LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

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\82N033022W.M
Title : SW846 8260

Signal : TIC: VN071959.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.434	69	76	86	rVB	446336	722565	1.50%	0.321%
2	3.134	185	195	213	rBV	2268267	5191470	10.75%	2.309%
3	3.516	249	260	279	rBV2	934145	2515982	5.21%	1.119%
4	3.992	332	341	359	rVB	388814	1059445	2.19%	0.471%
5	4.963	490	506	515	rBV3	137047	490933	1.02%	0.218%
6	5.081	515	526	530	rVV2	364262	1187027	2.46%	0.528%
7	5.181	531	543	568	rVB5	738898	4576871	9.48%	2.035%
8	5.616	601	617	635	rBV	525482	1814291	3.76%	0.807%
9	6.122	690	703	714	rBV2	187909	576131	1.19%	0.256%
10	6.469	752	762	775	rVB	306309	950566	1.97%	0.423%
11	6.604	775	785	793	rBV2	227317	695116	1.44%	0.309%
12	6.898	826	835	850	rVB	265037	779990	1.62%	0.347%
13	7.145	866	877	887	rBV	1830789	5306184	10.99%	2.360%
14	7.845	987	996	1005	rVB	472310	1158853	2.40%	0.515%
15	8.016	1015	1025	1030	rBV	401477	1012700	2.10%	0.450%
16	8.086	1030	1037	1046	rVV2	1467533	3896693	8.07%	1.733%
17	8.175	1046	1052	1064	rVB2	415031	1076872	2.23%	0.479%
18	8.457	1088	1100	1112	rBV	7577529	17843741	36.97%	7.935%
19	8.586	1114	1122	1128	rBV4	299820	878242	1.82%	0.391%
20	8.963	1177	1186	1199	rBV2	1420146	3325778	6.89%	1.479%
21	9.457	1254	1270	1277	rBV2	545446	1653964	3.43%	0.736%
22	9.969	1350	1357	1361	rBV2	345933	671432	1.39%	0.299%
23	10.321	1409	1417	1423	rBV	298368	582308	1.21%	0.259%
24	10.439	1429	1437	1442	rBV	1870792	3499366	7.25%	1.556%
25	10.504	1442	1448	1461	rVV	2888787	5605639	11.61%	2.493%
26	11.739	1650	1658	1666	rBV	1845048	3316215	6.87%	1.475%
27	11.839	1668	1675	1685	rVV	12233414	20510831	42.49%	9.121%
28	11.951	1685	1694	1706	rVB	25097836	48270489	100.00%	21.466%
29	12.274	1738	1749	1760	rBV	4097018	6884477	14.26%	3.062%
30	12.574	1793	1800	1810	rVB	1251077	1998821	4.14%	0.889%
31	12.727	1819	1826	1836	rVB	1457399	2483071	5.14%	1.104%
32	12.915	1848	1858	1863	rBV	2240353	3543925	7.34%	1.576%
33	12.980	1863	1869	1871	rVV	1908871	3140487	6.51%	1.397%
34	13.010	1871	1874	1878	rVV	2983102	4648237	9.63%	2.067%
35	13.057	1878	1882	1895	rVB	2285503	3567359	7.39%	1.586%
36	13.215	1901	1909	1919	rBV	3555510	5665106	11.74%	2.519%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

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\82N033022W.M
Title : SW846 8260

37	13.362	1923	1934	1949	rVV	10950611	17494457	36.24%	7.780%
38	13.698	1987	1991	2001	rVB	4990535	8704407	18.03%	3.871%
39	13.833	2008	2014	2015	rBV	546759	697958	1.45%	0.310%
40	13.874	2015	2021	2037	rVB	5889417	11376957	23.57%	5.059%
41	14.062	2047	2053	2058	rBV2	411008	686769	1.42%	0.305%
42	14.127	2058	2064	2067	rBV	489144	850572	1.76%	0.378%
43	14.209	2073	2078	2084	rVV	1152152	1755154	3.64%	0.781%
44	14.274	2084	2089	2092	rVV	317589	487809	1.01%	0.217%
45	14.321	2092	2097	2106	rVB2	1288693	2152439	4.46%	0.957%
46	14.533	2126	2133	2137	rBV	843127	1417962	2.94%	0.631%
47	14.574	2137	2140	2145	rVB	674805	938874	1.95%	0.418%
48	14.804	2174	2179	2185	rBV	797549	1256833	2.60%	0.559%
49	14.927	2191	2200	2206	rBV2	1407449	2889675	5.99%	1.285%
50	15.498	2283	2297	2309	rBV	1577868	3056107	6.33%	1.359%

