LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074262.D
Acq On : 02 Sep 2022 00:04
Operator : JC\MD
Sample : N4376-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

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\82N083022W.M
Title : SW846 8260

Signal : TIC: VN074262.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	50	58	62	rBV	54041	82359	1.43%	0.416%
2	2.398	82	87	95	rBV	160601	260785	4.52%	1.318%
3	3.087	196	204	213	rVB2	231011	517999	8.97%	2.618%
4	3.457	258	267	277	rBV2	31265	78852	1.37%	0.399%
5	4.998	519	529	535	rBV5	25807	89617	1.55%	0.453%
6	5.104	537	547	564	rVB4	70099	277444	4.81%	1.402%
7	5.287	564	578	597	rBV2	430656	1526010	26.44%	7.713%
8	5.539	607	621	636	rVB2	126056	449237	7.78%	2.270%
9	6.410	755	769	781	rBV2	50135	162128	2.81%	0.819%
10	7.063	867	880	891	rVB4	51067	181438	3.14%	0.917%
11	7.951	1021	1031	1036	rBV	192761	448644	7.77%	2.267%
12	8.016	1036	1042	1052	rVV	342181	800462	13.87%	4.046%
13	8.104	1052	1057	1069	rVB4	27099	65098	1.13%	0.329%
14	8.392	1094	1106	1115	rBV	2369656	5771888	100.00%	29.171%
15	8.904	1183	1193	1207	rBV	497351	1043160	18.07%	5.272%
16	9.951	1367	1371	1377	rVB2	35727	70898	1.23%	0.358%
17	10.139	1395	1403	1413	rBV2	49599	112718	1.95%	0.570%
18	10.380	1435	1444	1452	rBV	751611	1366502	23.68%	6.906%
19	10.580	1470	1478	1485	rBV3	55740	102750	1.78%	0.519%
20	10.657	1485	1491	1497	rVB2	58537	98269	1.70%	0.497%
21	11.069	1557	1561	1567	rVB	65758	115084	1.99%	0.582%
22	11.527	1631	1639	1645	rBV	51483	97448	1.69%	0.493%
23	11.686	1658	1666	1677	rBV	715966	1286586	22.29%	6.502%
24	11.786	1677	1683	1690	rVB	56822	105015	1.82%	0.531%
25	12.521	1801	1808	1814	rBV	151964	252032	4.37%	1.274%
26	12.668	1825	1833	1843	rBV	575067	983690	17.04%	4.972%
27	12.857	1856	1865	1872	rVB	142156	233669	4.05%	1.181%
28	13.610	1986	1993	2006	rBV	682808	1208101	20.93%	6.106%
29	13.780	2016	2022	2023	rBV	67937	94974	1.65%	0.480%
30	13.815	2023	2028	2034	rVB	645702	1053251	18.25%	5.323%
31	14.004	2055	2060	2067	rVB	48714	78173	1.35%	0.395%
32	14.151	2080	2085	2091	rBV	46727	72686	1.26%	0.367%
33	14.215	2091	2096	2100	rBV3	38543	68659	1.19%	0.347%
34	14.262	2100	2104	2111	rVB	141448	236810	4.10%	1.197%
35	14.474	2132	2140	2144	rBV2	66172	113959	1.97%	0.576%
36	14.868	2197	2207	2213	rBV3	83705	155034	2.69%	0.784%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074262.D
Acq On : 02 Sep 2022 00:04
Operator : JC\MD
Sample : N4376-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

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\82N083022W.M
Title : SW846 8260

37	15.433	2296	2303	2309	rVB2	31918	63154	1.09%	0.319%
38	16.733	2517	2524	2533	rVB3	27069	61534	1.07%	0.311%

Sum of corrected areas: 19786117

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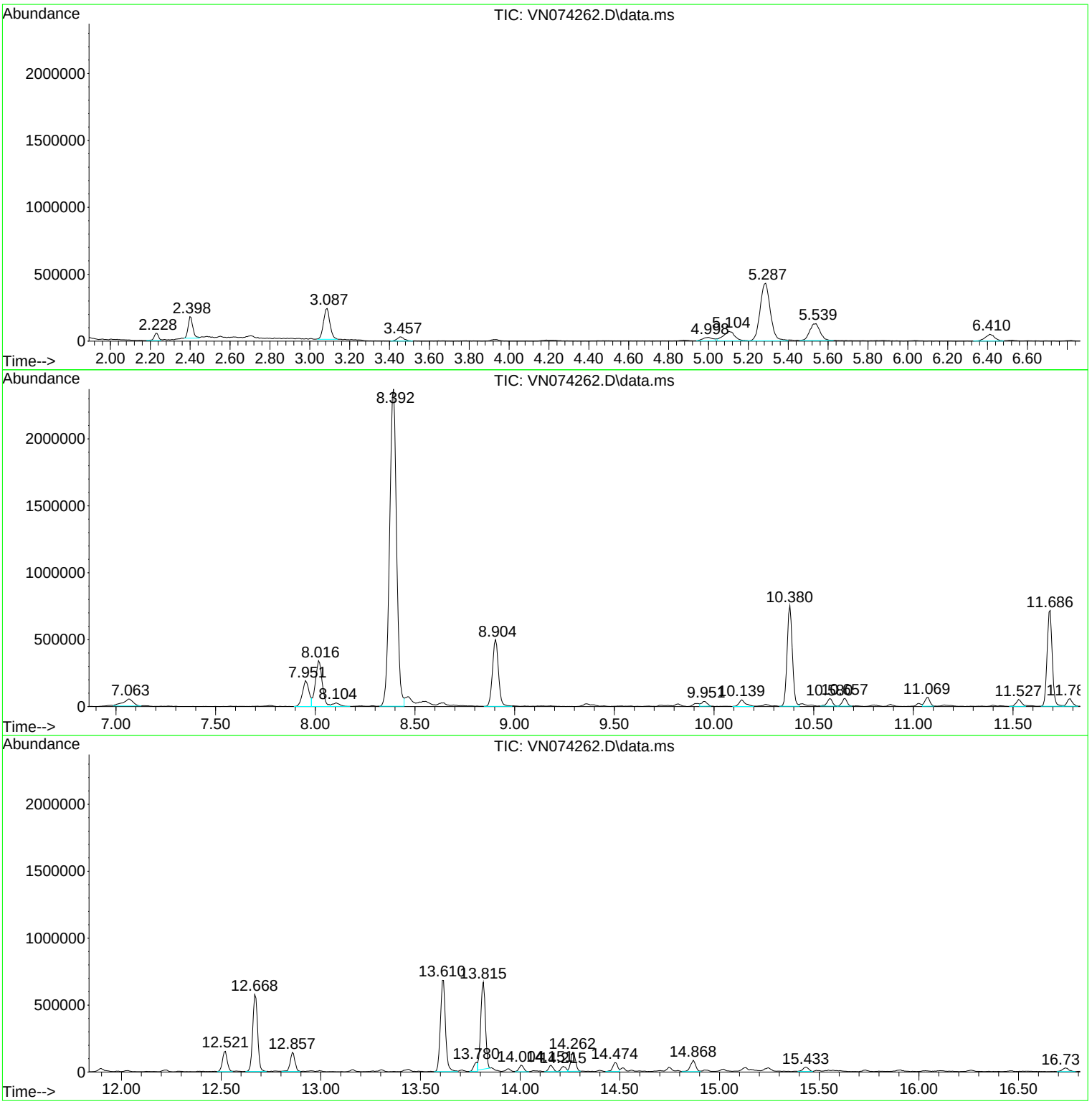
MSVOA_N
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



