LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

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: VN074595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.399	79	87	98	rBV	7415395	11028507	6.29%	1.636%
2	3.075	191	202	225	rBV	13184647	28383895	16.20%	4.211%
3	3.446	257	265	280	rVB	1426900	3295500	1.88%	0.489%
4	3.651	291	300	314	rBV	816760	1951799	1.11%	0.290%
5	5.087	532	544	580	rVB4	1364473	8037712	4.59%	1.193%
6	5.528	605	619	634	rBV2	949170	3262604	1.86%	0.484%
7	7.063	868	880	897	rVB	3329507	9670606	5.52%	1.435%
8	8.022	1035	1043	1052	rVB2	1929266	4627700	2.64%	0.687%
9	9.398	1261	1277	1285	rBV2	1396531	3772063	2.15%	0.560%
10	10.380	1435	1444	1448	rBV	987799	1857065	1.06%	0.276%
11	10.451	1448	1456	1472	rVB3	97682078	175209165	100.00%	25.997%
12	11.686	1658	1666	1675	rBV	2013375	3525451	2.01%	0.523%
13	11.786	1675	1683	1693	rBV	11478970	18307300	10.45%	2.716%
14	11.898	1693	1702	1715	rBV3	97525337	165074705	94.22%	24.493%
15	12.227	1748	1758	1766	rBV2	39408477	61797762	35.27%	9.169%
16	12.674	1826	1834	1845	rVB2	1715962	3137658	1.79%	0.466%
17	12.786	1845	1853	1858	rBV	1072427	1857662	1.06%	0.276%
18	12.863	1858	1866	1871	rVV	2640416	4430494	2.53%	0.657%
19	12.927	1871	1877	1881	rVV	19573243	31699272	18.09%	4.703%
20	12.957	1881	1882	1886	rVV	7400822	8604528	4.91%	1.277%
21	13.004	1886	1890	1900	rVB	10028966	14948042	8.53%	2.218%
22	13.163	1908	1917	1924	rBV	6890747	10940940	6.24%	1.623%
23	13.316	1932	1943	1949	rBV	32779716	50777563	28.98%	7.534%
24	13.615	1988	1994	1995	rBV2	1988603	2659740	1.52%	0.395%
25	13.651	1995	2000	2007	rVB	7174163	11789674	6.73%	1.749%
26	13.815	2024	2028	2032	rBV2	3877179	6453616	3.68%	0.958%
27	13.851	2032	2034	2045	rVB2	2267729	3456032	1.97%	0.513%
28	14.074	2066	2072	2075	rBV	1332626	2208786	1.26%	0.328%
29	14.157	2081	2086	2092	rVB	2402063	3757877	2.14%	0.558%
30	14.268	2101	2105	2114	rVB2	1547739	2607232	1.49%	0.387%
31	14.480	2133	2141	2145	rBV	1220811	2144423	1.22%	0.318%
32	14.521	2145	2148	2153	rVB	1518874	2109255	1.20%	0.313%
33	14.751	2182	2187	2192	rBV	1263755	1915512	1.09%	0.284%
34	14.874	2199	2208	2214	rBV2	2312939	4672350	2.67%	0.693%
35	15.439	2297	2304	2317	rVB	2153667	3997404	2.28%	0.593%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