Sum of corrected areas: 224867150

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Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
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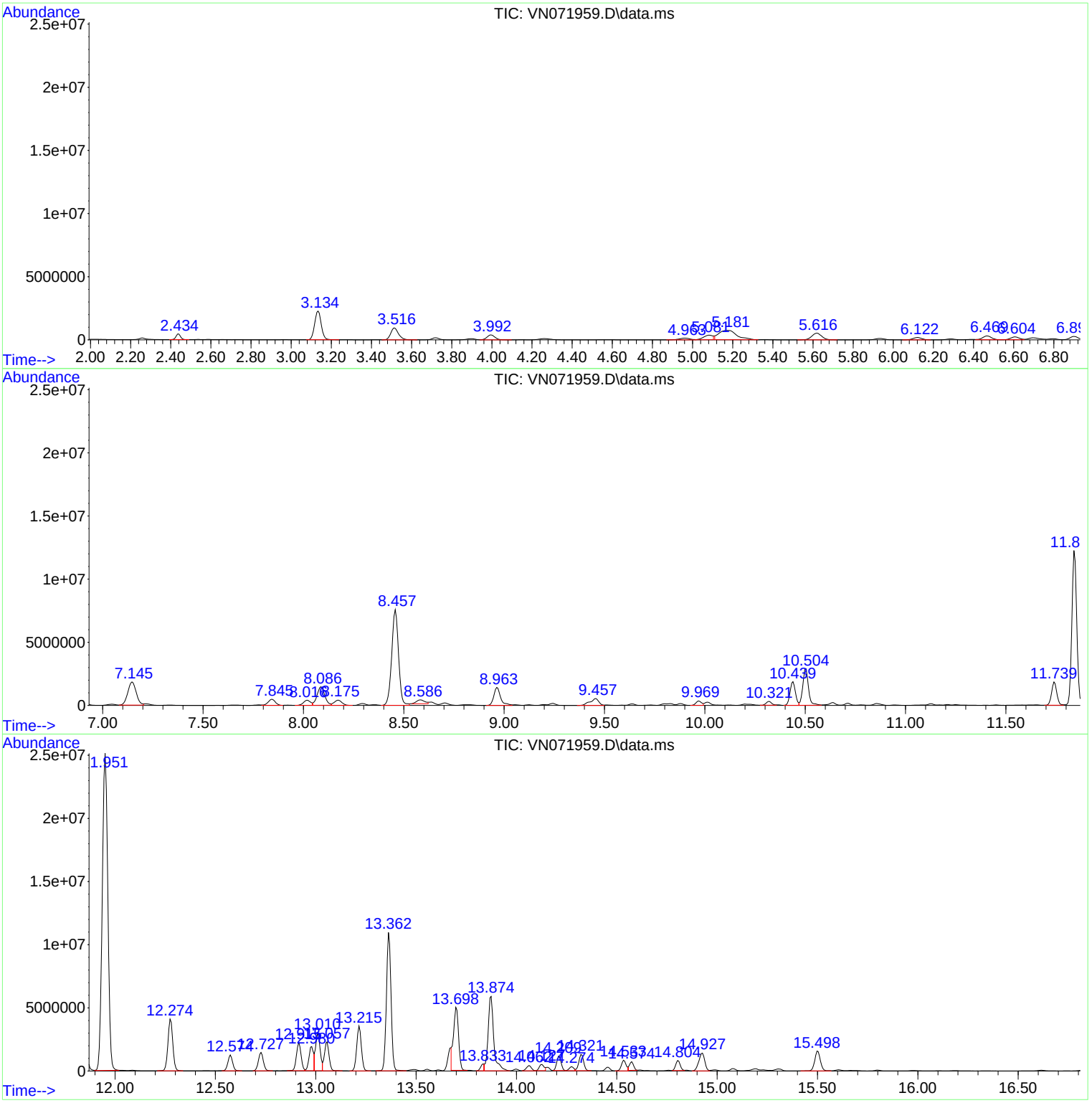
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

