LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074596.D
Acq On : 19 Sep 2022 19:19
Operator : JC\MD
Sample : N4566-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

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\82N091522W.M
Title : SW846 8260

Signal : TIC: VN074596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	47	58	78	rBV	6264021	10240156	1.50%	0.451%
2	2.393	78	86	109	rBV2	54194025	97885633	14.37%	4.313%
3	3.075	192	202	230	rBV	47215784	103249473	15.16%	4.549%
4	3.357	241	250	257	rBV	4774447	10591209	1.56%	0.467%
5	3.445	257	265	289	rVB	9111062	21150551	3.11%	0.932%
6	3.651	289	300	317	rBV	13892518	32269659	4.74%	1.422%
7	3.828	318	330	358	rVB	4937033	13079053	1.92%	0.576%
8	5.098	531	546	584	rVB2	9431691	41040614	6.03%	1.808%
9	6.610	791	803	815	rBV3	2674363	11063351	1.62%	0.487%
10	7.063	868	880	903	rVB	9655844	27761656	4.08%	1.223%
11	8.022	1034	1043	1052	rBV3	4827199	12193405	1.79%	0.537%
12	8.522	1117	1128	1135	rBV3	2429259	6994821	1.03%	0.308%
13	9.392	1261	1276	1284	rBV2	2987239	8017225	1.18%	0.353%
14	10.445	1449	1455	1461	rVV	4069044	6907181	1.01%	0.304%
15	11.704	1659	1669	1676	rBV2	2980114	6969072	1.02%	0.307%
16	11.792	1676	1684	1694	rBV2	115773182	189476291	27.82%	8.348%
17	11.910	1694	1704	1715	rBV7	216594775	681017404	100.00%	30.006%
18	12.233	1747	1759	1767	rBV3	195889379	432250970	63.47%	19.045%
19	12.862	1858	1866	1871	rVV	8166543	13296949	1.95%	0.586%
20	12.927	1871	1877	1881	rVV2	61403756	96676196	14.20%	4.260%
21	12.962	1881	1883	1886	rVV	21548577	25417690	3.73%	1.120%
22	13.004	1886	1890	1898	rVB	28291664	42194529	6.20%	1.859%
23	13.162	1909	1917	1924	rBV	19962960	31515030	4.63%	1.389%
24	13.315	1934	1943	1950	rBV3	126730876	193477086	28.41%	8.525%
25	13.651	1988	2000	2010	rVV	28233485	50158910	7.37%	2.210%
26	13.821	2023	2029	2045	rVB3	24862450	53470282	7.85%	2.356%
27	14.157	2081	2086	2092	rVB	5401555	8427258	1.24%	0.371%
28	14.868	2199	2207	2213	rBV3	5286579	11159530	1.64%	0.492%
29	15.439	2292	2304	2316	rVB	17642686	31639254	4.65%	1.394%

Sum of corrected areas: 2269590438

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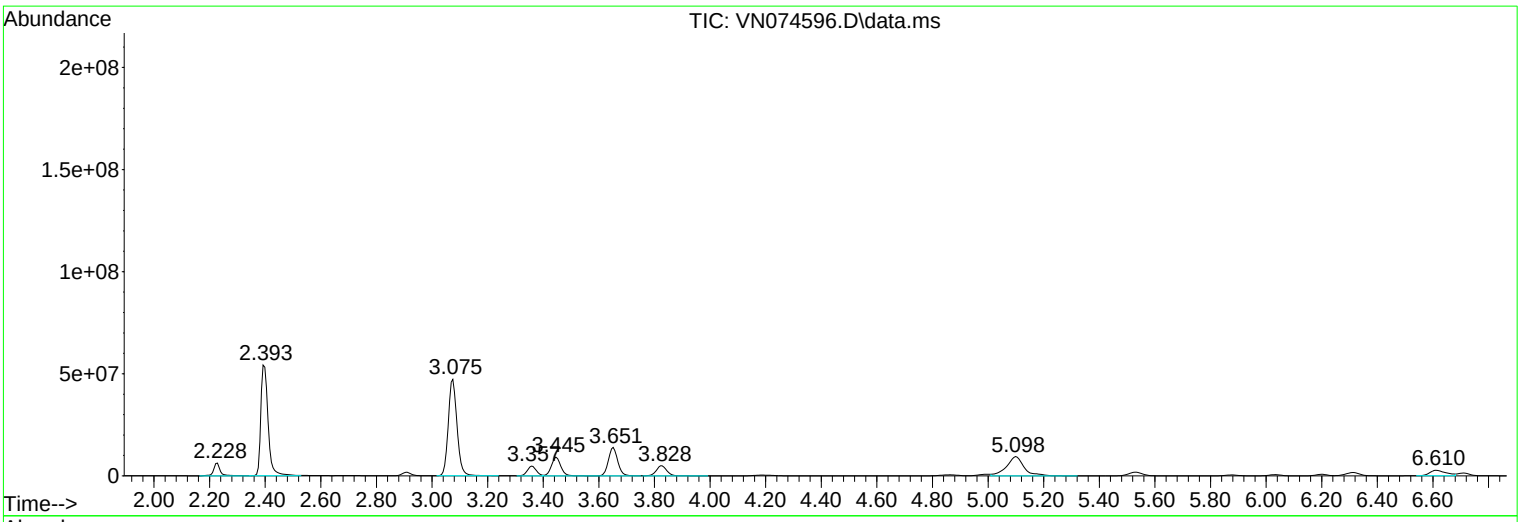
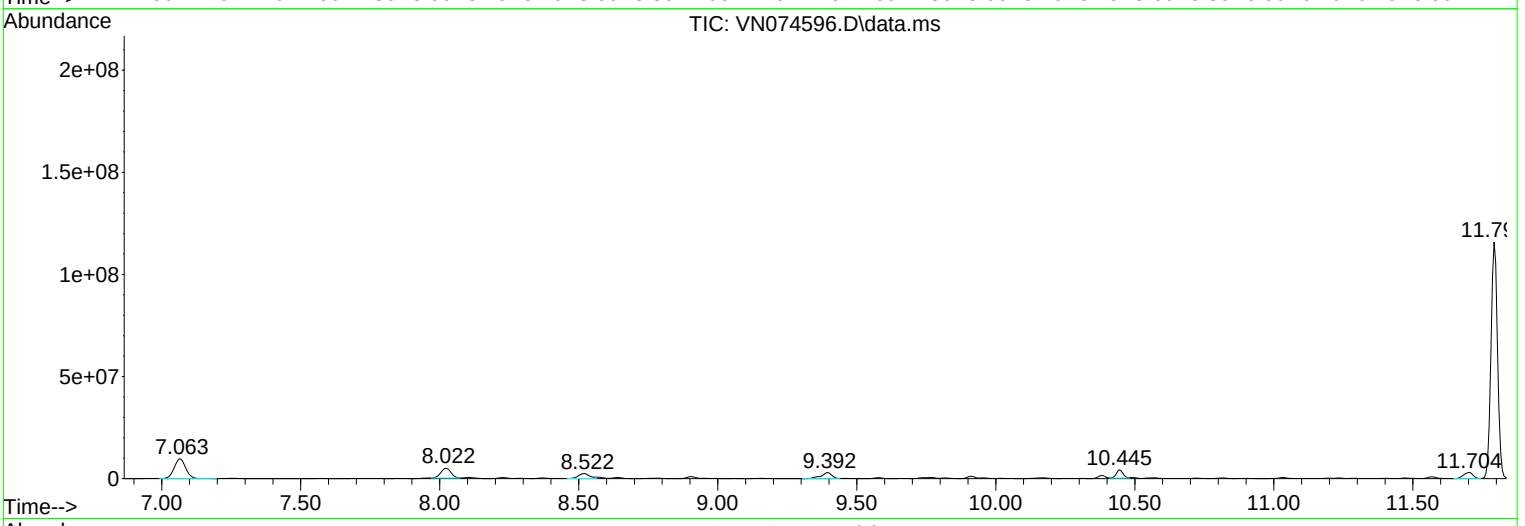
ALS Vial : 22 Sample Multiplier: 1

