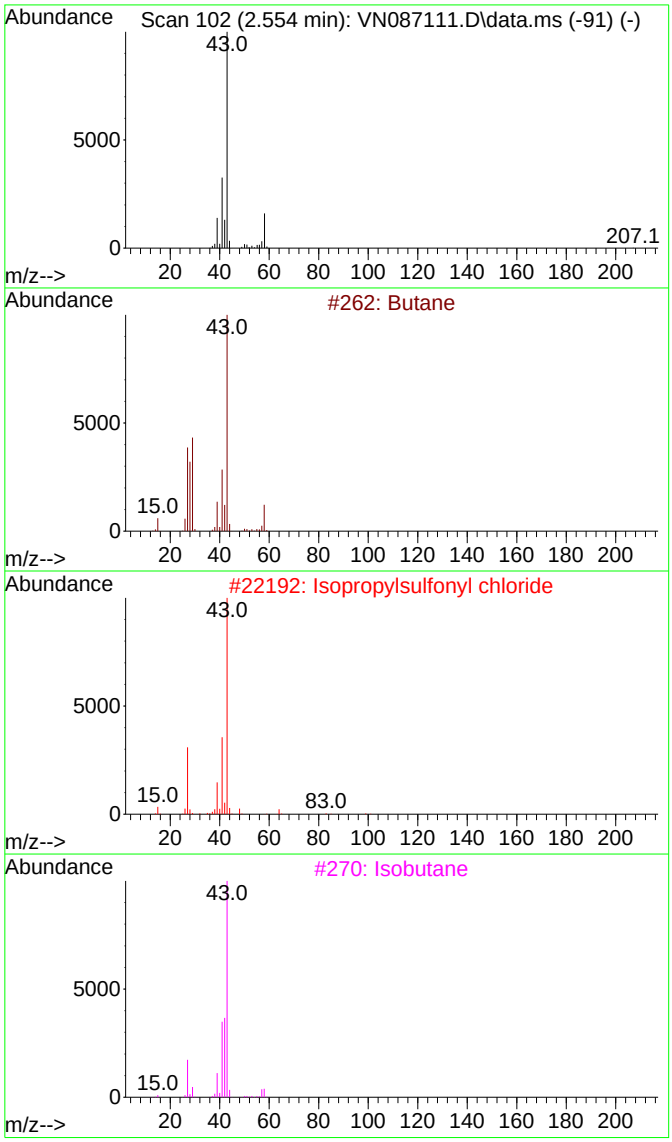
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

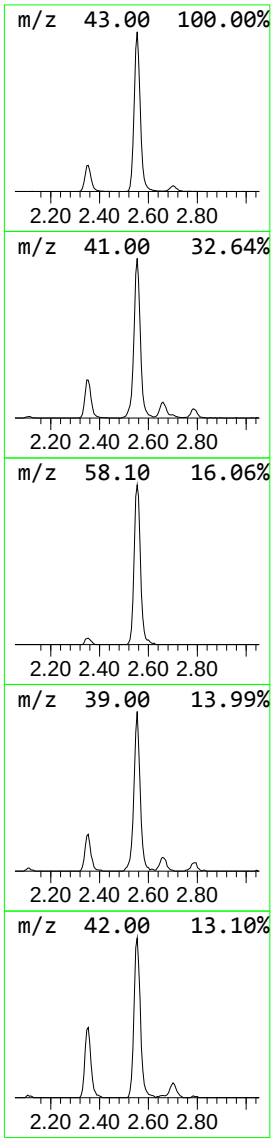
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.554	28.87 ug/l	708118	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Acetone	58	C3H6O	000067-64-1	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