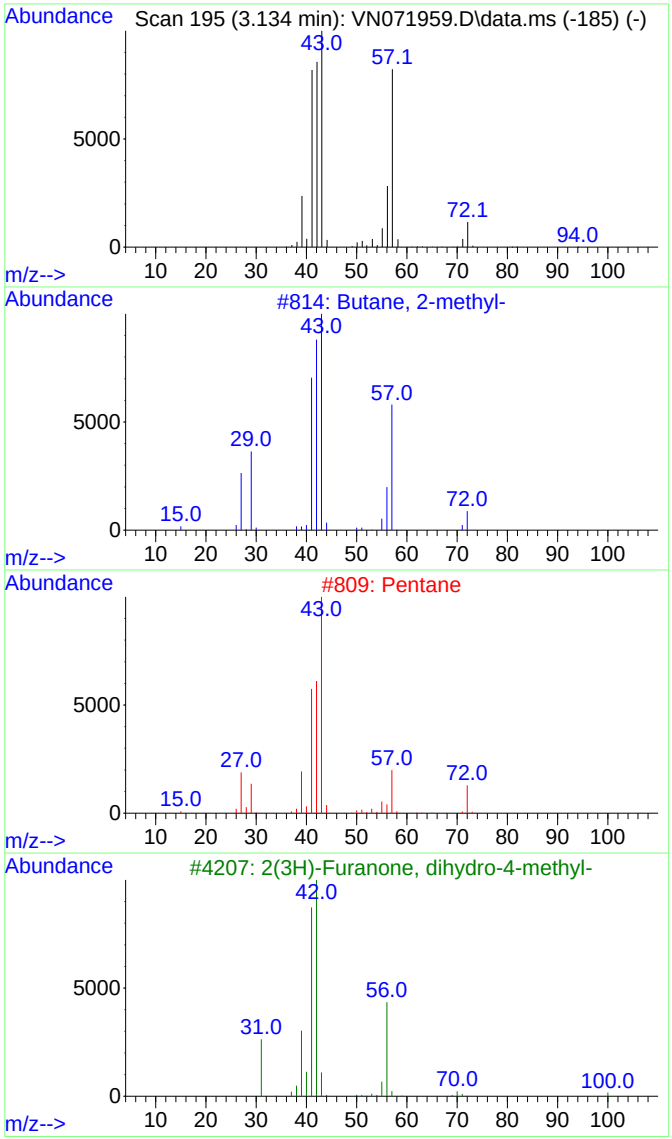
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

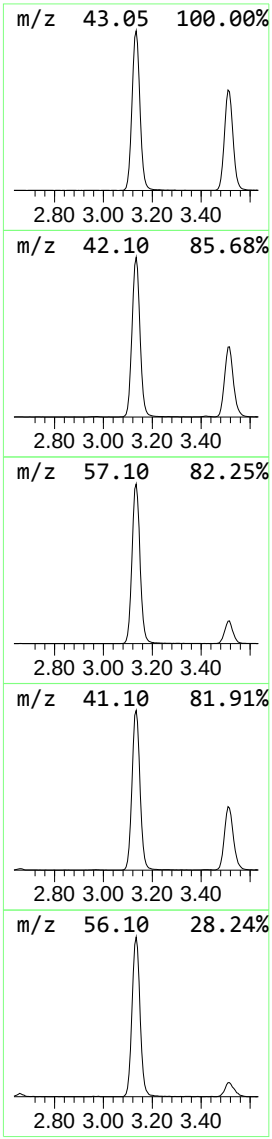
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	66.61 ug/l	5191470	Pentafluorobenzene	8.080

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	46
3	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	36
4	3-Buten-1-ol	72	C4H8O	000627-27-0	25
5	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

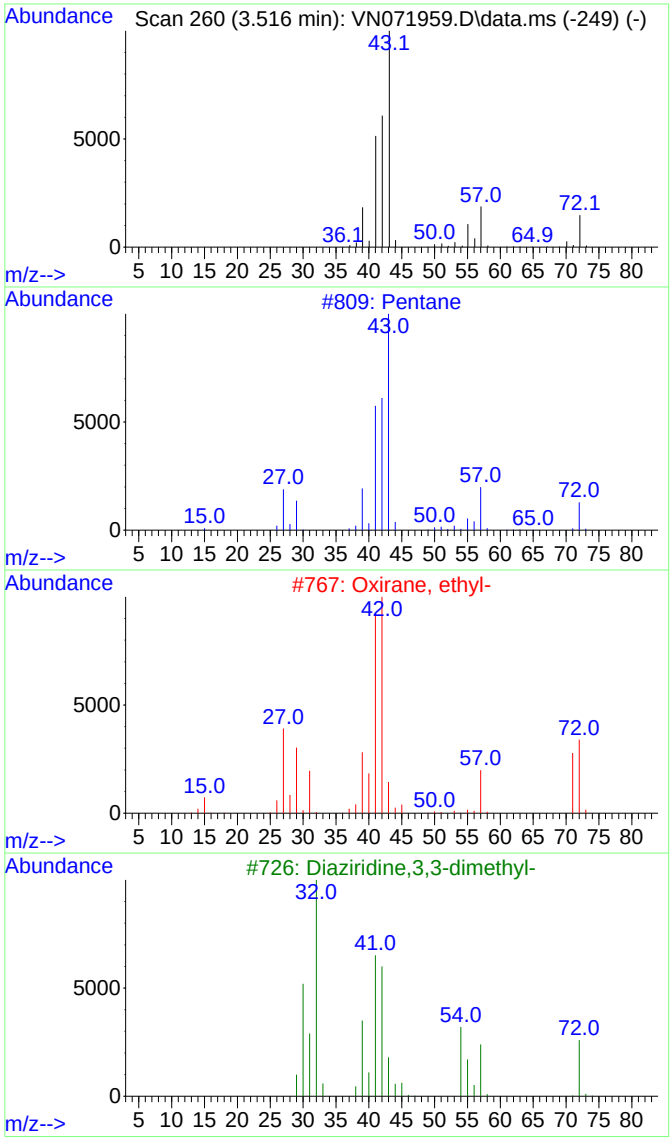
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