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Data File : VN074262.D
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

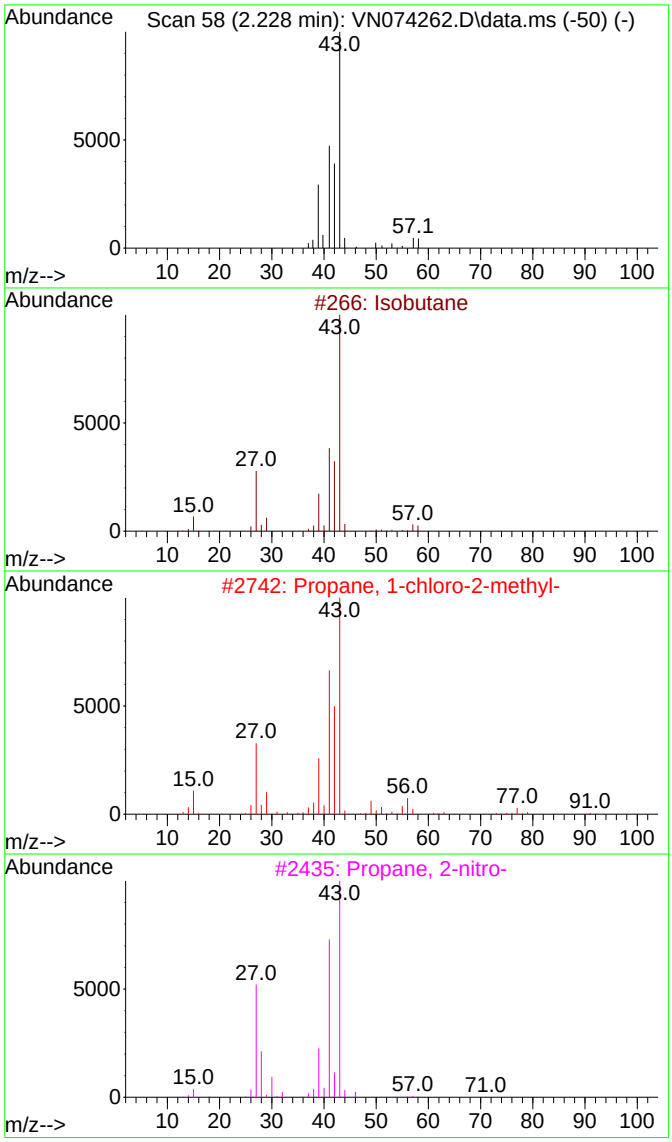
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

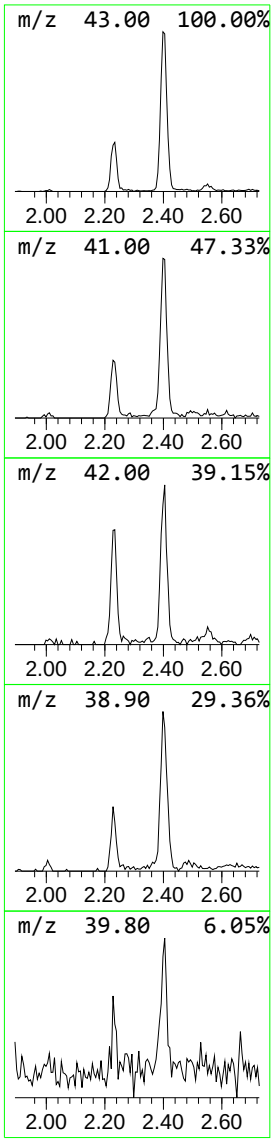
****

Peak Number 1 Isobutane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	5.14 ug/l	82359	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	78
2	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	9
3	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
4	5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	4





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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