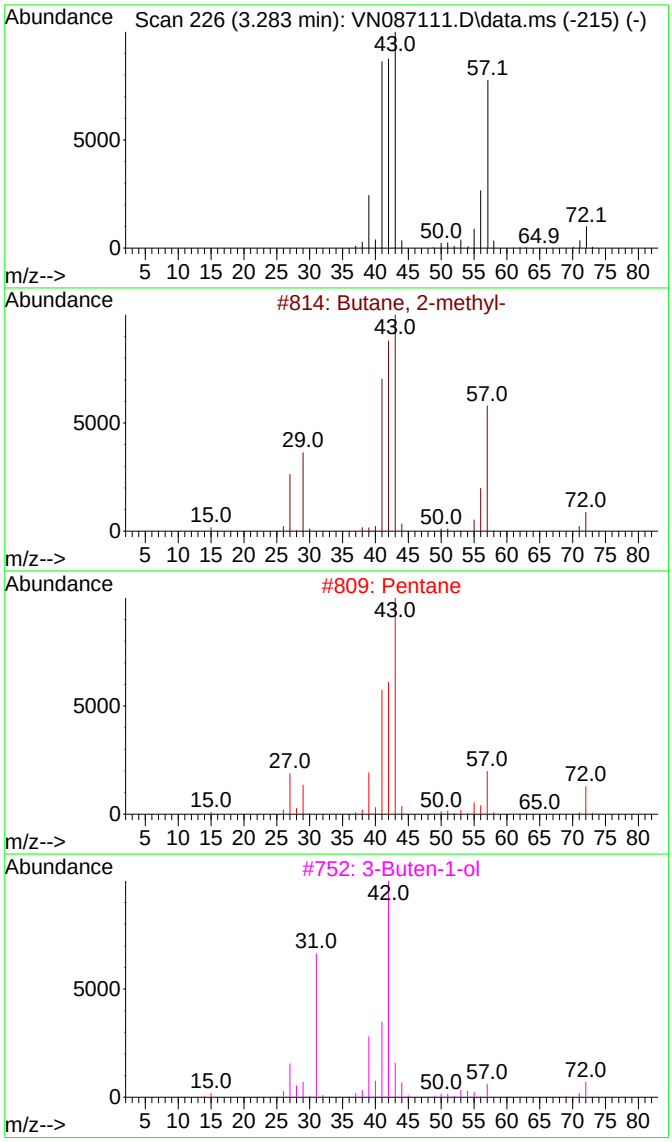
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

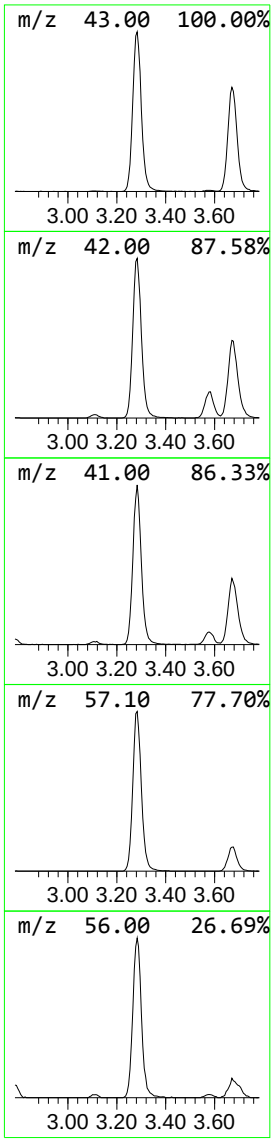
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.283	57.83 ug/l	1418170	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	38
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

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

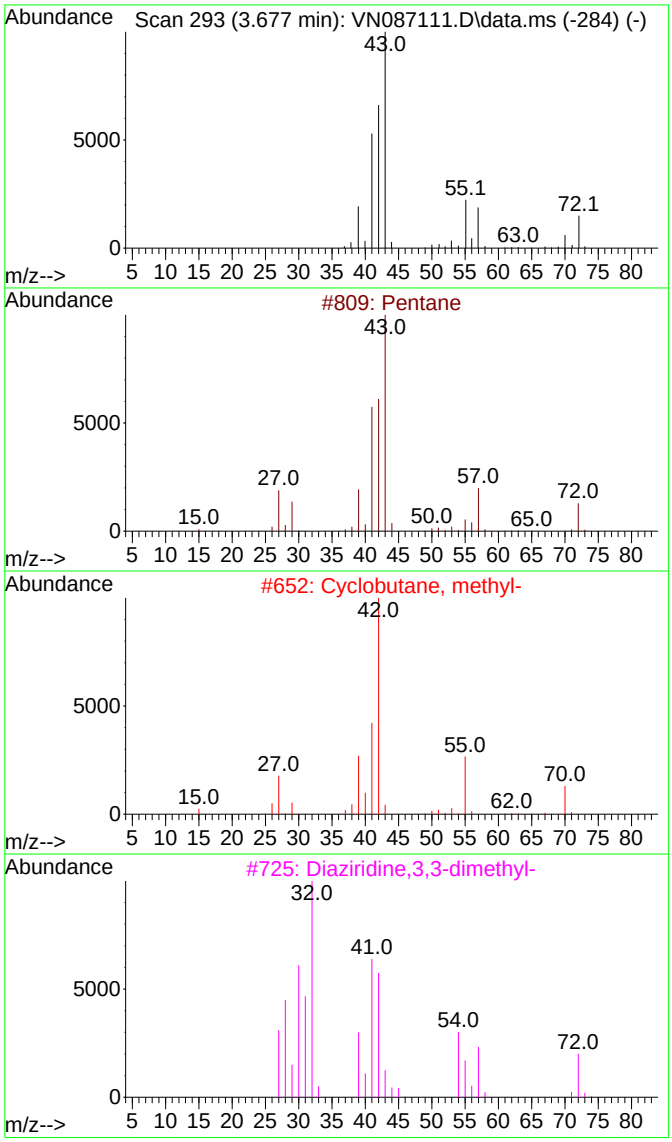
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