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

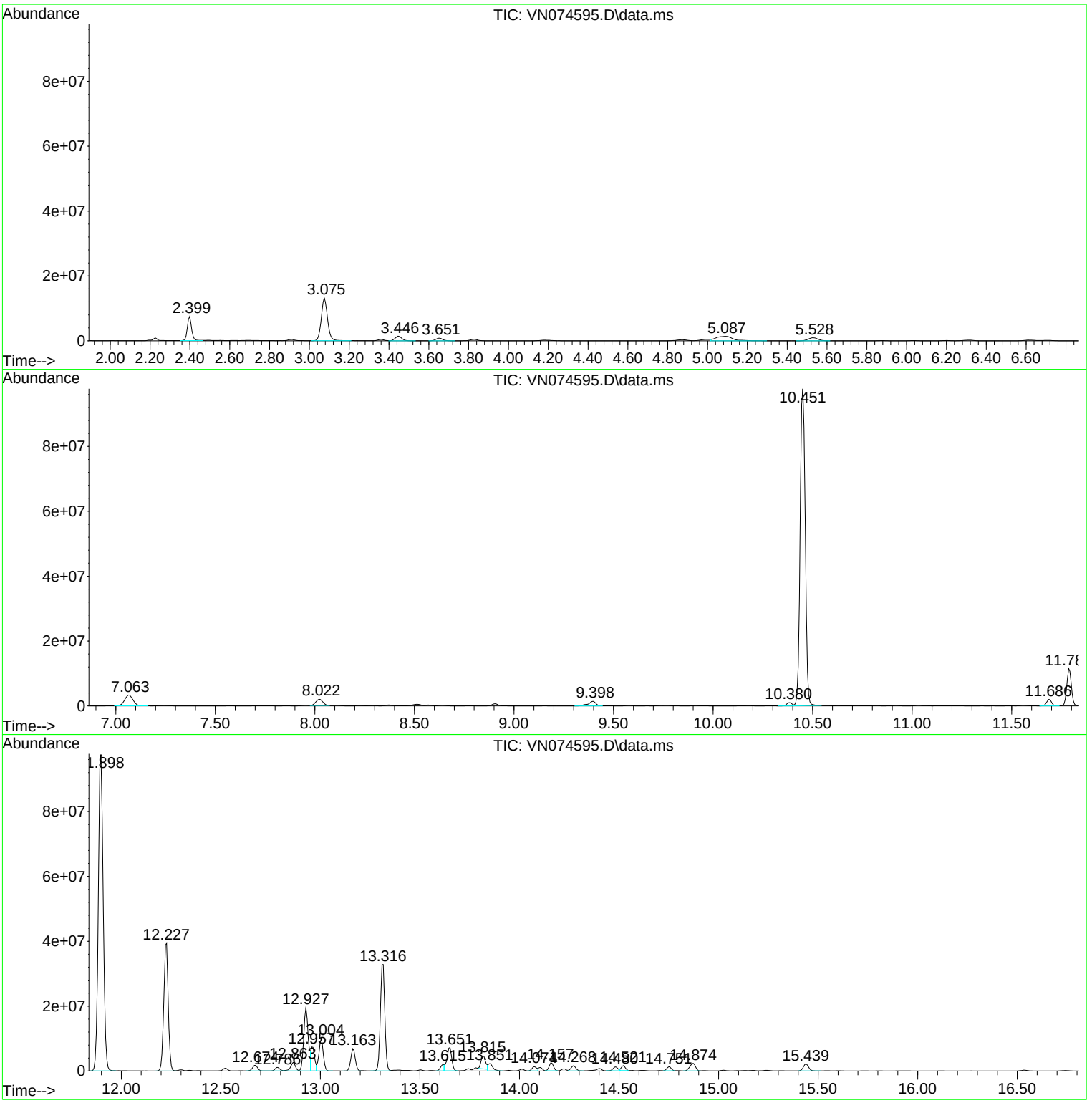
Sum of corrected areas: 673969894

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
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Instrument :
MSVOA_N
ClientSampleId :
MW-7

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

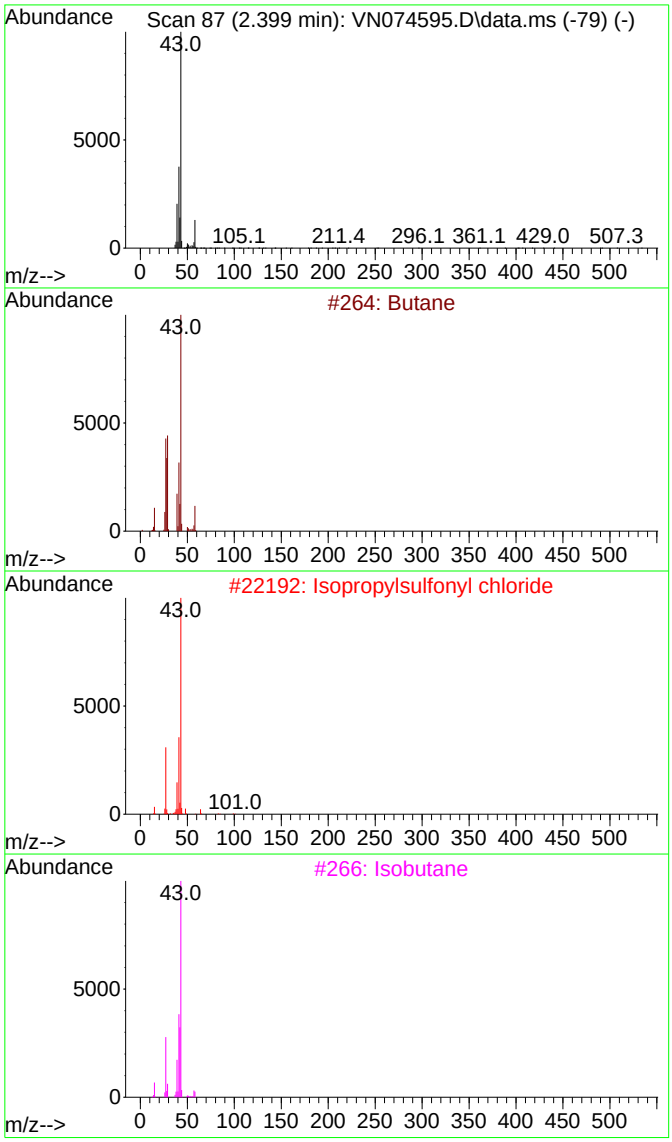
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

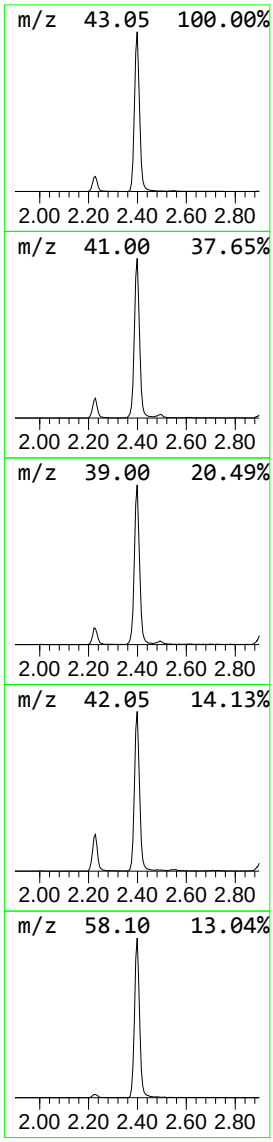
****

Peak Number 1 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	119.16 ug/l	11028500	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	64
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	Diazene, dimethyl-	58	C2H6N2	000503-28-6	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