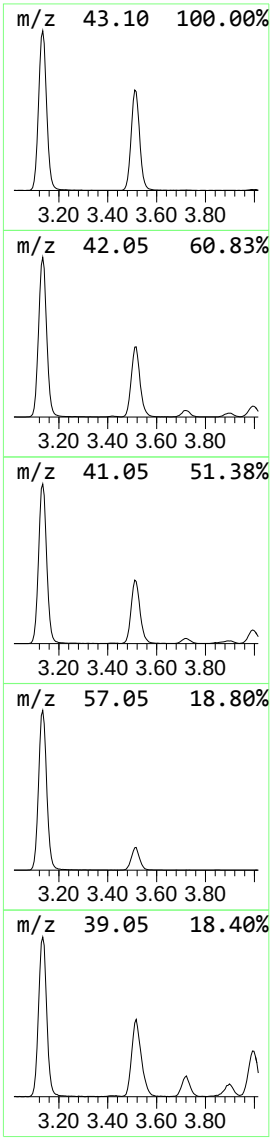
****

Peak Number 2 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.516	32.28 ug/l	2515980	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	42
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	Tetrahydrofuran	72	C4H8O	000109-99-9	9
5	2-Butanone	72	C4H8O	000078-93-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

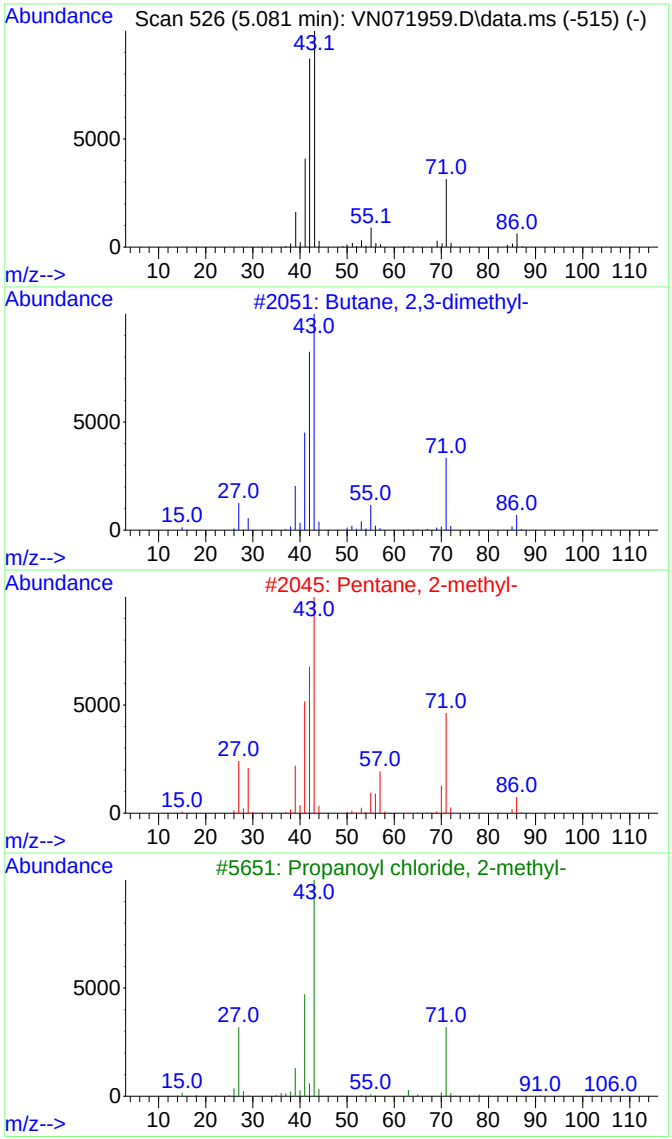
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