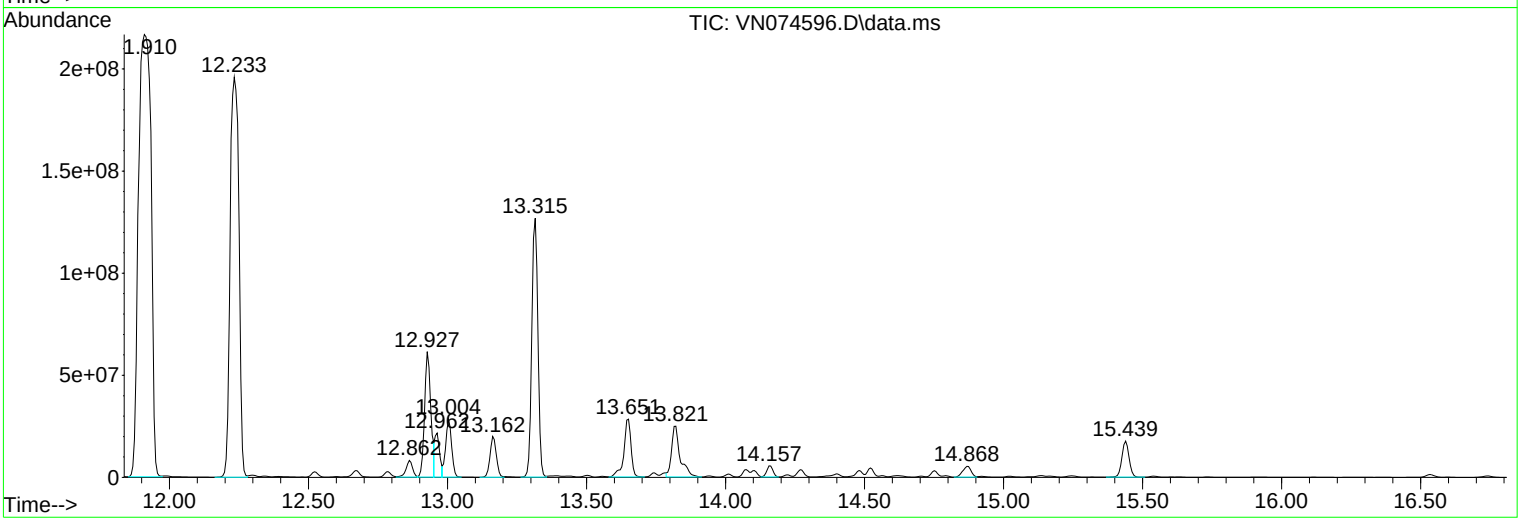
Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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