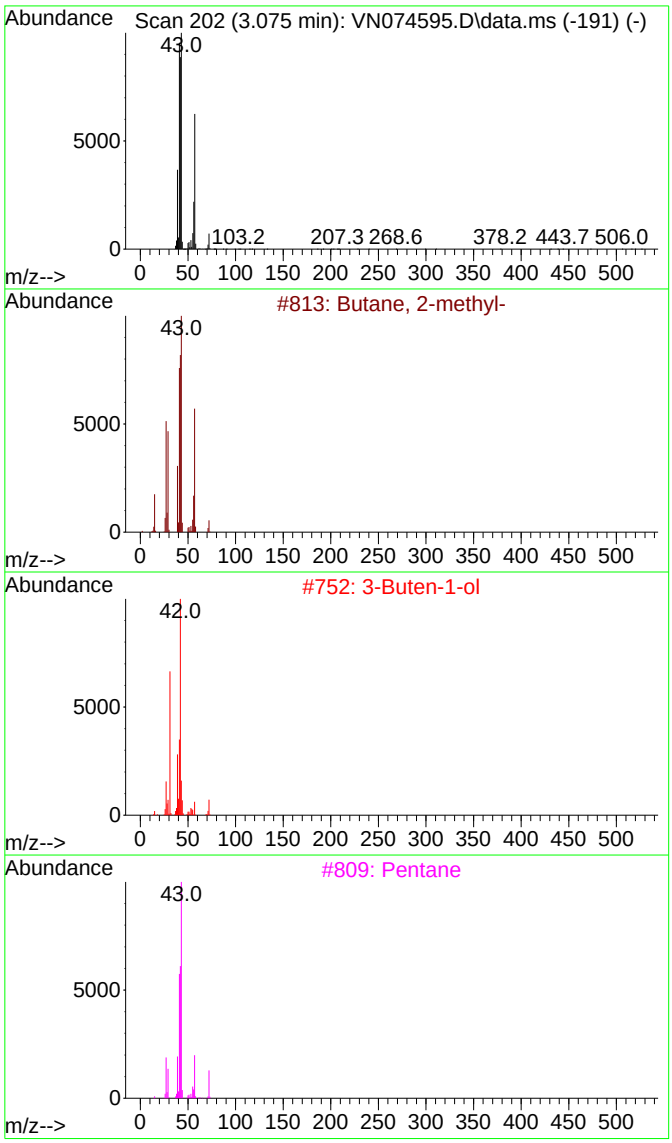
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

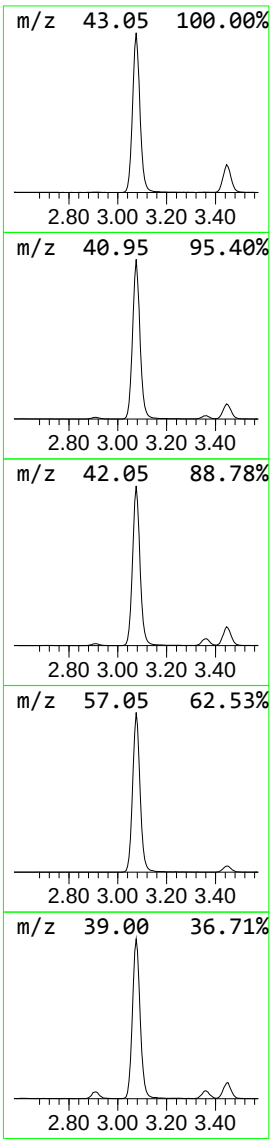
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.075	306.67 ug/l	28383900	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5	1-Butene	56	C4H8	000106-98-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

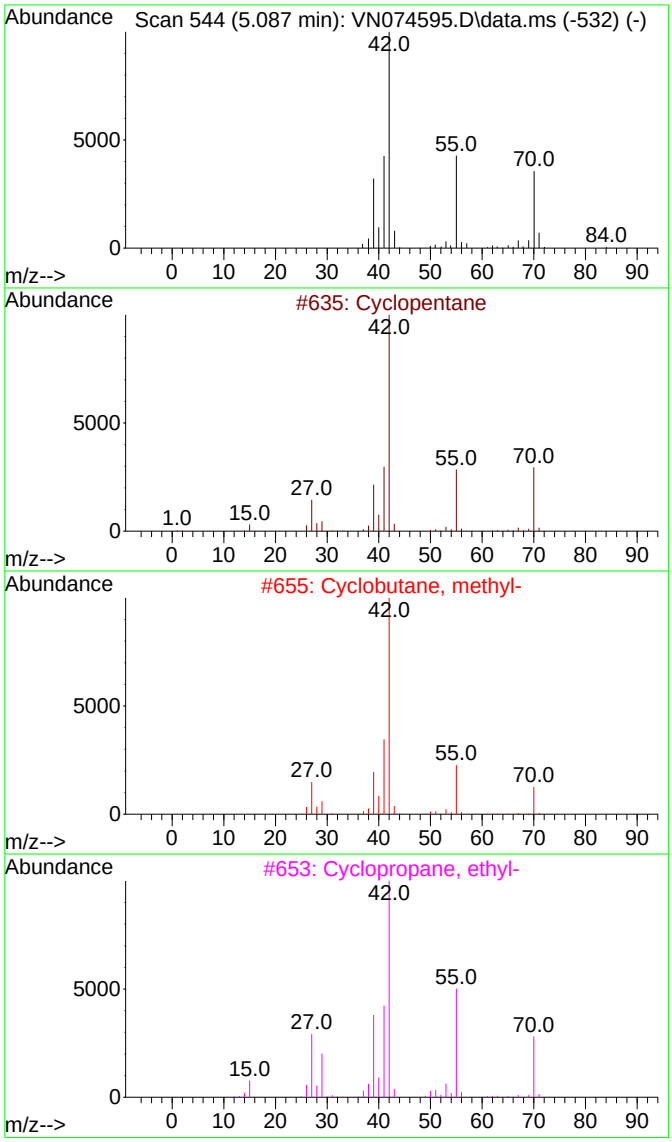
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