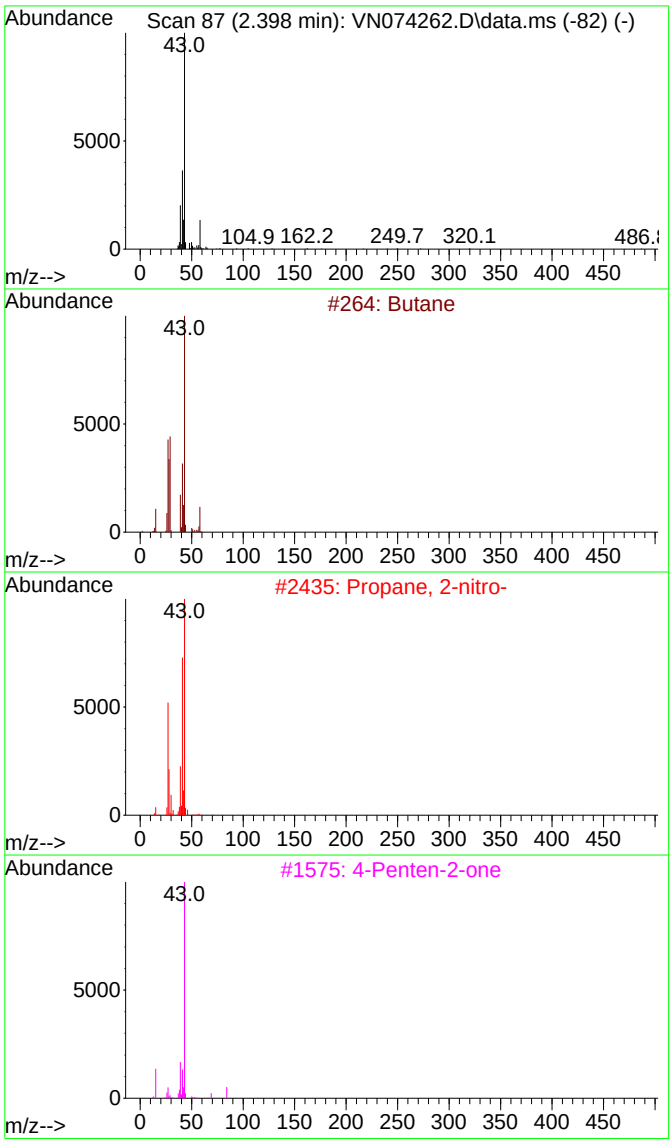
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

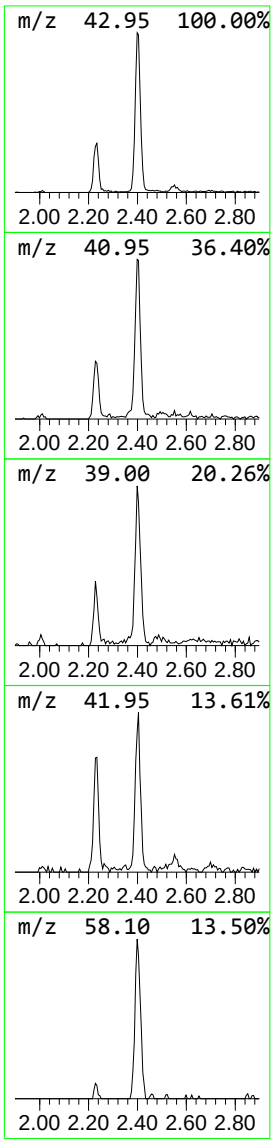
****

Peak Number 2 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.398	16.29 ug/l	260785	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	58
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3	4-Penten-2-one	84	C5H8O	013891-87-7	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074262.D
Acq On : 02 Sep 2022 00:04
Operator : JC\MD
Sample : N4376-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

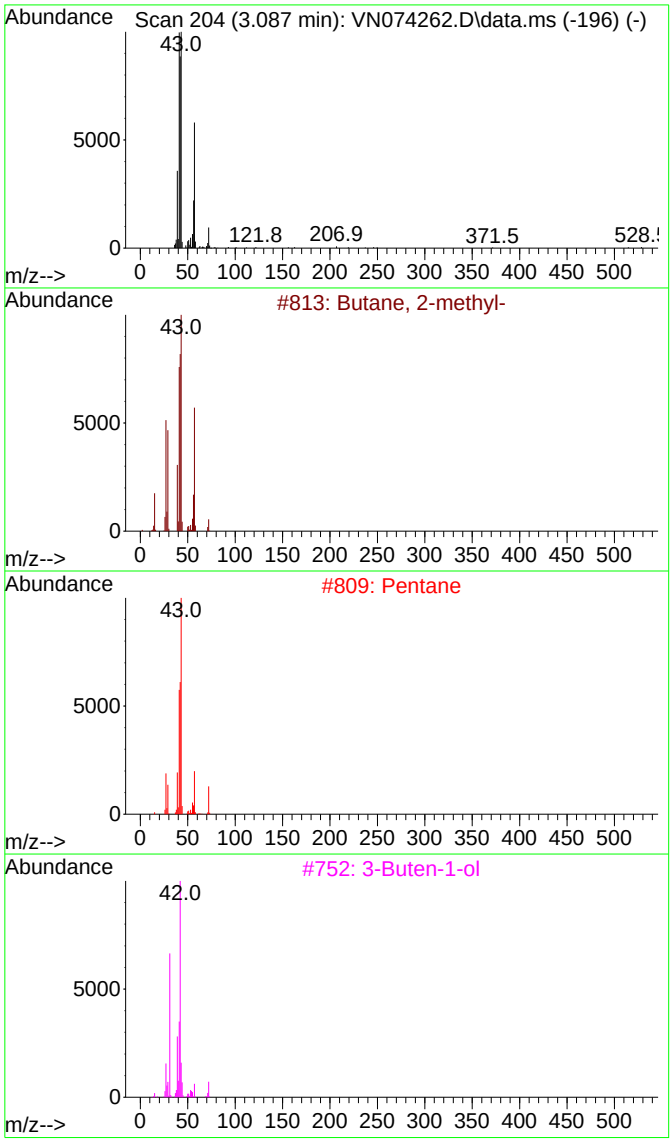
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