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TIC Library : C:\Database\NIST20.L
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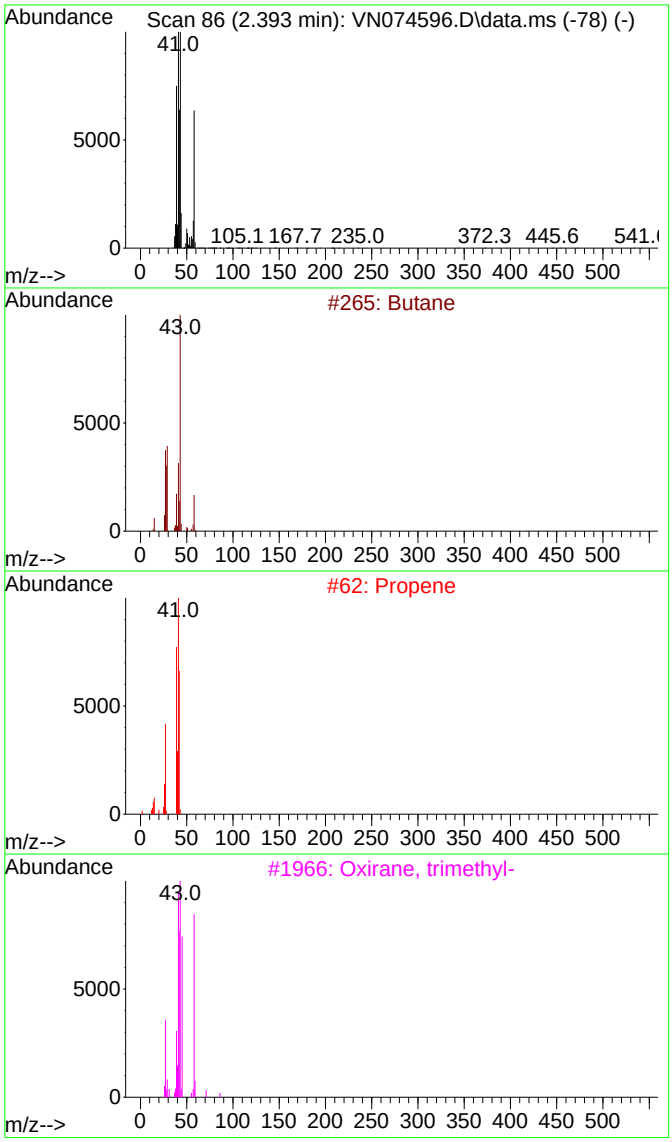
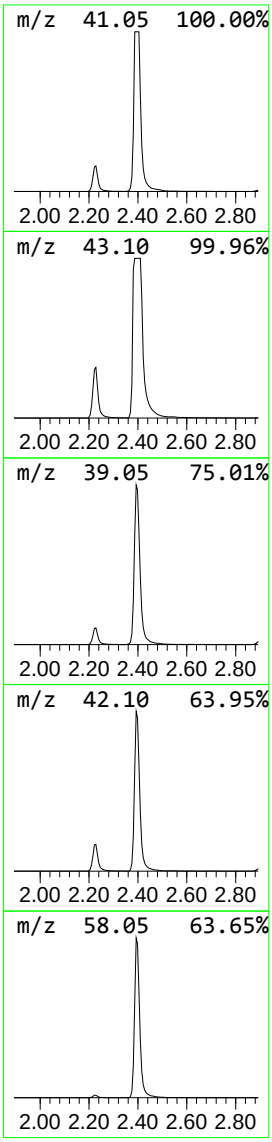
****
Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.393	401.39 ug/l	97885600	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Propene	42	C3H6	000115-07-1	9
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	9
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5
5	Acetone	58	C3H6O	000067-64-1	5





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ClientSampleId :
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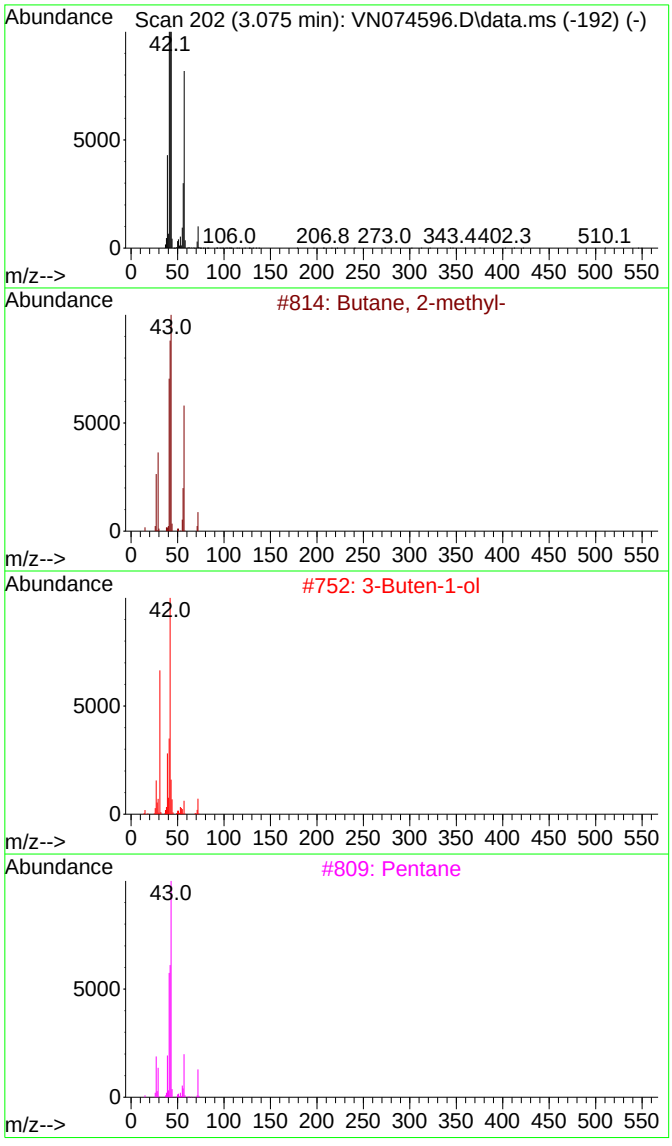
Quant Title : SW846 8260

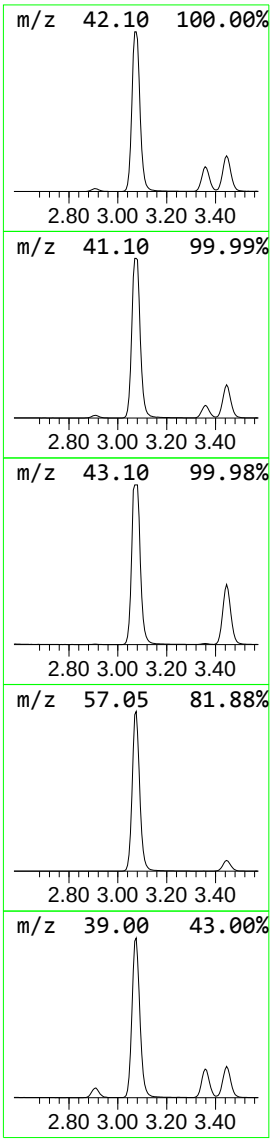
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.075	423.38 ug/l	103249000	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	3-Buten-1-ol	72	C4H8O	000627-27-0	35
3	Pentane	72	C5H12	000109-66-0	33
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	27
5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	25