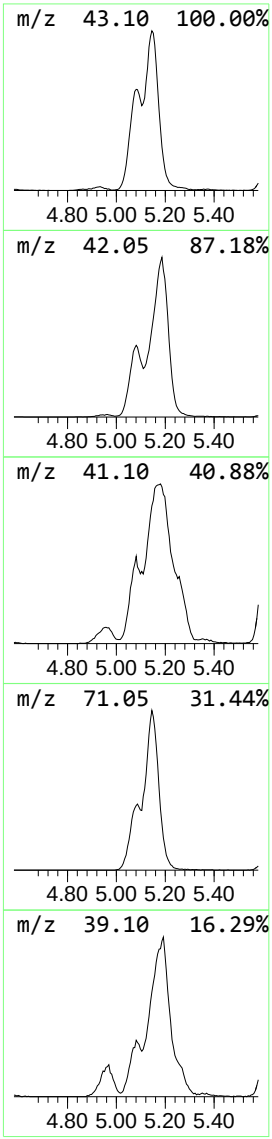
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	15.23 ug/l	1187030	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	58
3	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	27
4	Pyrrolidine	71	C4H9N	000123-75-1	22
5	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

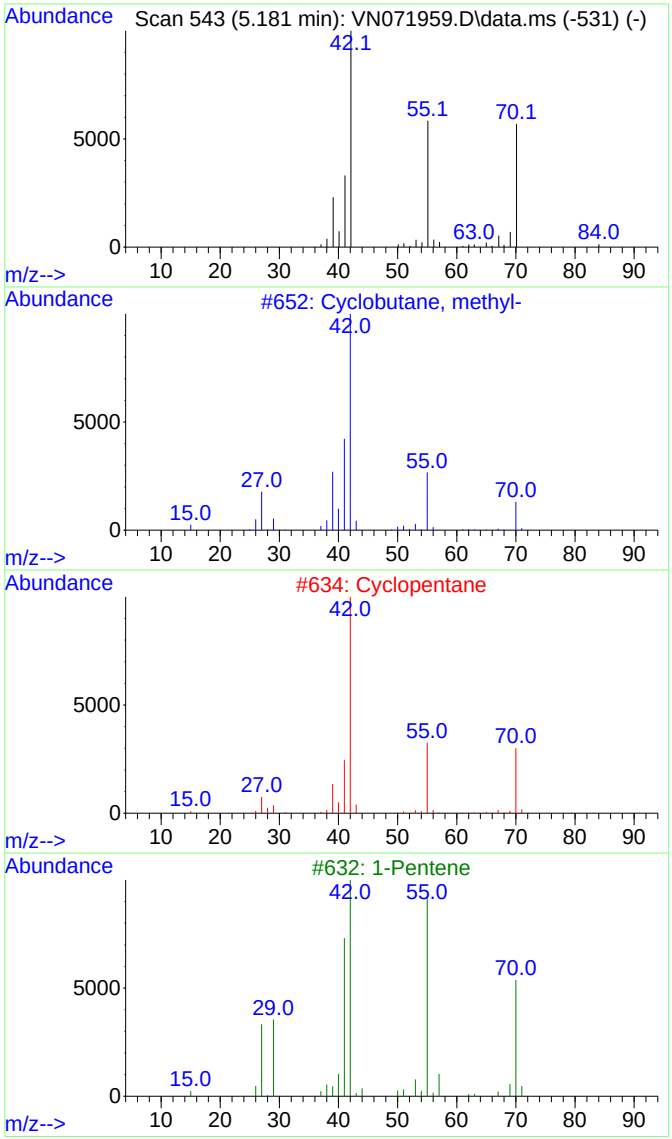
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

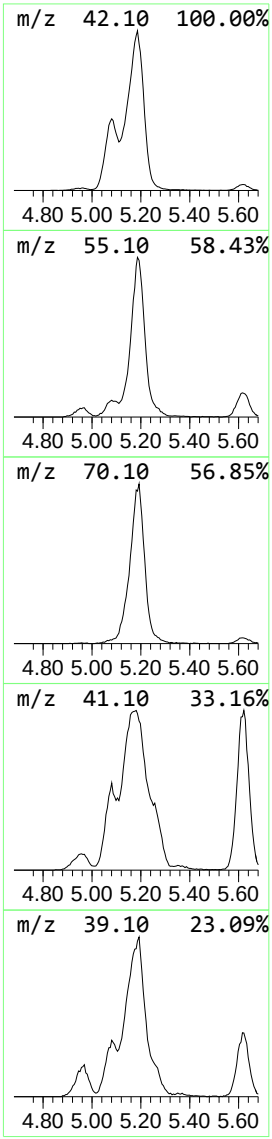
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclobutane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	58.73 ug/l	4576870	Pentafluorobenzene	8.080

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	56
4	1-Pentanol	88	C5H12O	000071-41-0	40
5	2-Pentene, (E)-	70	C5H10	000646-04-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