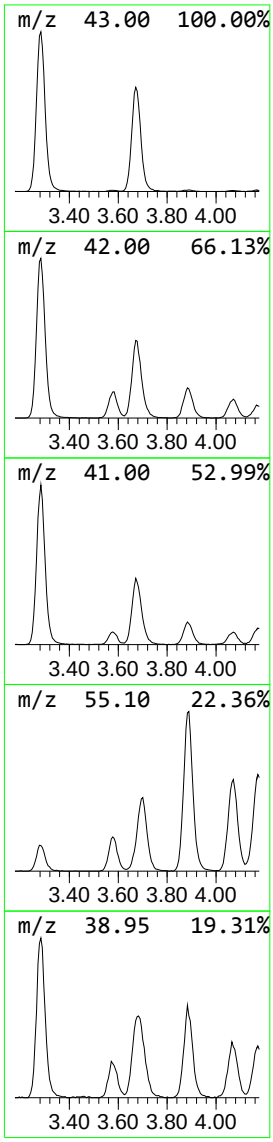
****

Peak Number 3 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.677	34.05 ug/l	835129	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	87
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	46
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	Tetrahydrofuran	72	C4H8O	000109-99-9	25
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

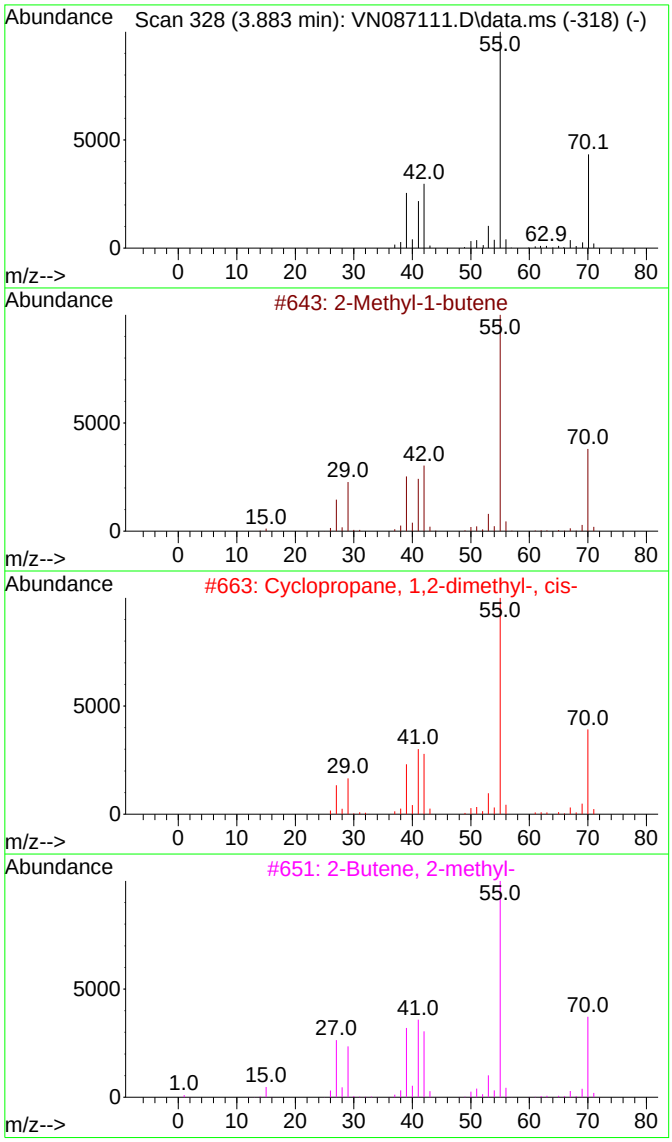
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

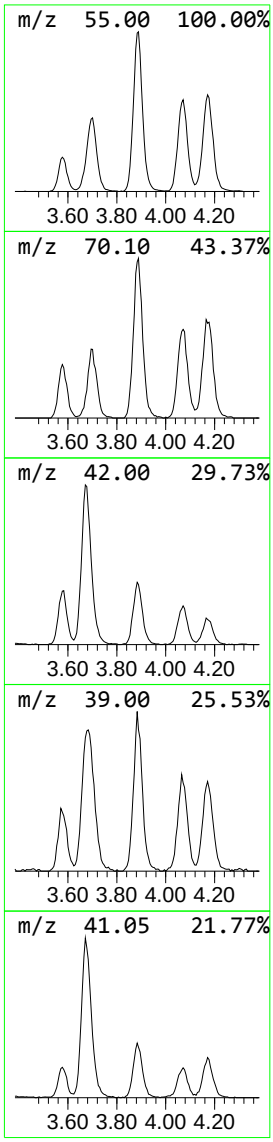
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Methyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.883	20.49 ug/l	502482	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1-butene	70	C5H10	000563-46-2	91
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
3	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
4	2-Pentene, (E)-	70	C5H10	000646-04-8	90
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	90