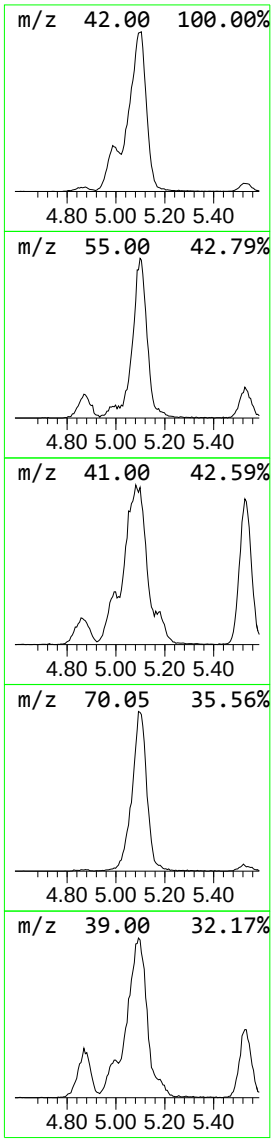
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	86.84 ug/l	8037710	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	78
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	64
4	1-Pentene	70	C5H10	000109-67-1	56
5	Cyclobutanone	70	C4H6O	001191-95-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

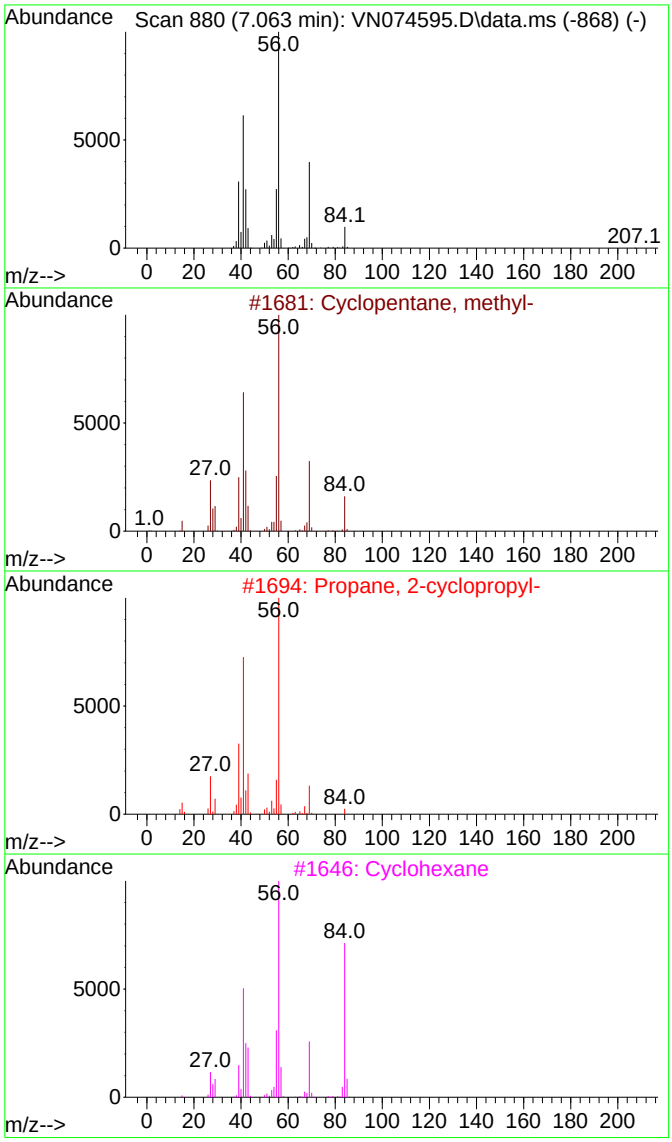
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

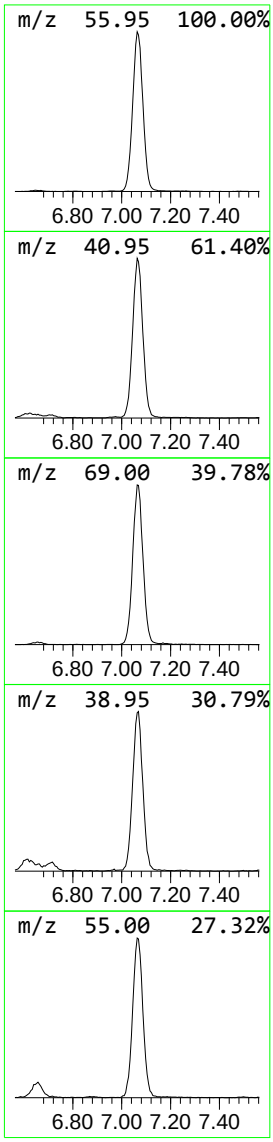
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.063	104.49 ug/l	9670610	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
3	Cyclohexane	84	C6H12	000110-82-7	78
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Cyclobutane, butyl-	112	C8H16	013152-44-8	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