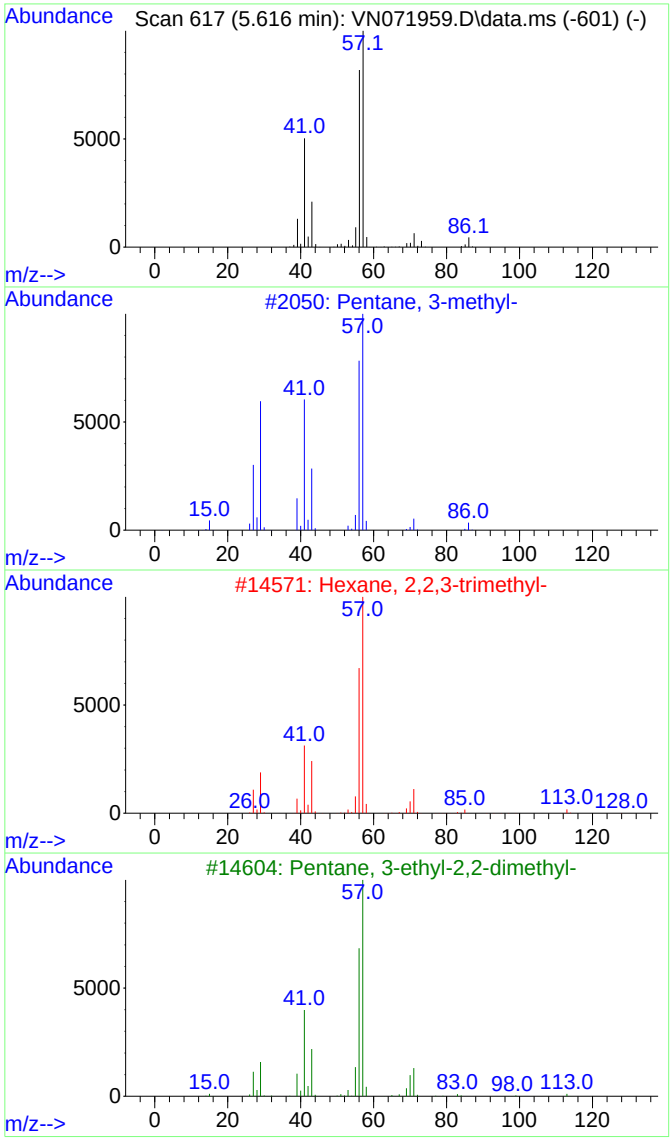
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

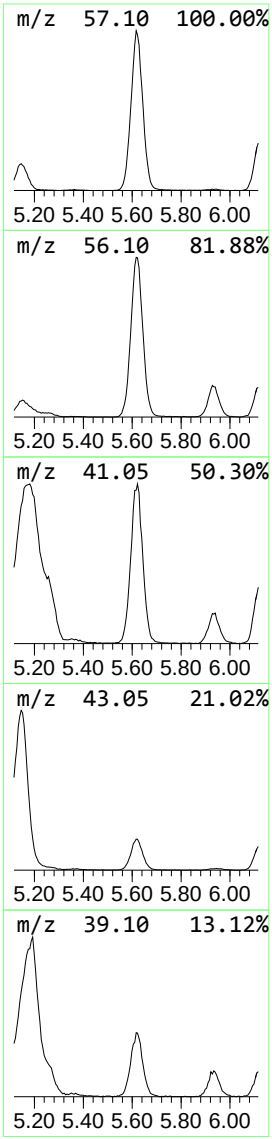
****

Peak Number 5 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.616	23.28 ug/l	1814290	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	78
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	72
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

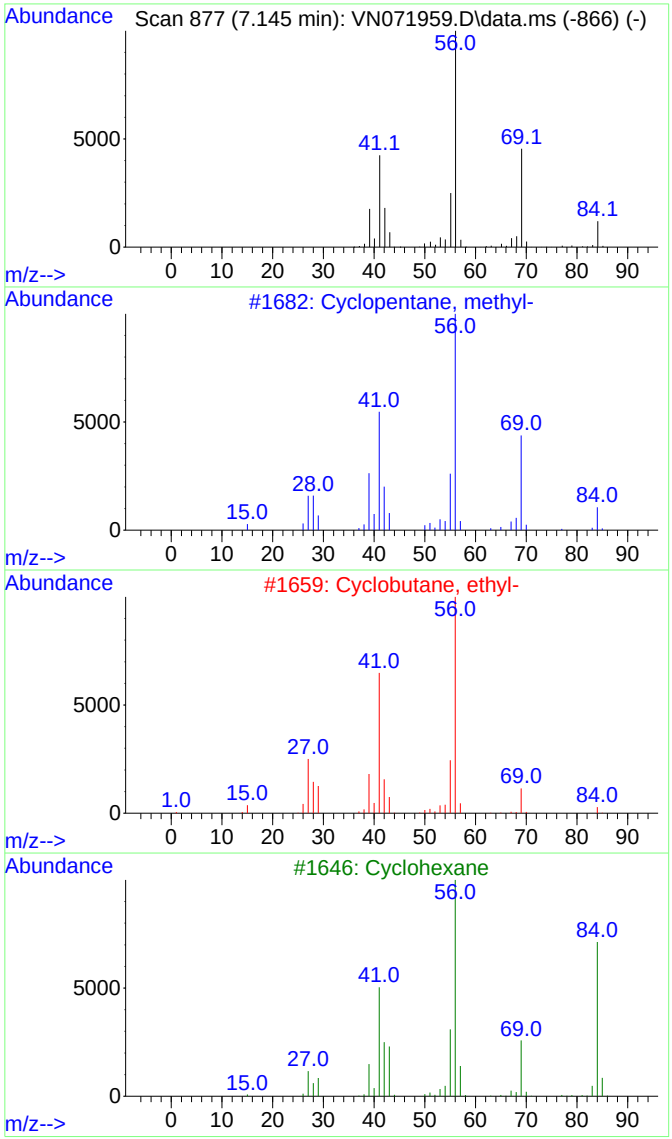
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