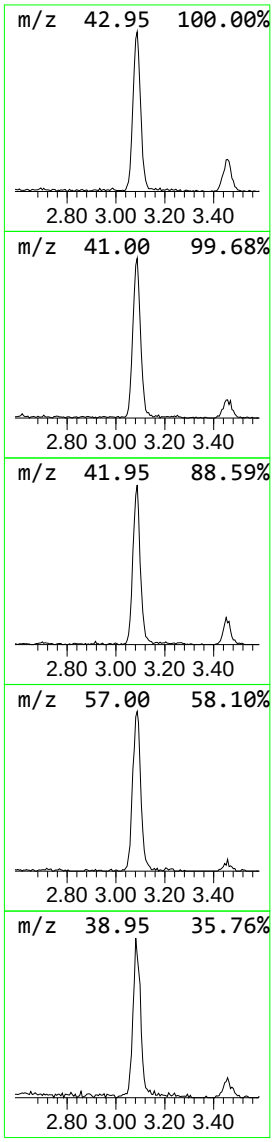
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	32.36 ug/l	517999	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Pentane	72	C5H12	000109-66-0	33
3	3-Buten-1-ol	72	C4H8O	000627-27-0	25
4	1-Butene	56	C4H8	000106-98-9	9
5	Azetidine	57	C3H7N	000503-29-7	9





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Data File : VN074262.D
Acq On : 02 Sep 2022 00:04
Operator : JC\MD
Sample : N4376-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

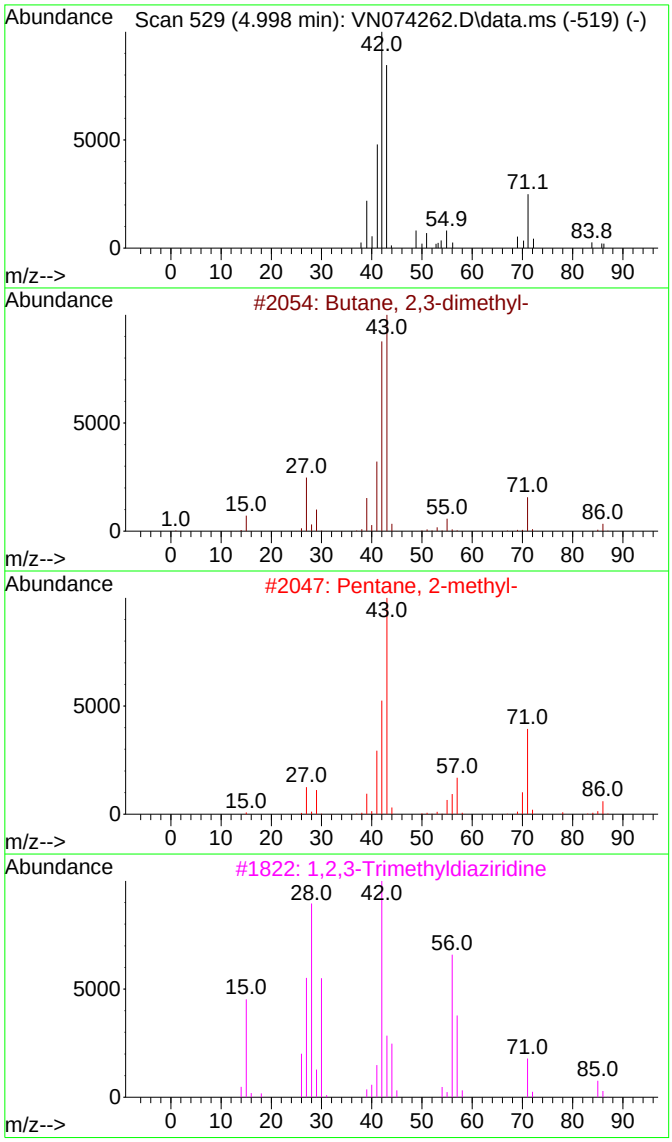
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

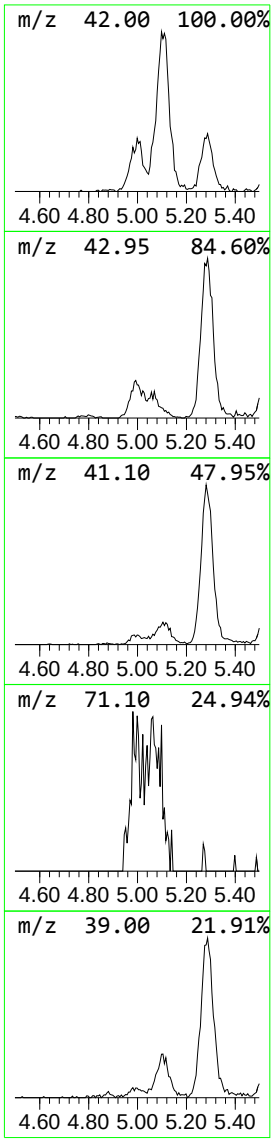
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	5.60 ug/l	89617	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
3	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	9
4	1-Pentene	70	C5H10	000109-67-1	9
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074262.D
Acq On : 02 Sep 2022 00:04
Operator : JC\MD
Sample : N4376-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