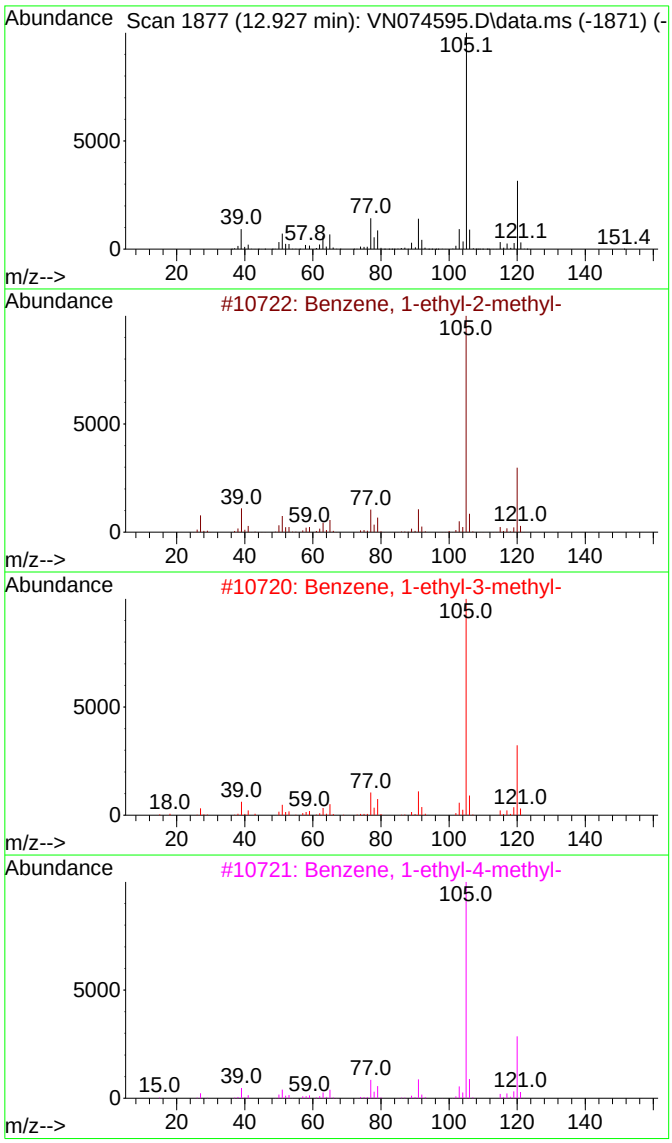
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

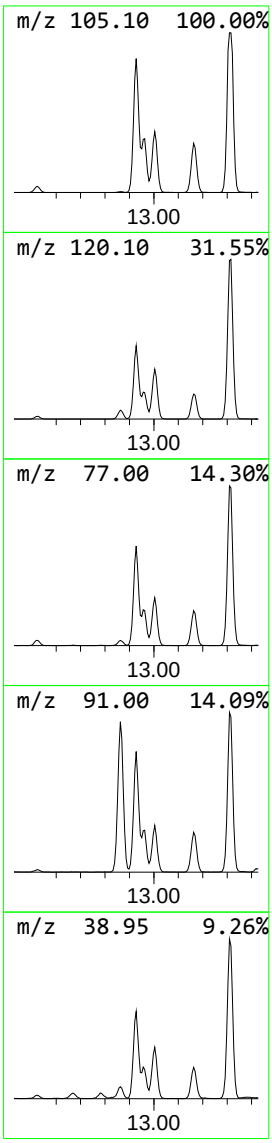
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.927	595.91 ug/l	31699300	1,4-Dichlorobenzene-d4	13.616

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	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

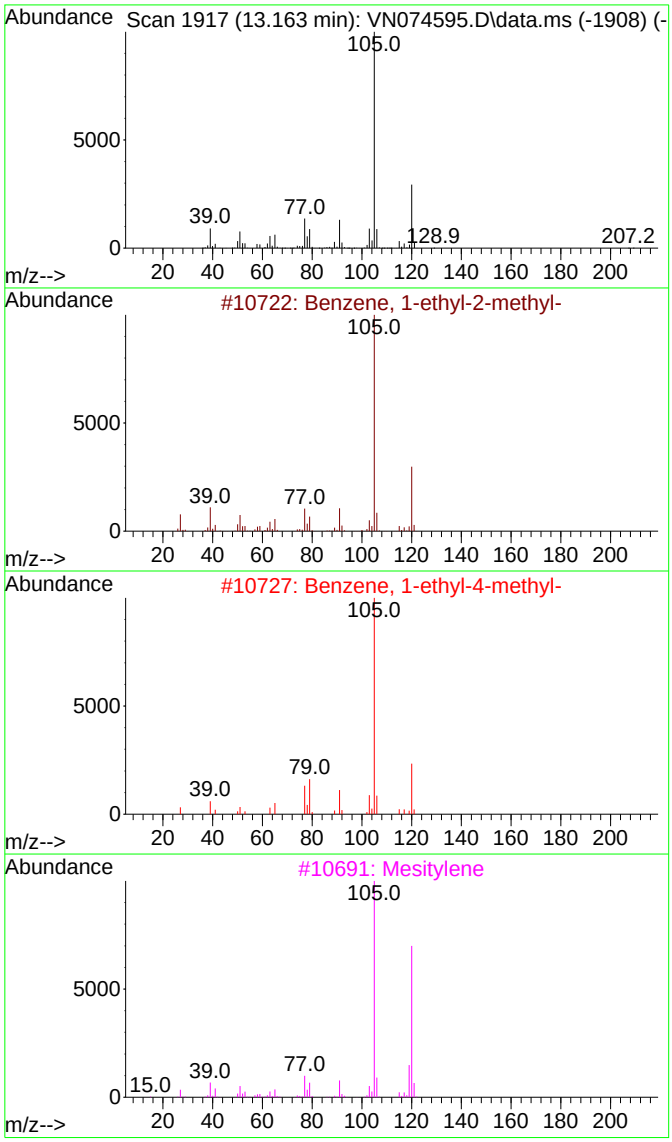
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