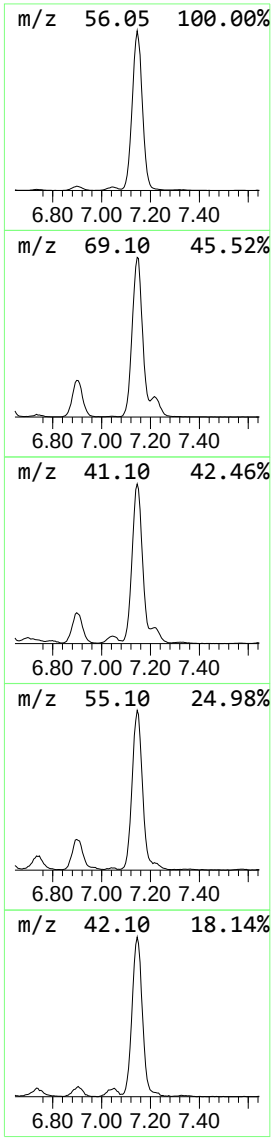
****

Peak Number 6 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	68.09 ug/l	5306180	Pentafluorobenzene	8.080

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	72
3	Cyclohexane	84	C6H12	000110-82-7	64
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	46





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Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

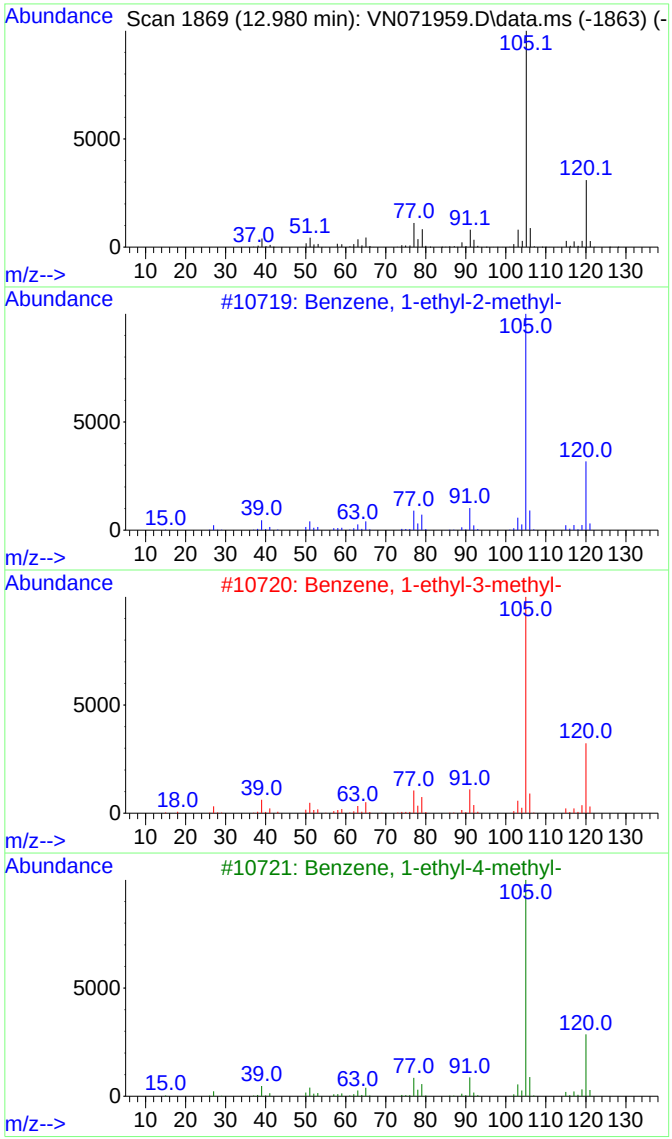
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