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MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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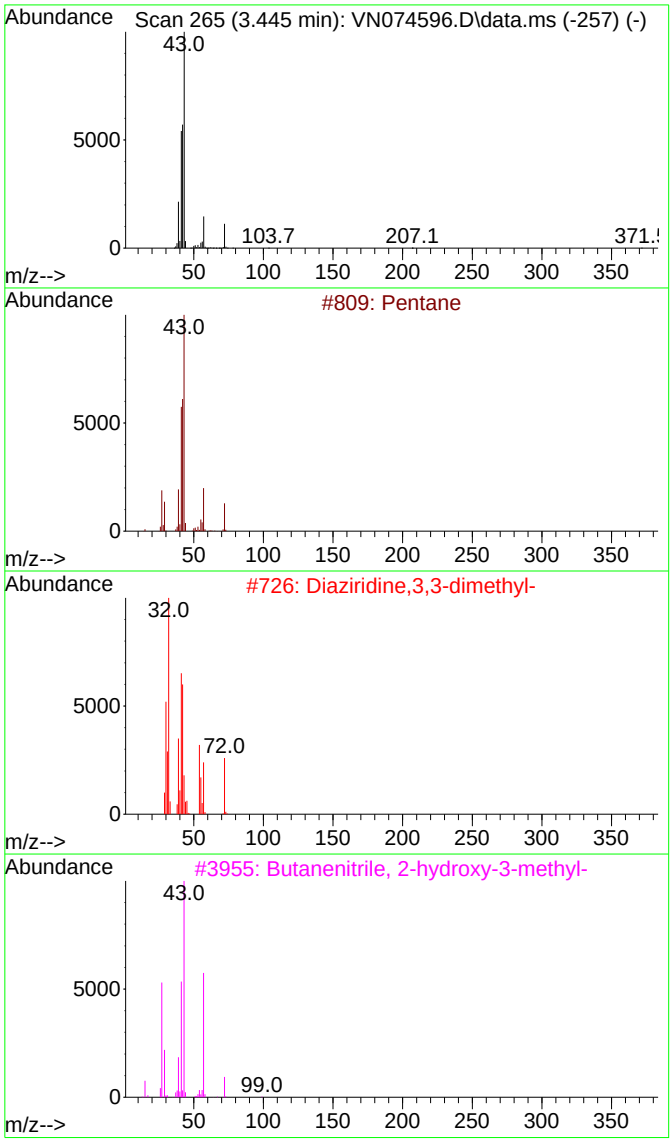
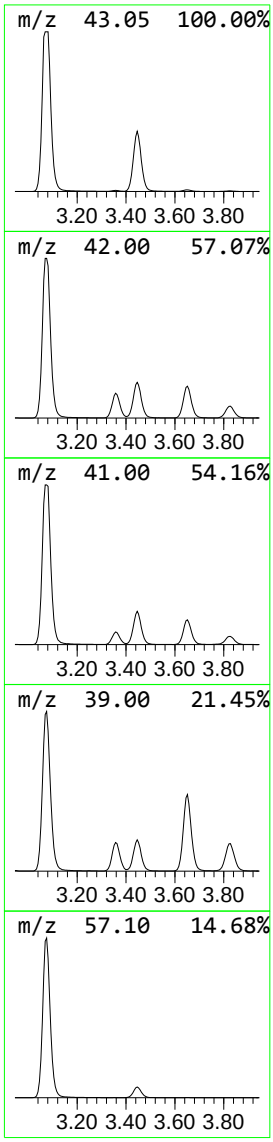
****
Peak Number 3 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.445	86.73 ug/l	21150600	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
3	Butanenitrile, 2-hydroxy-3-methyl-	99	C5H9NO	010021-64-4	17
4	Butane, 2-methyl-	72	C5H12	000078-78-4	9
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	9





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

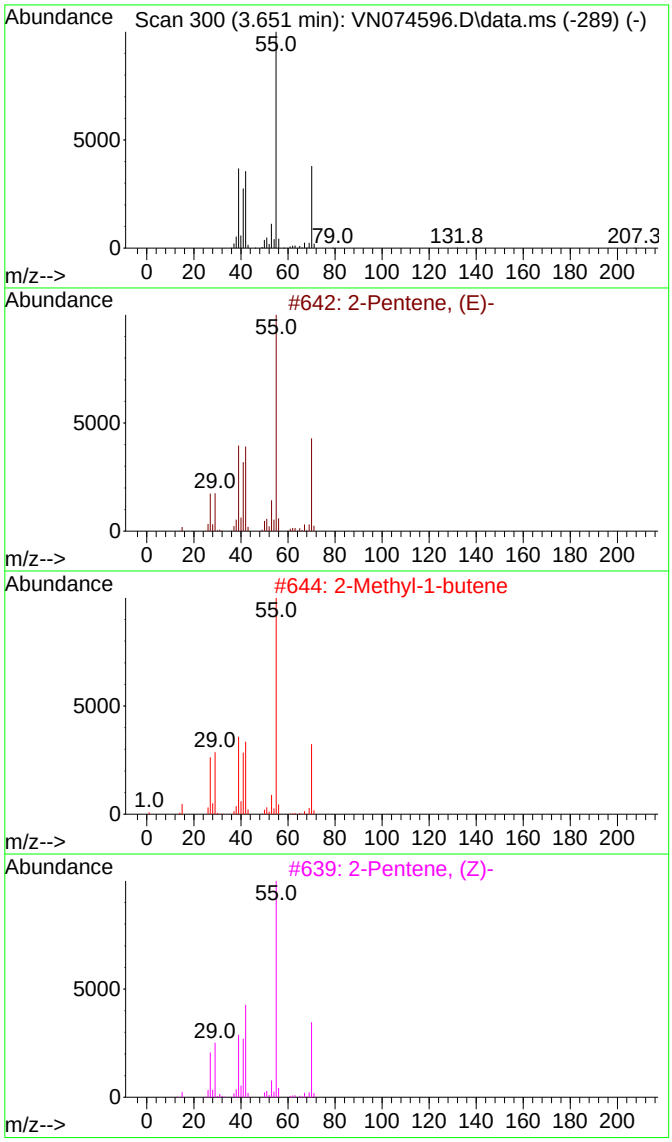
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