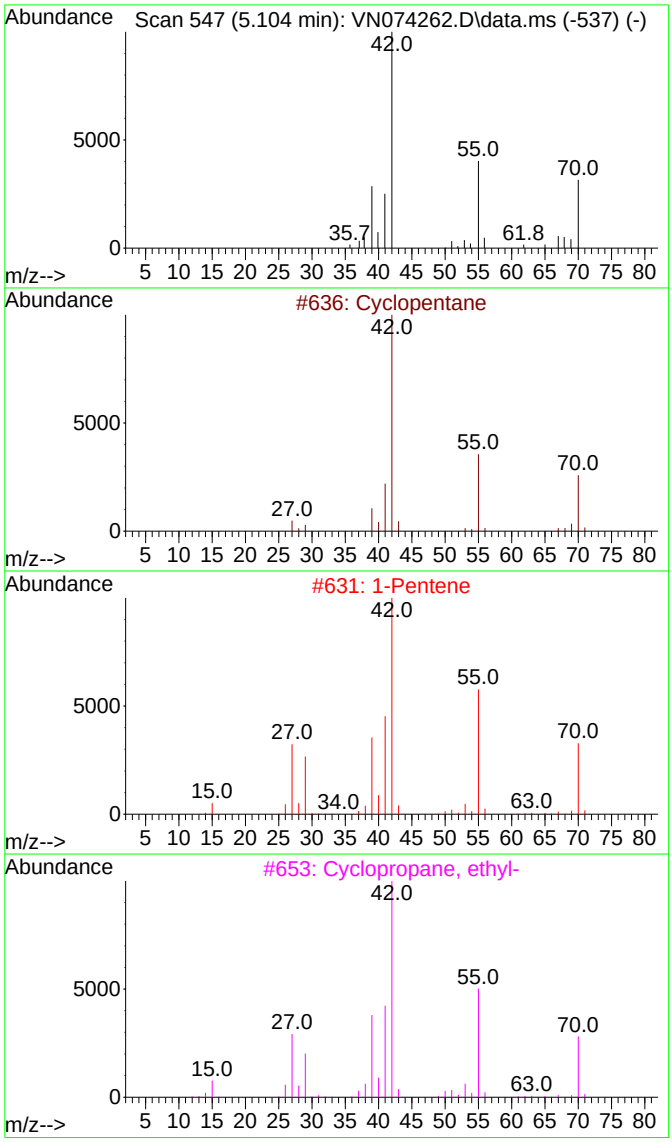
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

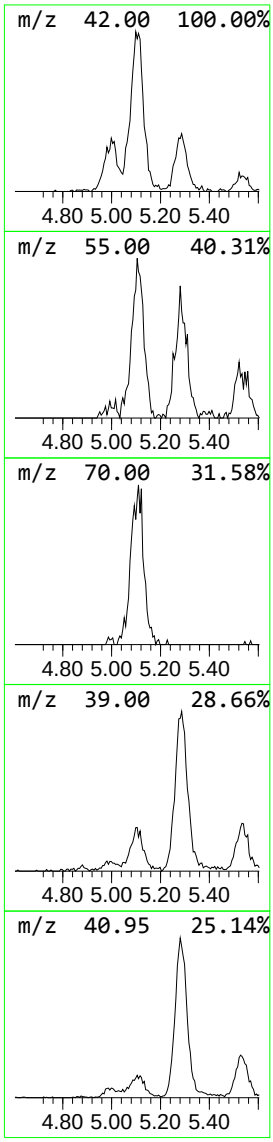
****

Peak Number 5 Cyclopentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	17.33 ug/l	277444	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	80
2	1-Pentene	70	C5H10	000109-67-1	50
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	45
4	Cyclobutanone	70	C4H6O	001191-95-3	42
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	9





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Acq On : 02 Sep 2022 00:04
Operator : JC\MD
Sample : N4376-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

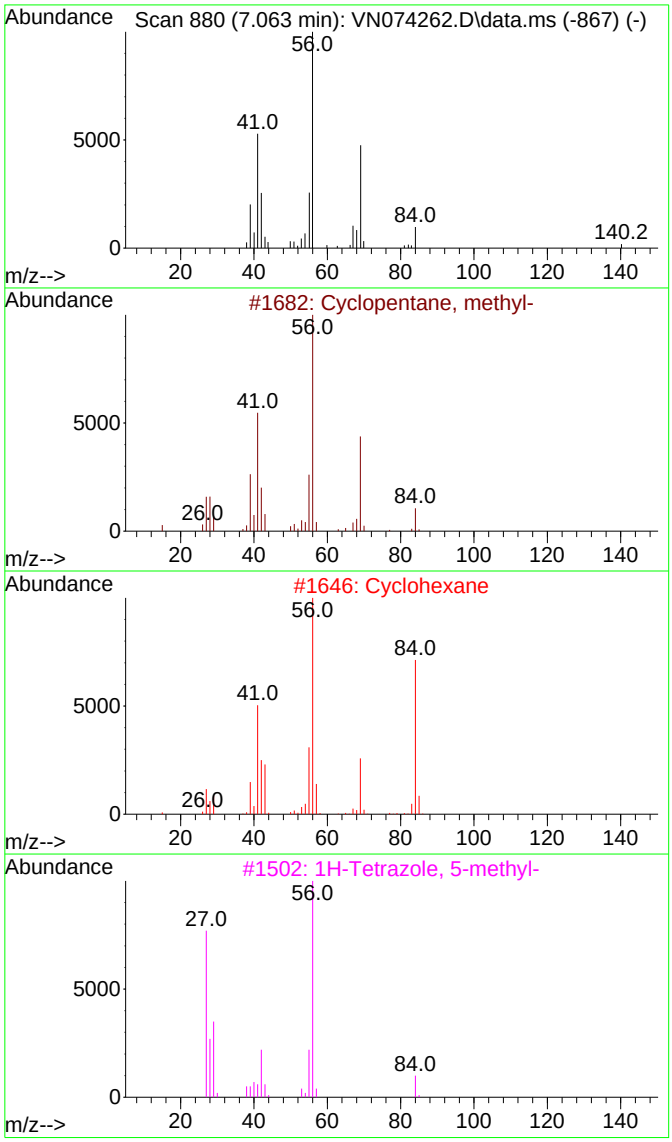
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