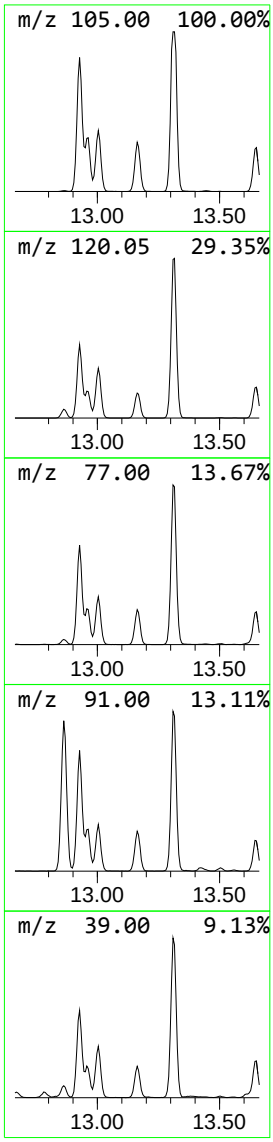
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	205.68 ug/l	10940900	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

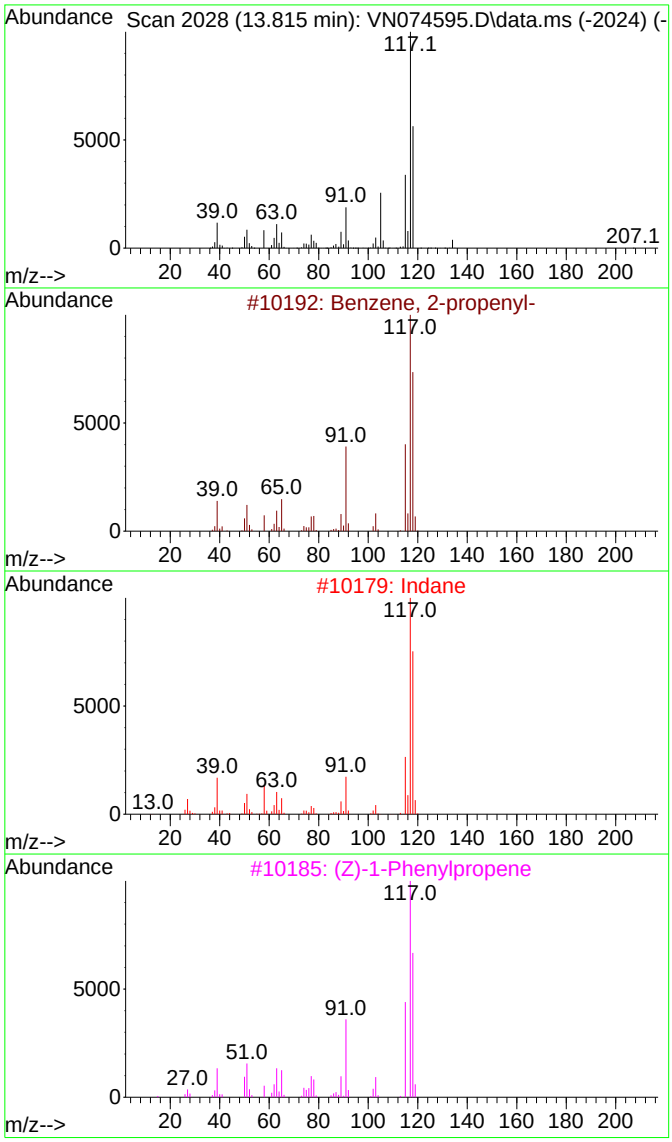
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

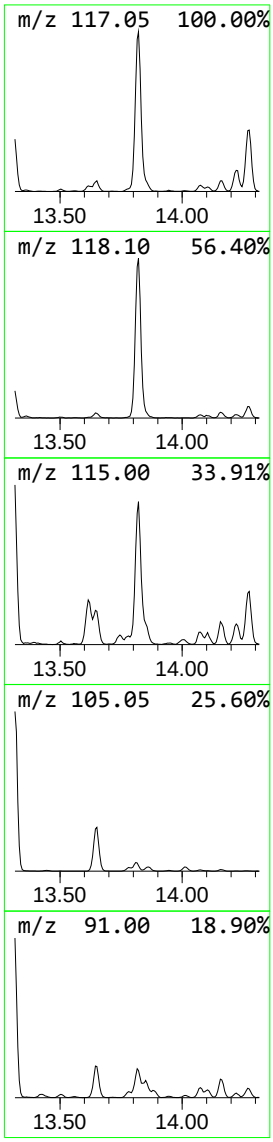
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-propenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	121.32 ug/l	6453620	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
2	Indane	118	C9H10	000496-11-7	70
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	70
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	58