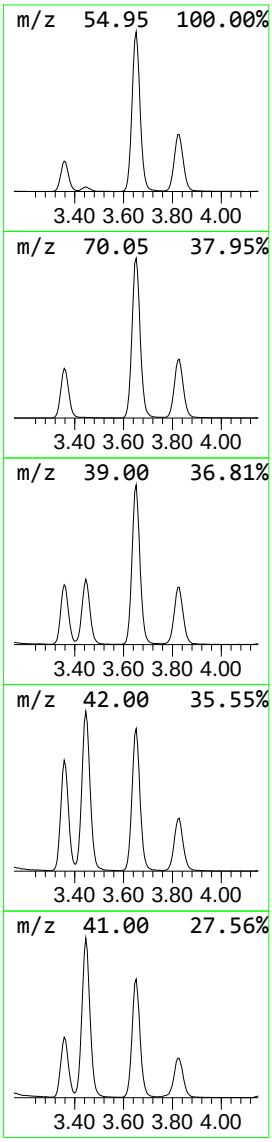
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.651	132.32 ug/l	32269700	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	93
2	2-Methyl-1-butene	70	C5H10	000563-46-2	90
3	2-Pentene, (Z)-	70	C5H10	000627-20-3	90
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
5	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87





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Operator : JC\MD
Sample : N4566-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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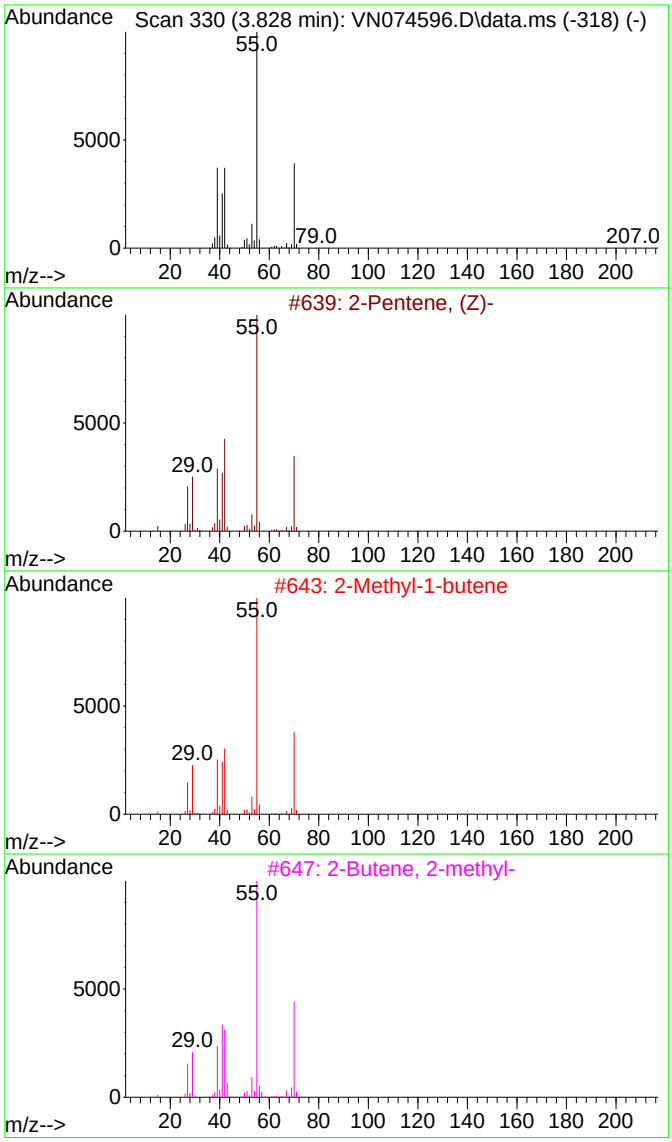
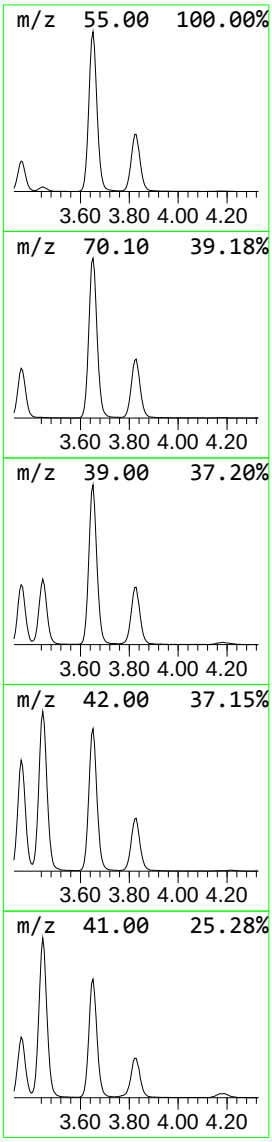
****
Peak Number 5 2-Pentene, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.828	53.63 ug/l	13079100	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-	70	C5H10	000627-20-3	90
2	2-Methyl-1-butene	70	C5H10	000563-46-2	87
3	2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
4	2-Pentene	70	C5H10	000109-68-2	86
5	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86