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Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

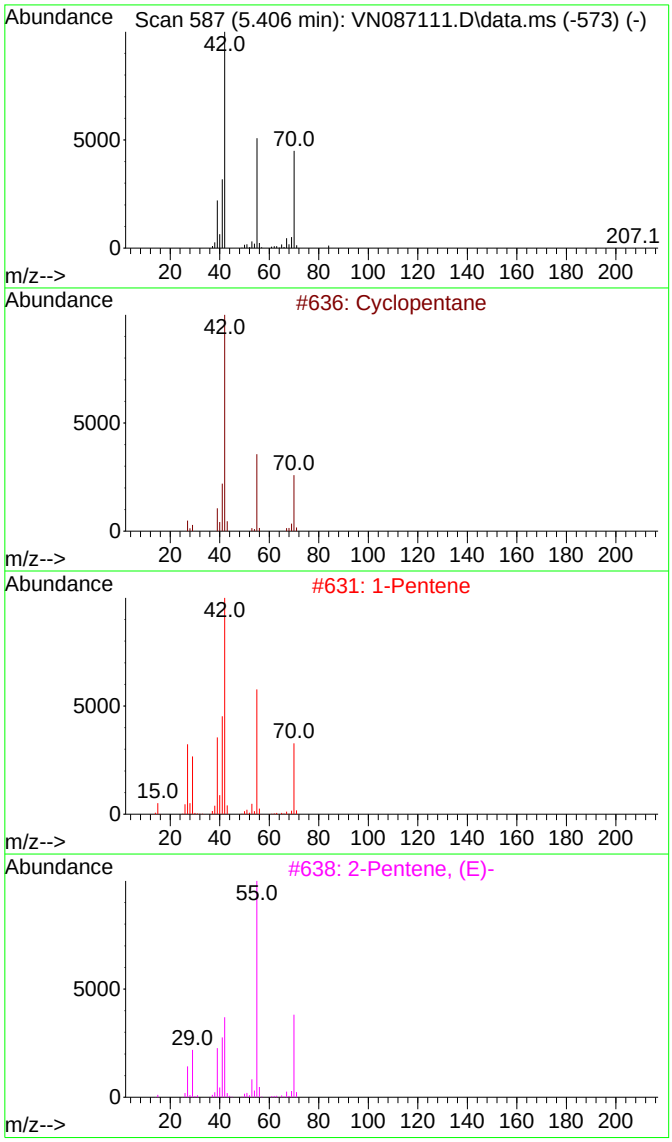
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

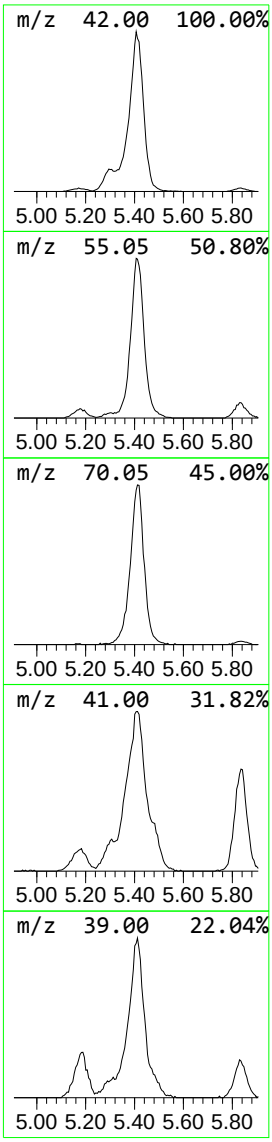
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.406	51.09 ug/l	1253030	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	1-Pentene	70	C5H10	000109-67-1	50
3	2-Pentene, (E)-	70	C5H10	000646-04-8	35
4	3-Buten-1-ol	72	C4H8O	000627-27-0	25
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	23





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ALS Vial : 13 Sample Multiplier: 1