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

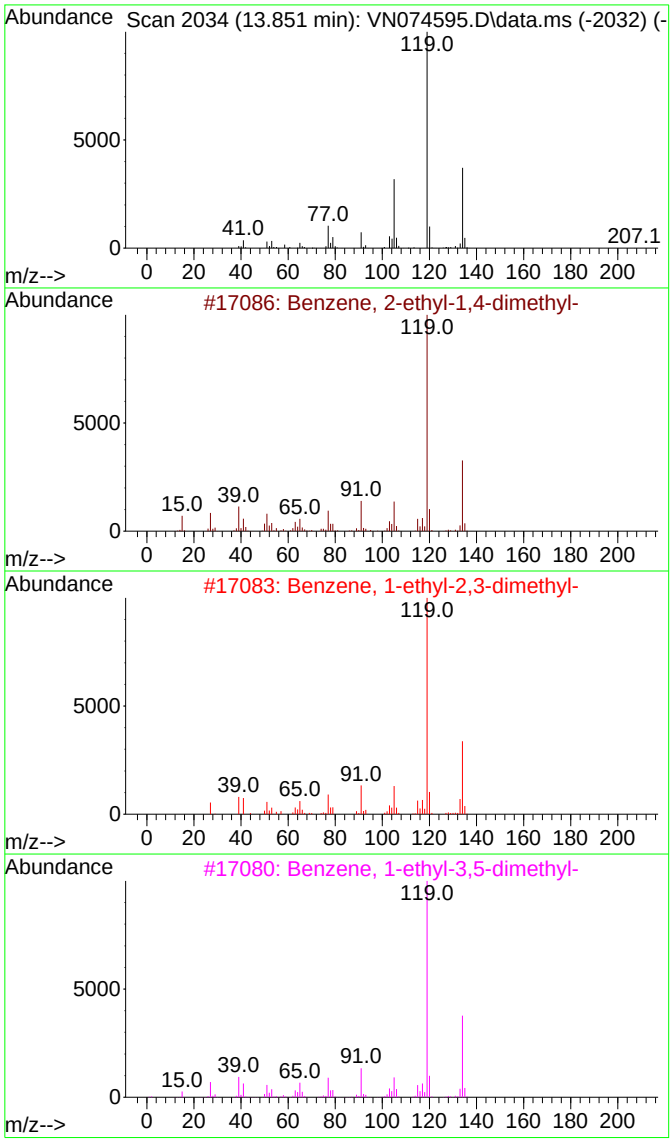
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

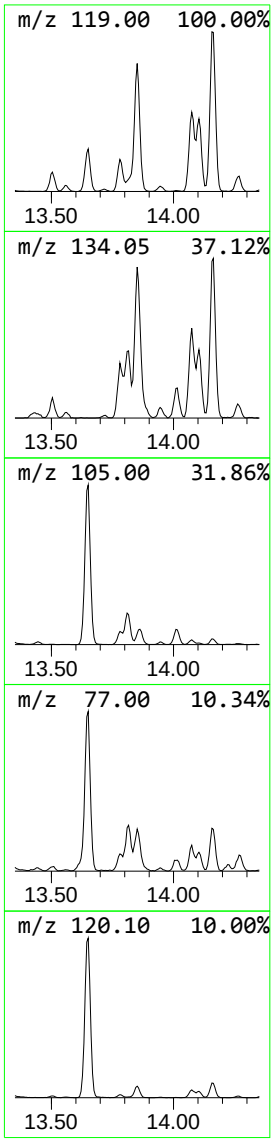
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	64.97 ug/l	3456030	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	86
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	86
3	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	80
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	80
5	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

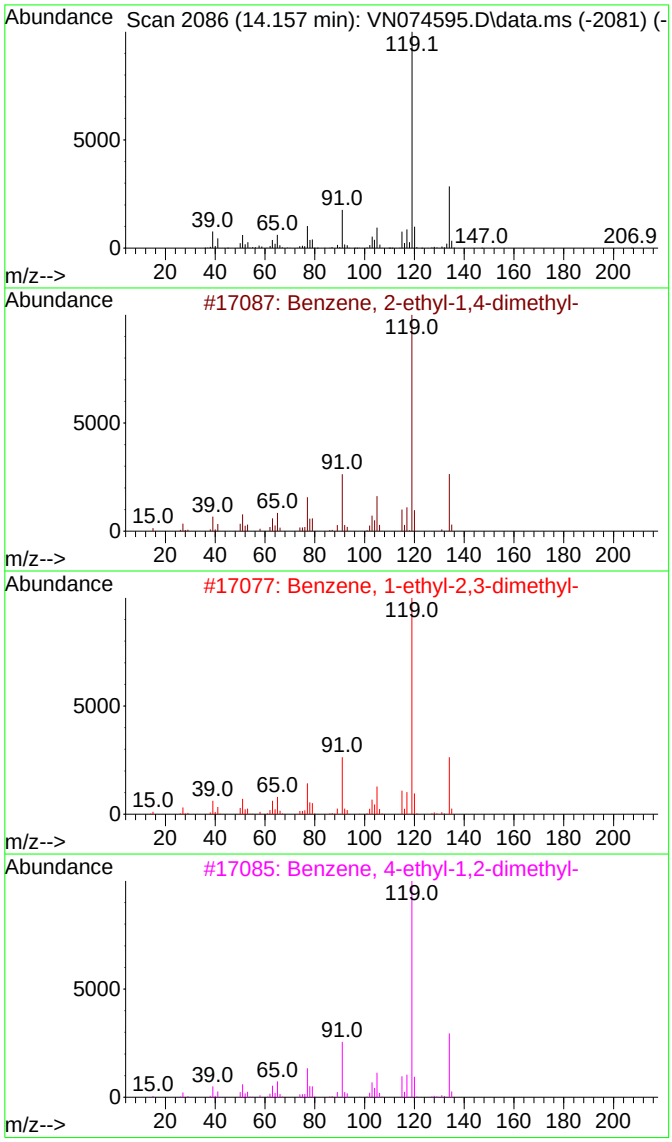
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