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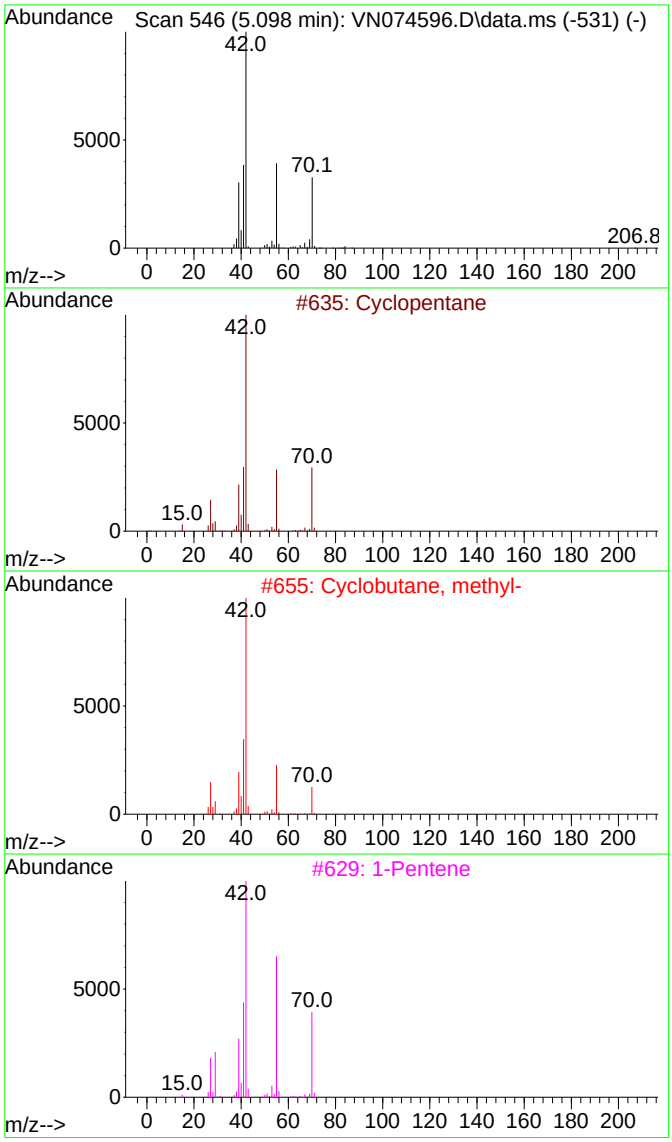
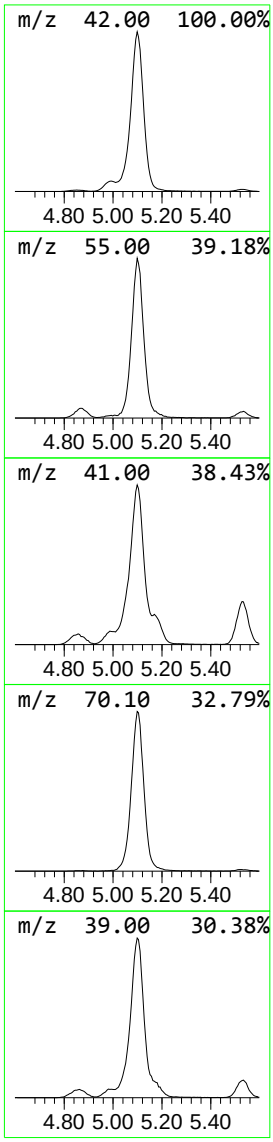
****

Peak Number 6 Cyclopentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	168.29 ug/l	41040600	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
3	1-Pentene	70	C5H10	000109-67-1	50
4	Cyclobutanone	70	C4H6O	001191-95-3	50
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	25





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TIC Library : C:\Database\NIST20.L
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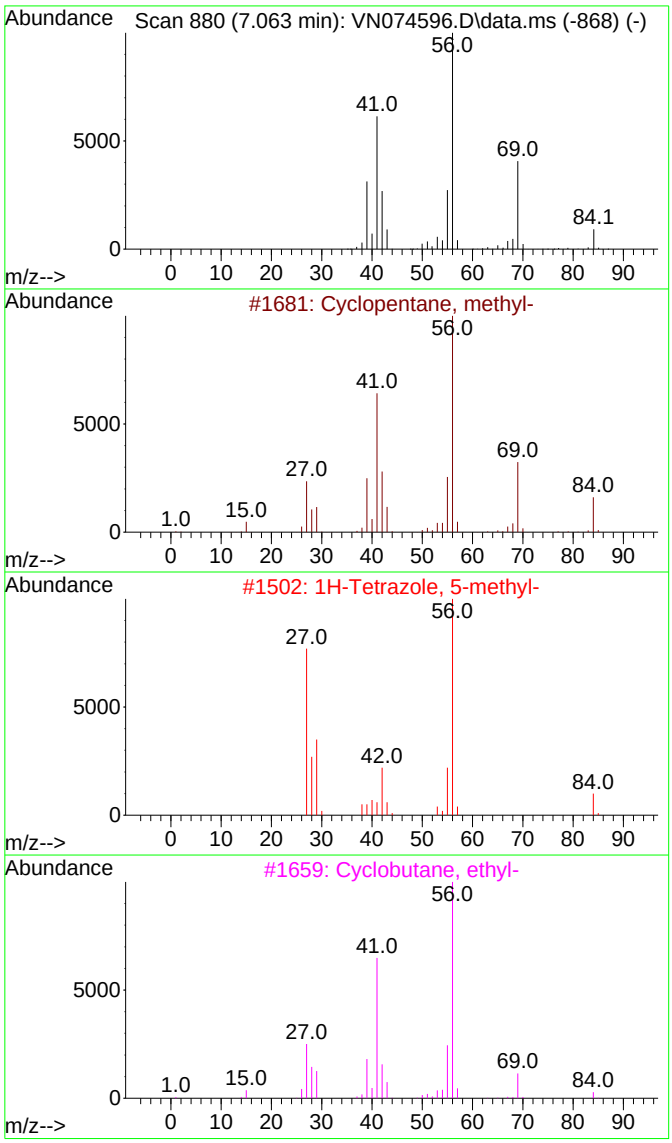
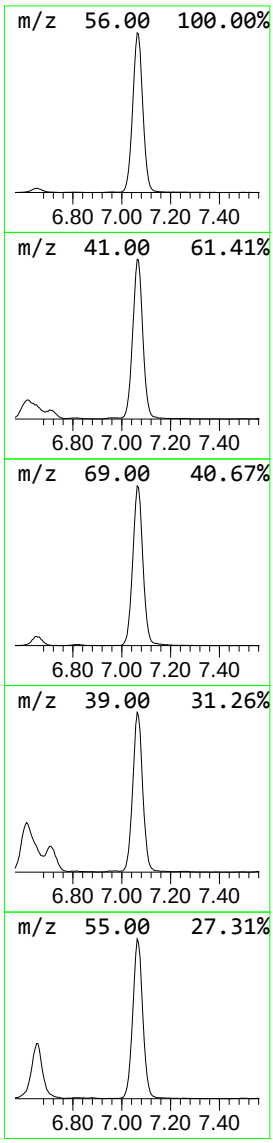
****
Peak Number 7 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	113.84 ug/l	27761700	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclobutane, butyl-	112	C8H16	013152-44-8	64
5	Cyclohexane	84	C6H12	000110-82-7	56