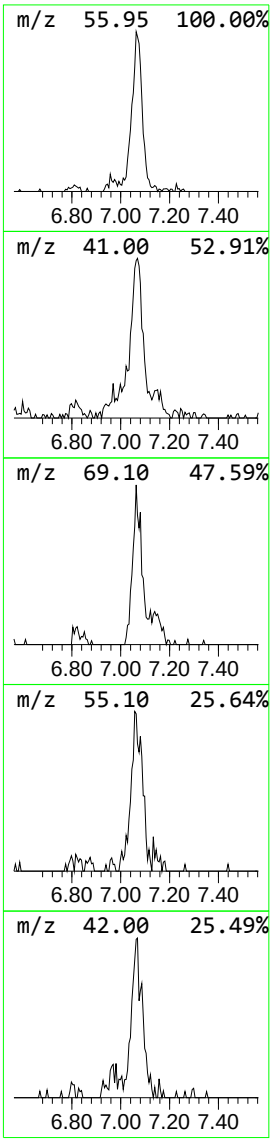
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	11.33 ug/l	181438	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclohexane	84	C6H12	000110-82-7	72
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	53
5	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	50





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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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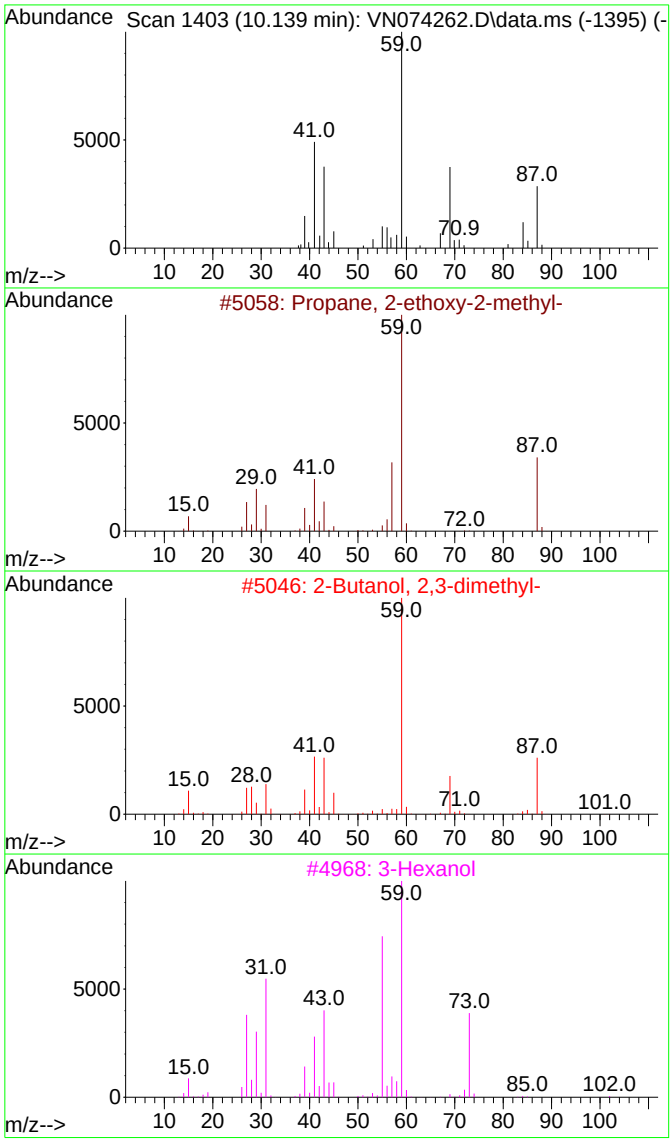
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

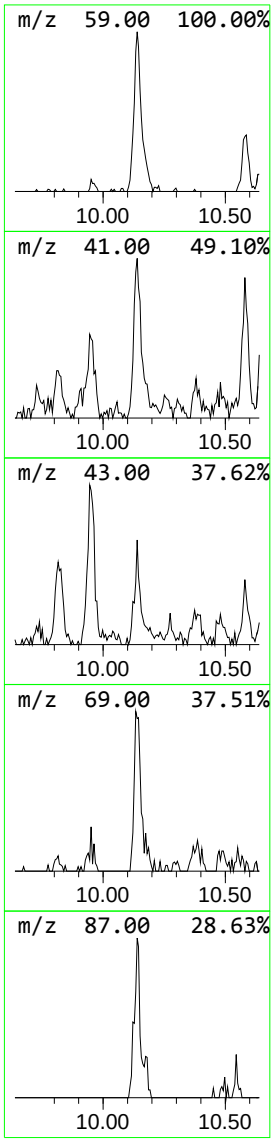
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propane, 2-ethoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.139	5.40 ug/l	112718	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
2	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	50
3	3-Hexanol	102	C6H14O	000623-37-0	50
4	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	50
5	Butane, 2-methoxy-	88	C5H12O	006795-87-5	49





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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