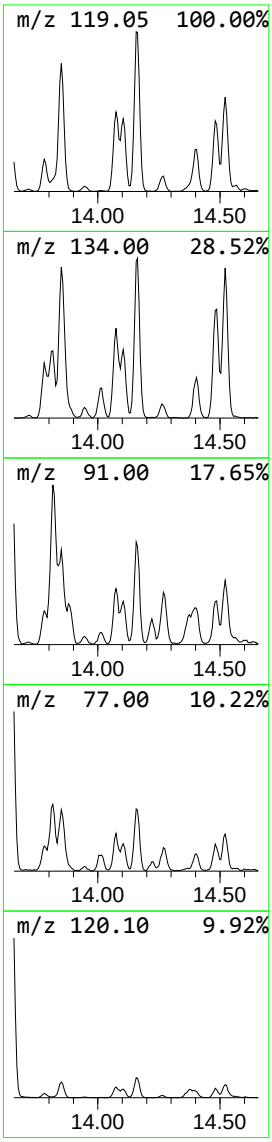
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	70.64 ug/l	3757880	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
4	o-Cymene	134	C10H14	000527-84-4	95
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

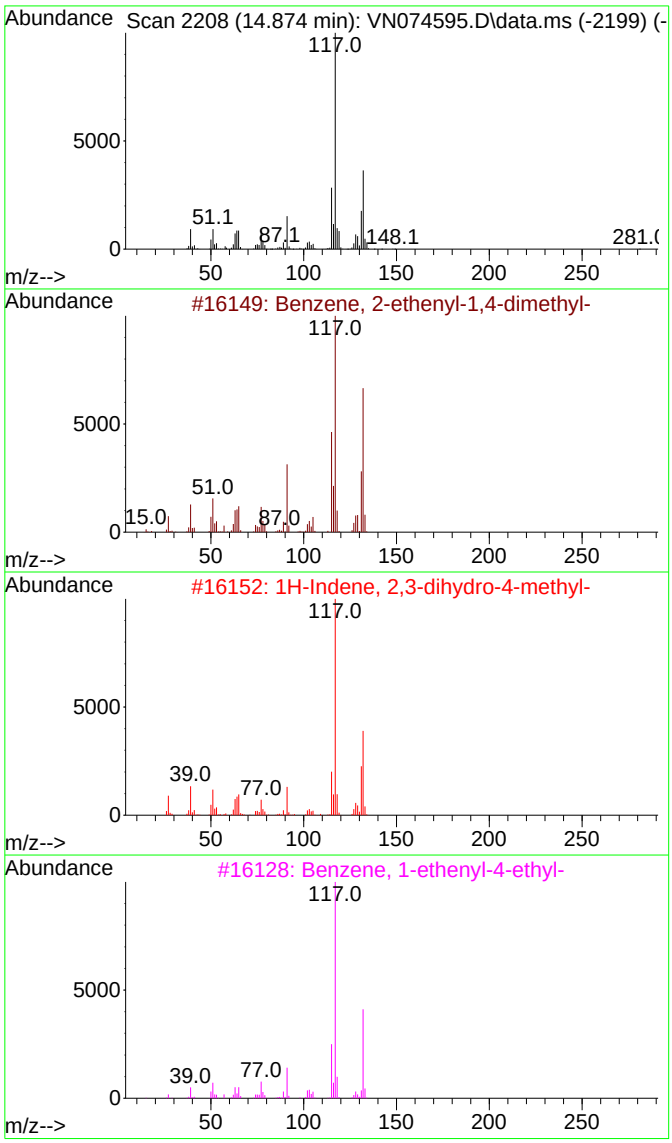
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

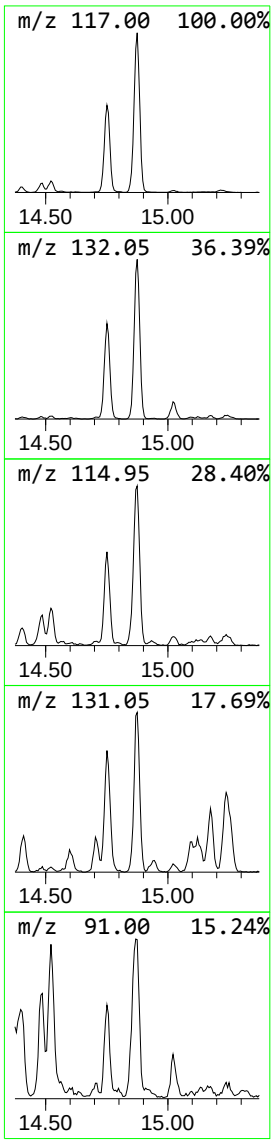
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.874	87.83 ug/l	4672350	1,4-Dichlorobenzene-d4	13.616

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
Data File : VN074595.D
Acq On : 19 Sep 2022 18:55
Operator : JC\MD
Sample : N4566-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

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	2.399	119.2	ug/l	11028500	1	8.016	4627700	50.0
Butane, 2-methyl-	3.075	306.7	ug/l	28383900	1	8.016	4627700	50.0
Cyclopentane	5.087	86.8	ug/l	8037710	1	8.016	4627700	50.0
Cyclopentane, m...	7.063	104.5	ug/l	9670610	1	8.016	4627700	50.0
Benzene, 1-ethy...	12.927	595.9	ug/l	31699300	4	13.616	2659740	50.0
Benzene, 1-ethy...	13.163	205.7	ug/l	10940900	4	13.616	2659740	50.0
Benzene, 2-prop...	13.816	121.3	ug/l	6453620	4	13.616	2659740	50.0
Benzene, 2-ethy...	13.851	65.0	ug/l	3456030	4	13.616	2659740	50.0
Benzene, 1-ethy...	14.157	70.6	ug/l	3757880	4	13.616	2659740	50.0
Benzene, 2-ethe...	14.874	87.8	ug/l	4672350	4	13.616	2659740	50.0