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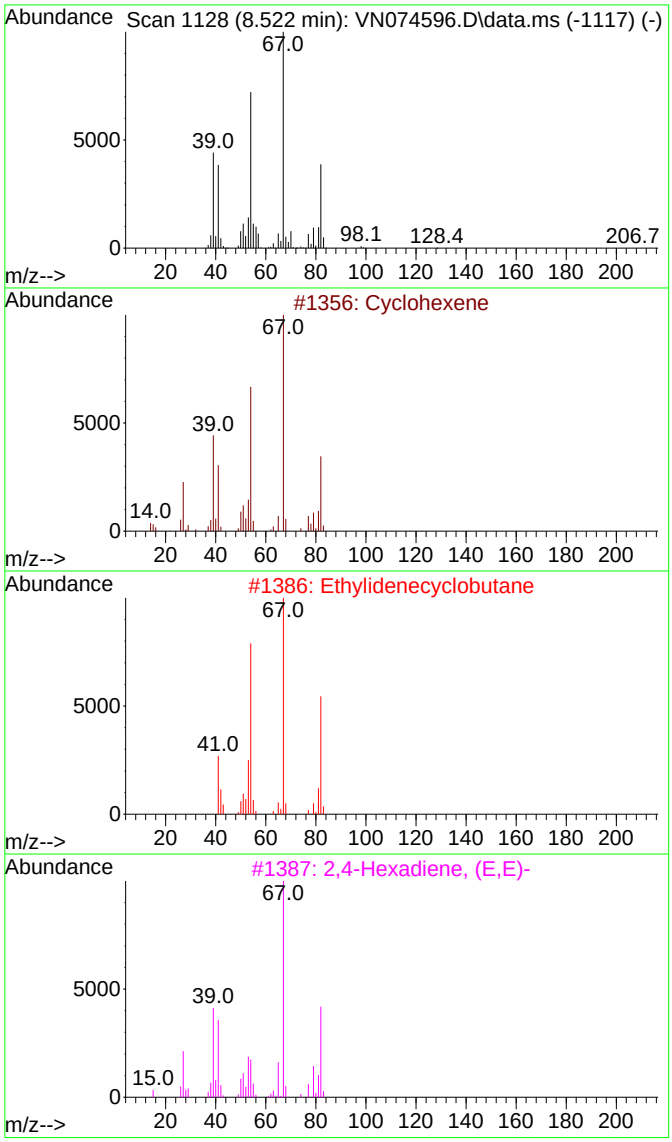
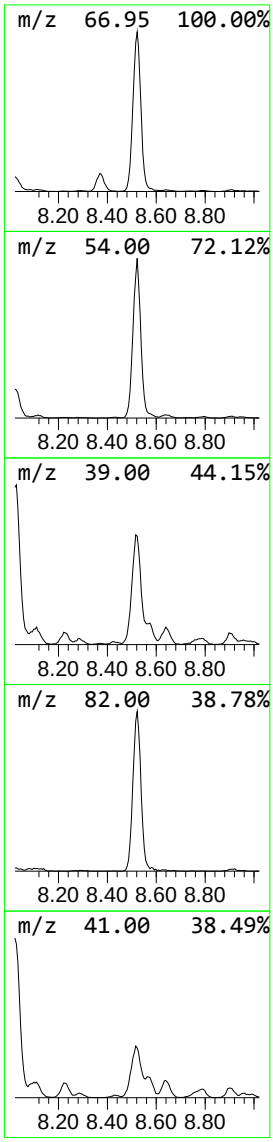
****
Peak Number 8 Ethylidenecyclobutane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.522	50.00 ug/l	6994820	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	94
2	Ethylidenecyclobutane	82	C6H10	001528-21-8	87
3	2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	81
4	C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	81
5	1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	80





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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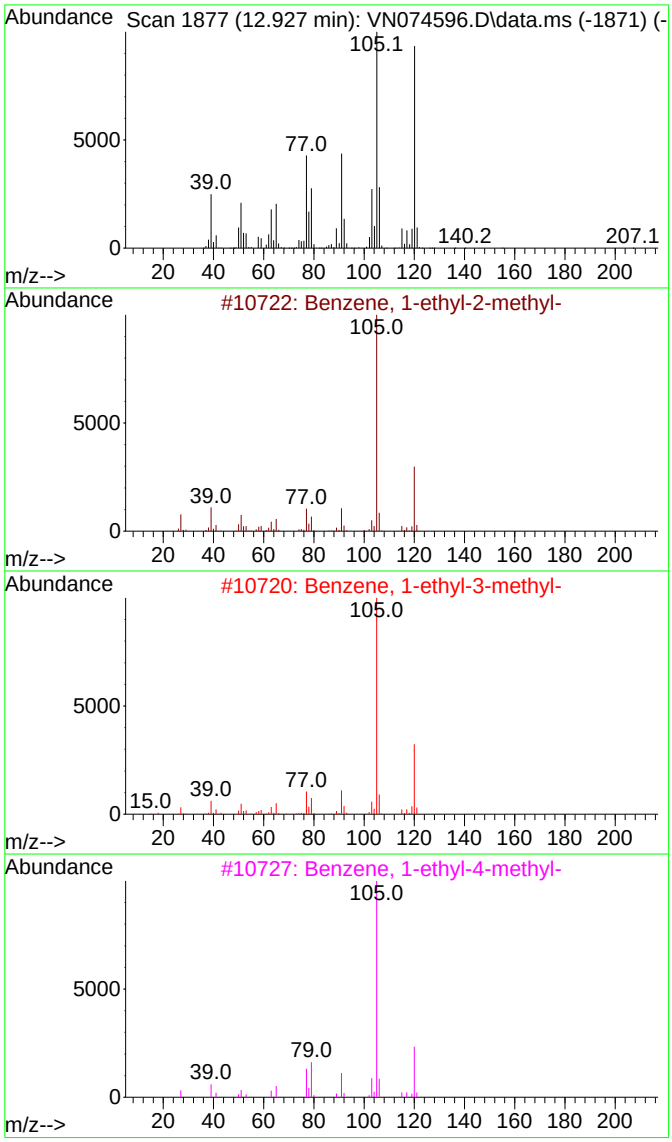
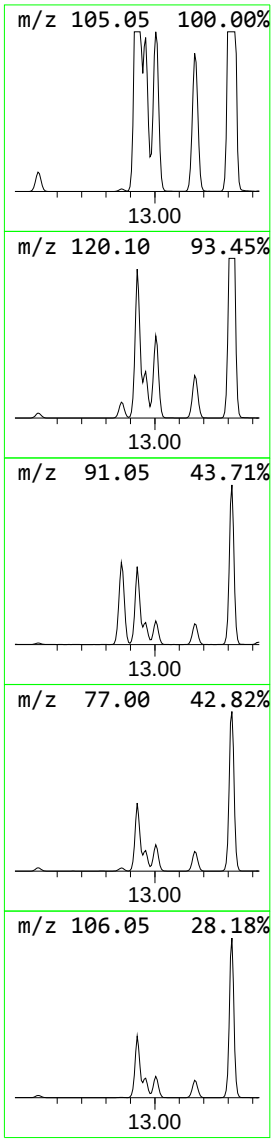
****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.927	96.37 ug/l	96676200	1,4-Dichlorobenzene-d4	13.615