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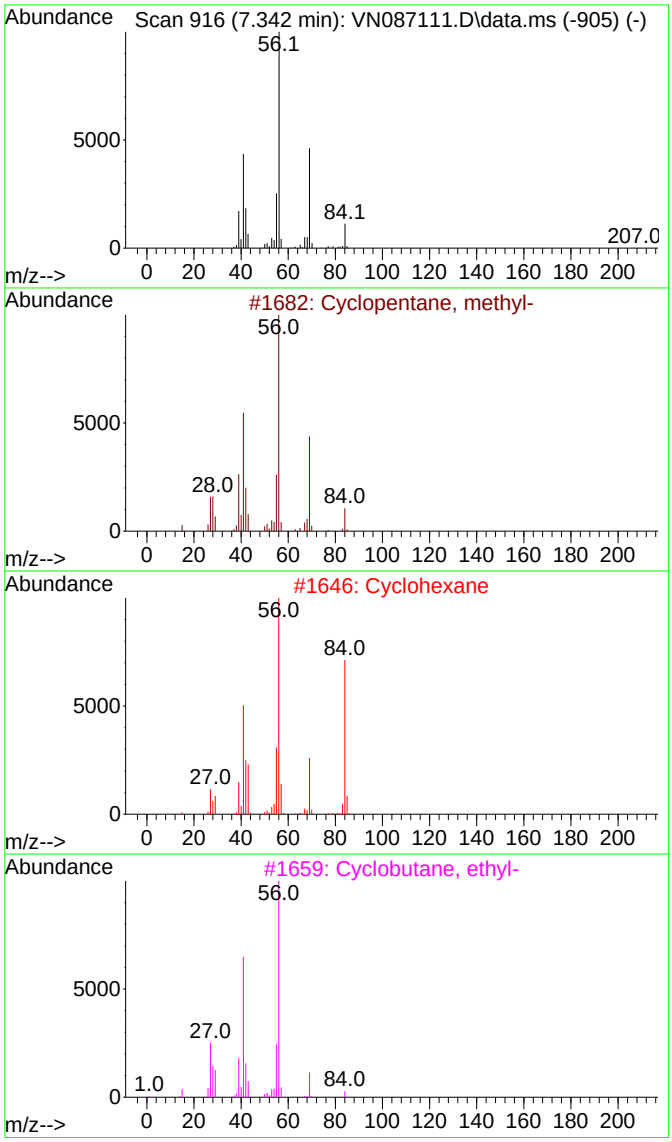
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

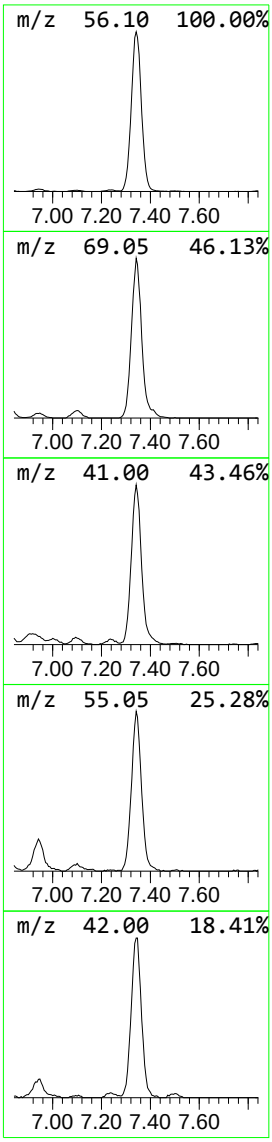
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.342	47.63 ug/l	1168120	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	1-Hexene	84	C6H12	000592-41-6	52





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Data File : VN087111.D
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

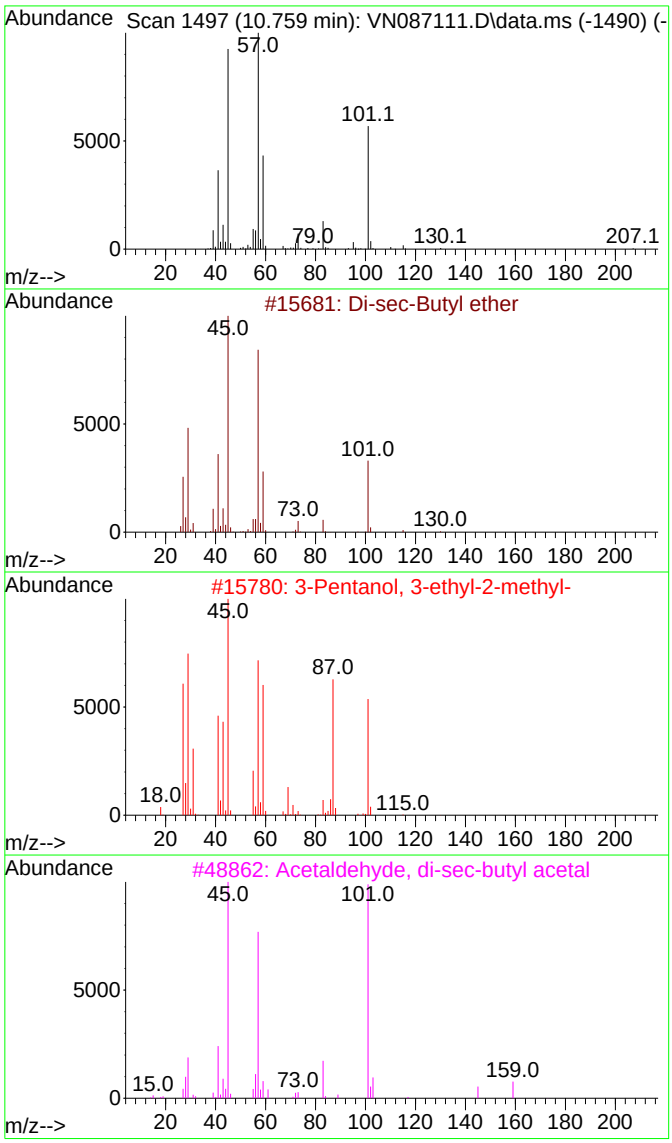
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