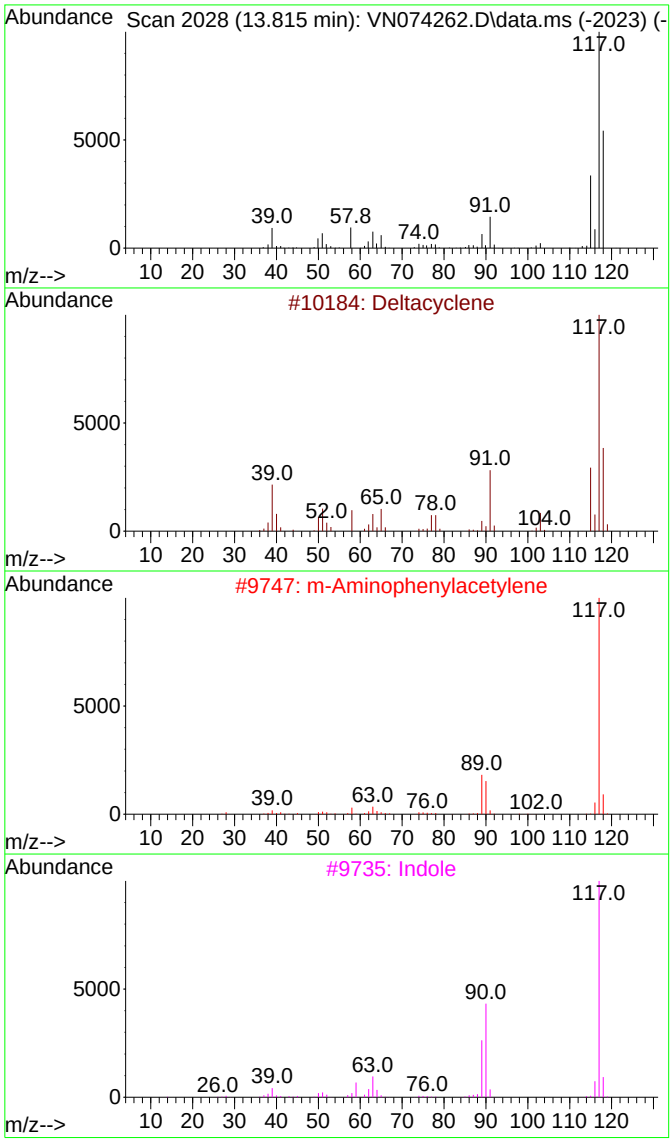
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

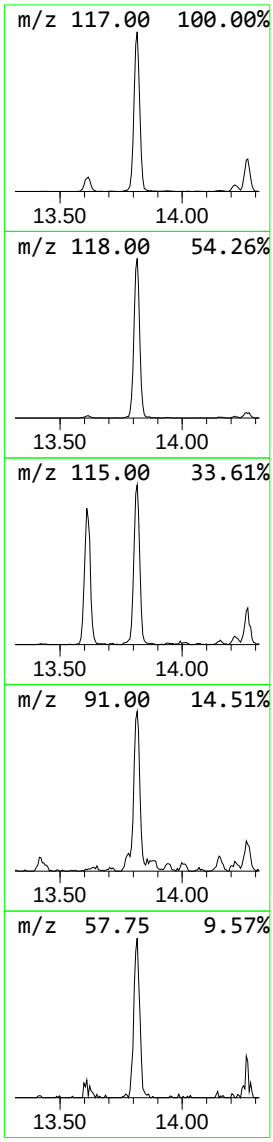
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown13.815 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	43.59 ug/l	1053250	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	72
2	m-Aminophenylacetylene	117	C8H7N	054060-30-9	47
3	Indole	117	C8H7N	000120-72-9	43
4	Benzene, (isocyanomethyl)-	117	C8H7N	010340-91-7	38
5	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	38





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

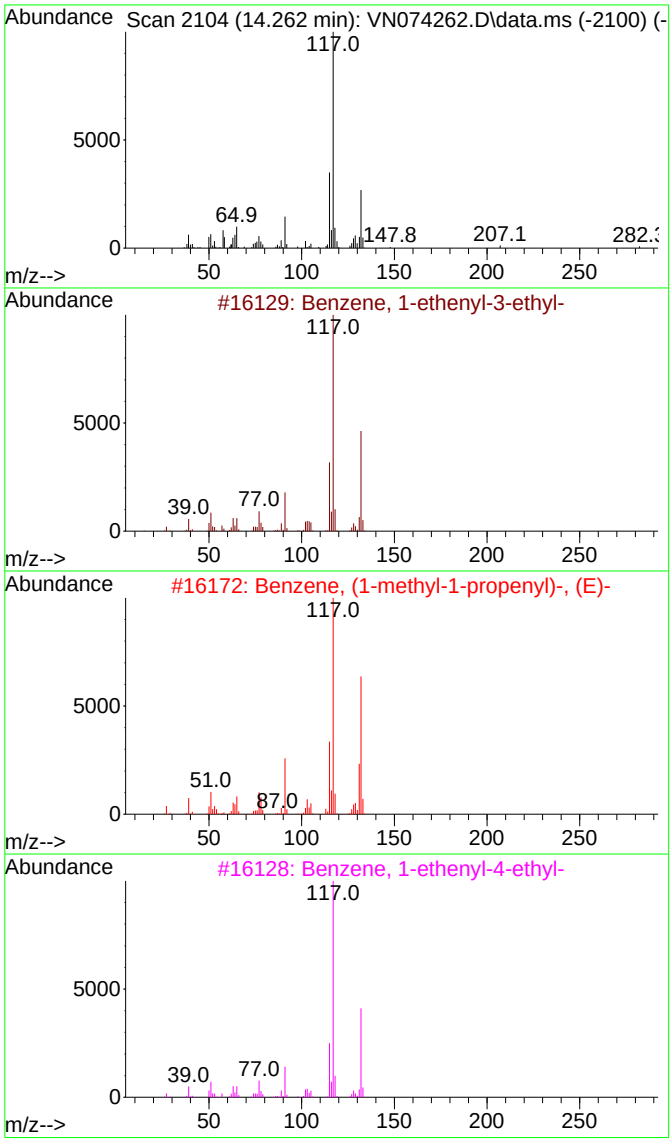
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