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	81
4	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	74
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074596.D
Acq On : 19 Sep 2022 19:19
Operator : JC\MD
Sample : N4566-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

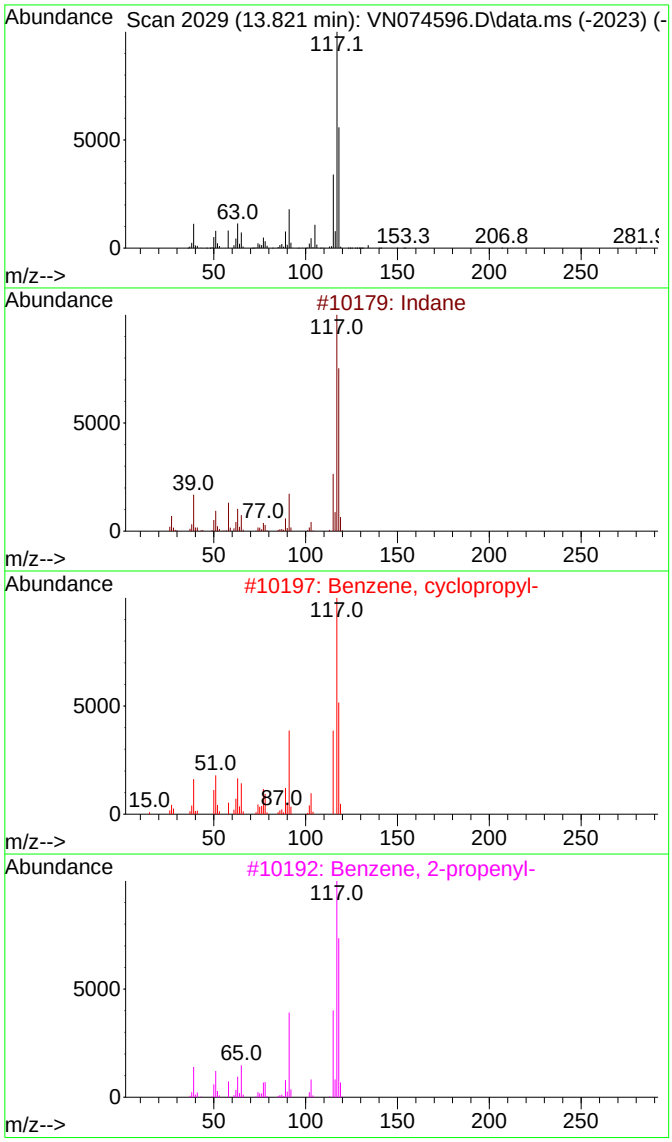
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

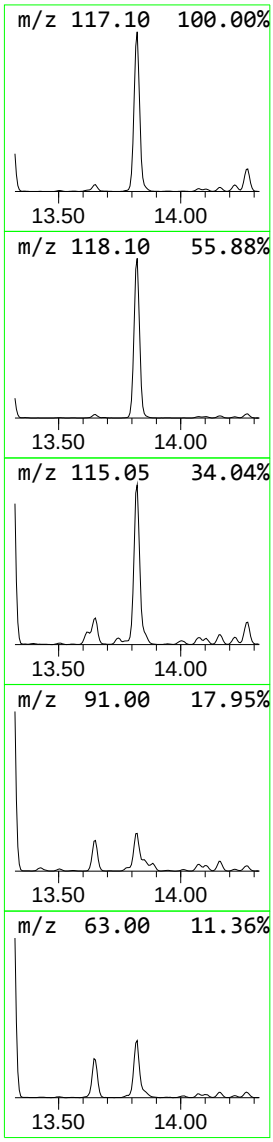
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	53.30 ug/l	53470300	1,4-Dichlorobenzene-d4	13.615

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	76
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074596.D
Acq On : 19 Sep 2022 19:19
Operator : JC\MD
Sample : N4566-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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	2.393	401.4	ug/l	97885600	1	8.016	12193400	50.0
Butane, 2-methyl-	3.075	423.4	ug/l	103249000	1	8.016	12193400	50.0
Pentane	3.445	86.7	ug/l	21150600	1	8.016	12193400	50.0
2-Pentene, (E)-	3.651	132.3	ug/l	32269700	1	8.016	12193400	50.0
2-Pentene, (Z)-	3.828	53.6	ug/l	13079100	1	8.016	12193400	50.0
Cyclopentane	5.098	168.3	ug/l	41040600	1	8.016	12193400	50.0
Cyclopentane, m...	7.063	113.8	ug/l	27761700	1	8.016	12193400	50.0
Ethylidenecyclo...	8.522	50.0	ug/l	6994820	2	8.904	6994820	50.0
Benzene, 1-ethy...	12.927	96.4	ug/l	96676200	4	13.615	50158900	50.0
Indane	13.821	53.3	ug/l	53470300	4	13.615	50158900	50.0