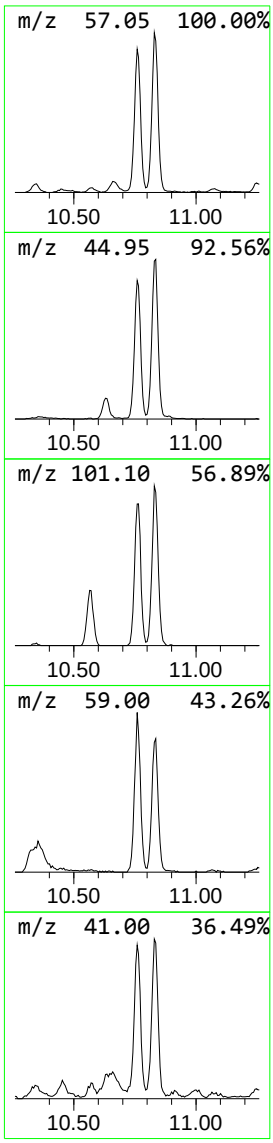
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Di-sec-Butyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.759	21.79 ug/l	433672	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	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	72
3	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	59
4	Butane, 1,1'-[ethylidenebis(oxy)...	174	C10H22O2	000871-22-7	53
5	Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

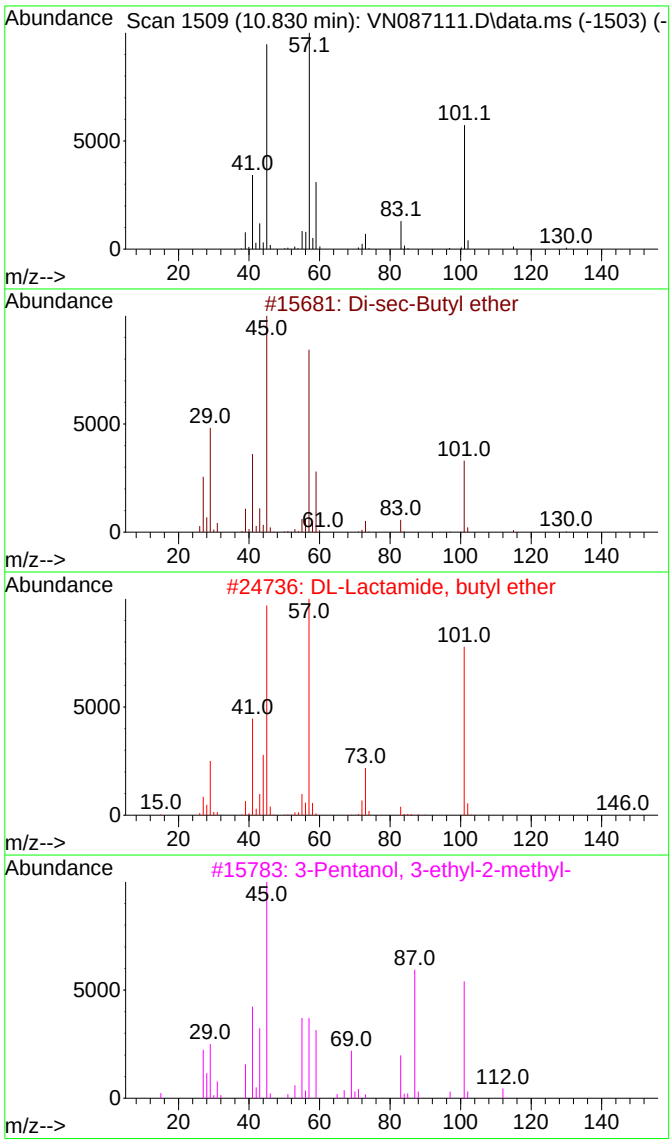
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