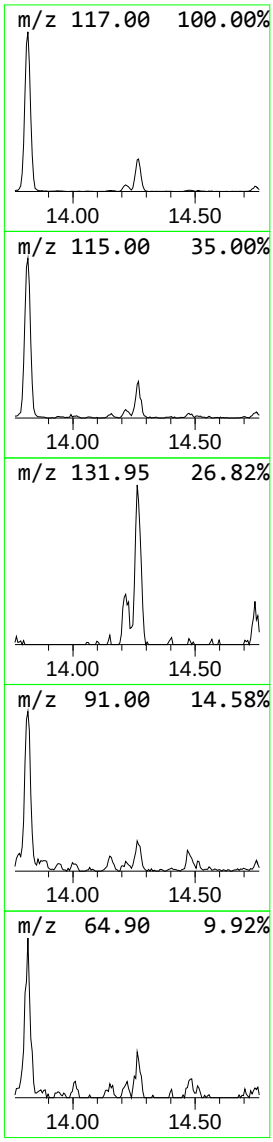
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.262	9.80 ug/l	236810	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	86
5	Indan, 1-methyl-	132	C10H12	000767-58-8	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074262.D
Acq On : 02 Sep 2022 00:04
Operator : JC\MD
Sample : N4376-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

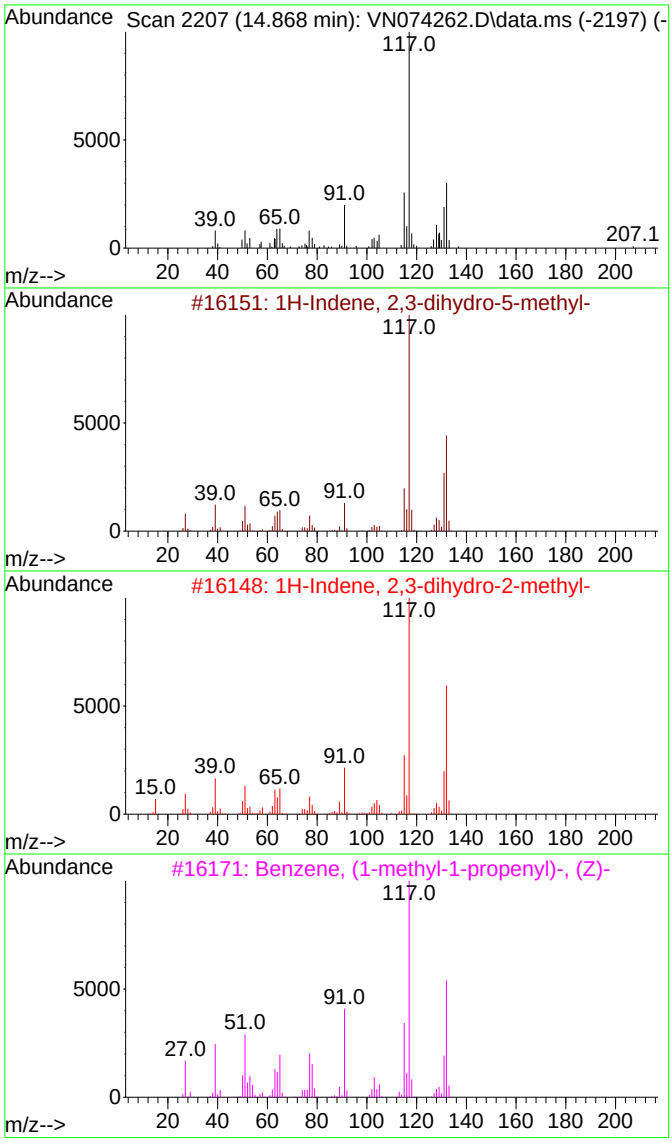
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

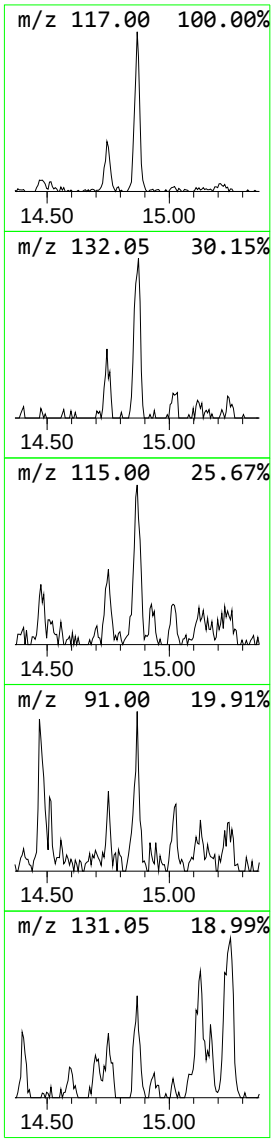
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	6.42 ug/l	155034	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	87
2	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	83
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81
5	Indan, 1-methyl-	132	C10H12	000767-58-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074262.D
Acq On : 02 Sep 2022 00:04
Operator : JC\MD
Sample : N4376-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.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
Isobutane	2.228	5.1	ug/l	82359	1	8.016	800462	50.0
Butane	2.398	16.3	ug/l	260785	1	8.016	800462	50.0
Butane, 2-methyl-	3.087	32.4	ug/l	517999	1	8.016	800462	50.0
Butane, 2,3-dim...	4.998	5.6	ug/l	89617	1	8.016	800462	50.0
Cyclopentane	5.104	17.3	ug/l	277444	1	8.016	800462	50.0
Cyclopentane, m...	7.063	11.3	ug/l	181438	1	8.016	800462	50.0
Propane, 2-etho...	10.139	5.4	ug/l	112718	2	8.904	1043160	50.0
unknown13.815	13.815	43.6	ug/l	1053250	4	13.610	1208100	50.0
Benzene, 1-ethe...	14.262	9.8	ug/l	236810	4	13.610	1208100	50.0
1H-Indene, 2,3-...	14.868	6.4	ug/l	155034	4	13.610	1208100	50.0