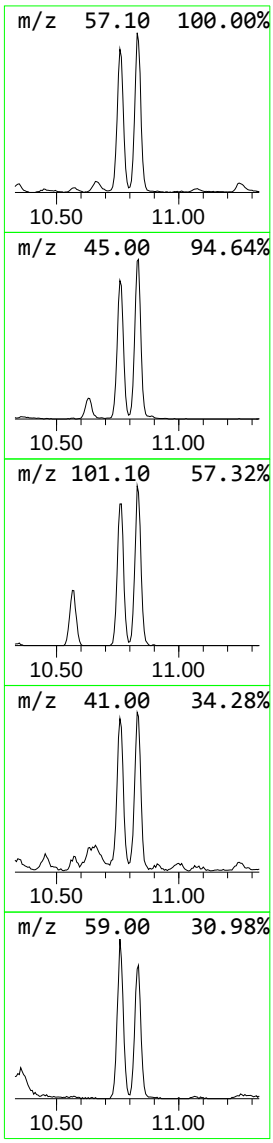
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 DL-Lactamide, butyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.829	20.94 ug/l	416798	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	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	59
3	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	56
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5	Sulfurous acid, di(2-methyl-4-me...	282	C12H26O5S	1000309-20-7	42





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Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

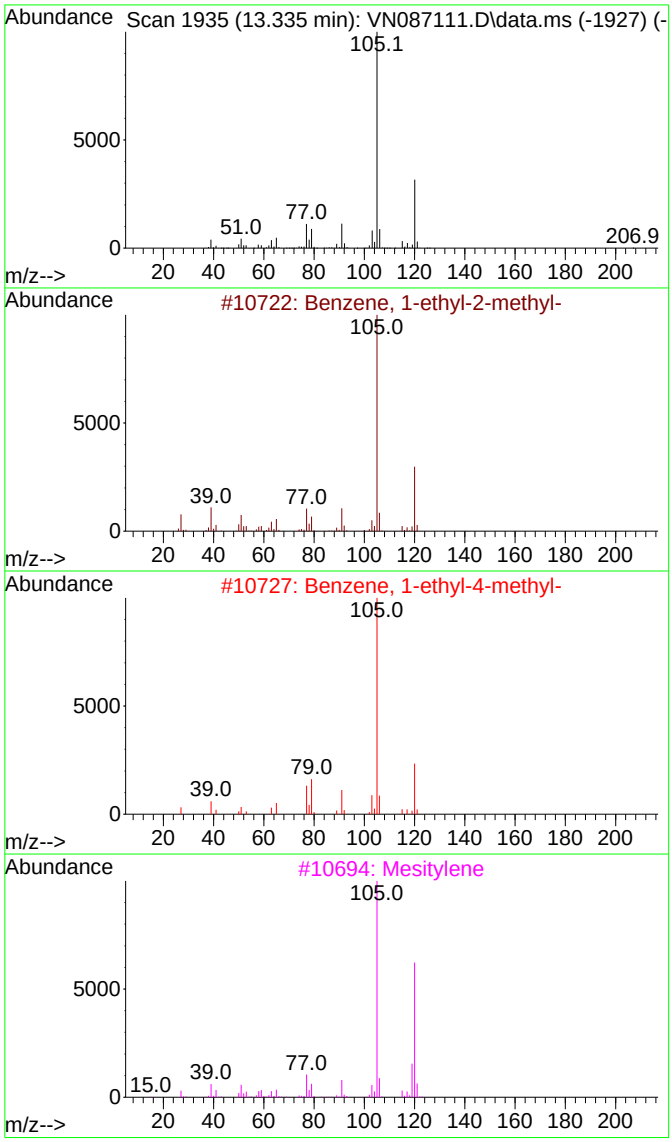
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

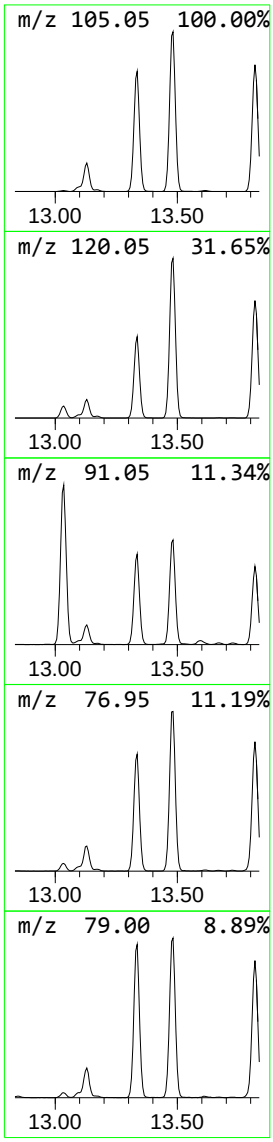
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	38.96 ug/l	7942350	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	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

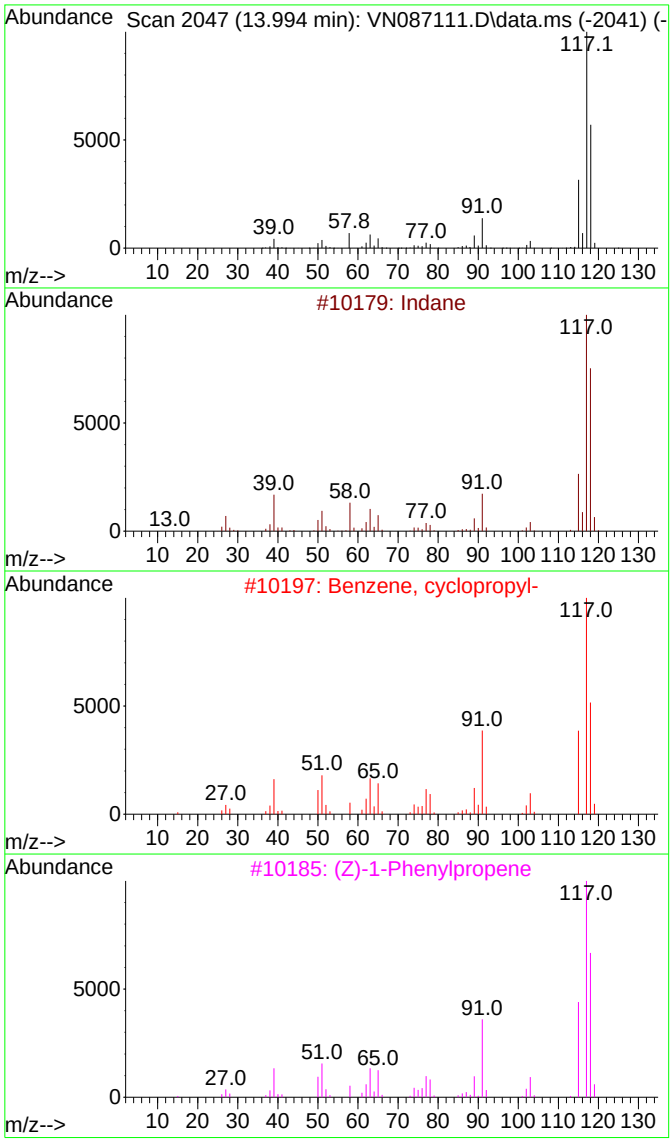
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

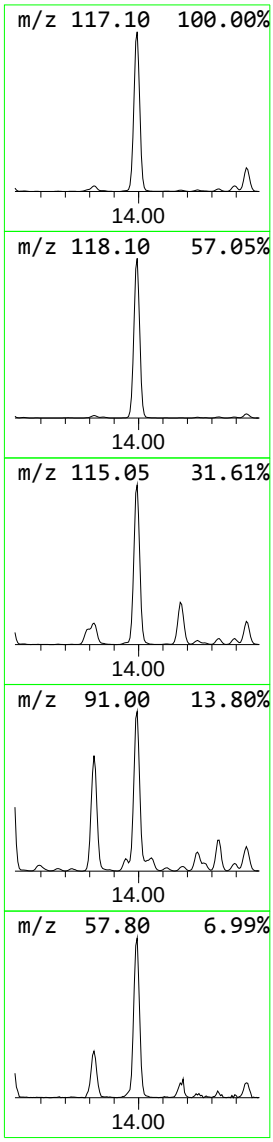
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	47.02 ug/l	9584710	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	72
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061925\
Data File : VN087111.D
Acq On : 19 Jun 2025 15:03
Operator : JC\MD
Sample : Q2333-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane	2.554	28.9	ug/l	708118	1	8.230	1226240	50.0
Butane, 2-methyl-	3.283	57.8	ug/l	1418170	1	8.230	1226240	50.0
Pentane	3.677	34.0	ug/l	835129	1	8.230	1226240	50.0
2-Methyl-1-butene	3.883	20.5	ug/l	502482	1	8.230	1226240	50.0
Cyclopentane	5.406	51.1	ug/l	1253030	1	8.230	1226240	50.0
Cyclopentane, m...	7.342	47.6	ug/l	1168120	1	8.230	1226240	50.0
Di-sec-Butyl ether	10.759	21.8	ug/l	433672	3	11.865	995084	50.0
DL-Lactamide, b...	10.829	20.9	ug/l	416798	3	11.865	995084	50.0
Benzene, 1-ethy...	13.335	39.0	ug/l	7942350	4	13.788	10192700	50.0
Indane	13.994	47.0	ug/l	9584710	4	13.788	10192700	50.0