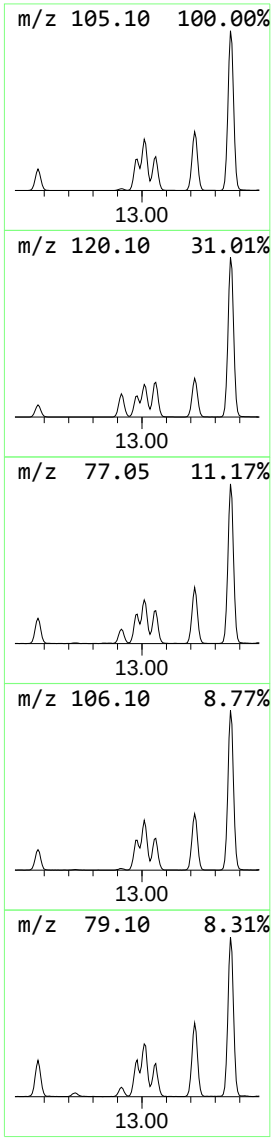
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	18.04 ug/l	3140490	1,4-Dichlorobenzene-d4	13.668

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	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

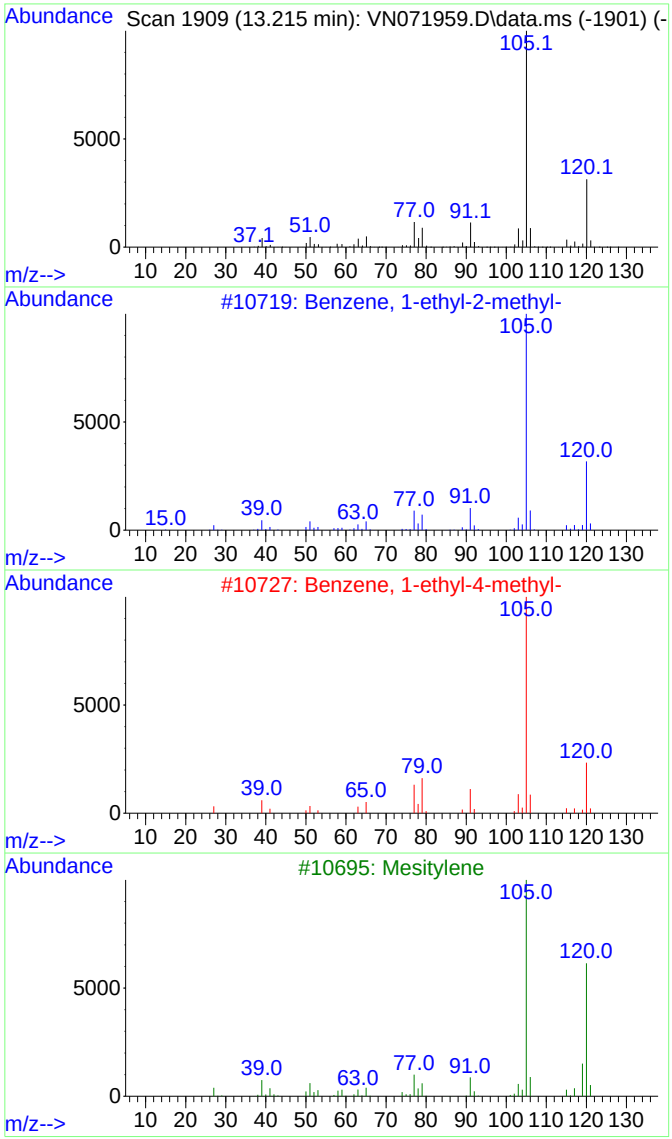
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

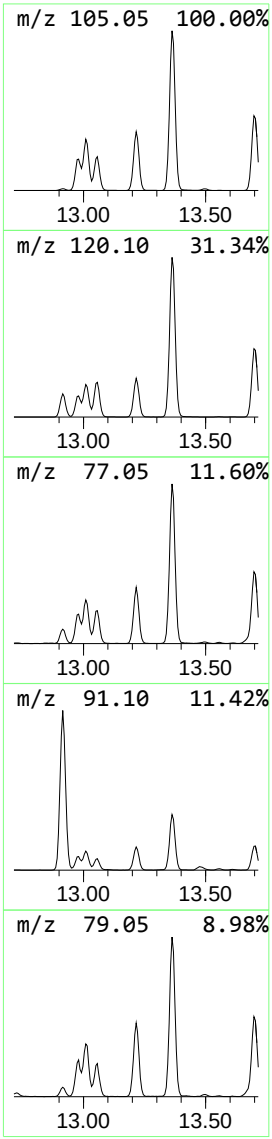
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.215	32.54 ug/l	5665110	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	90
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90





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Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

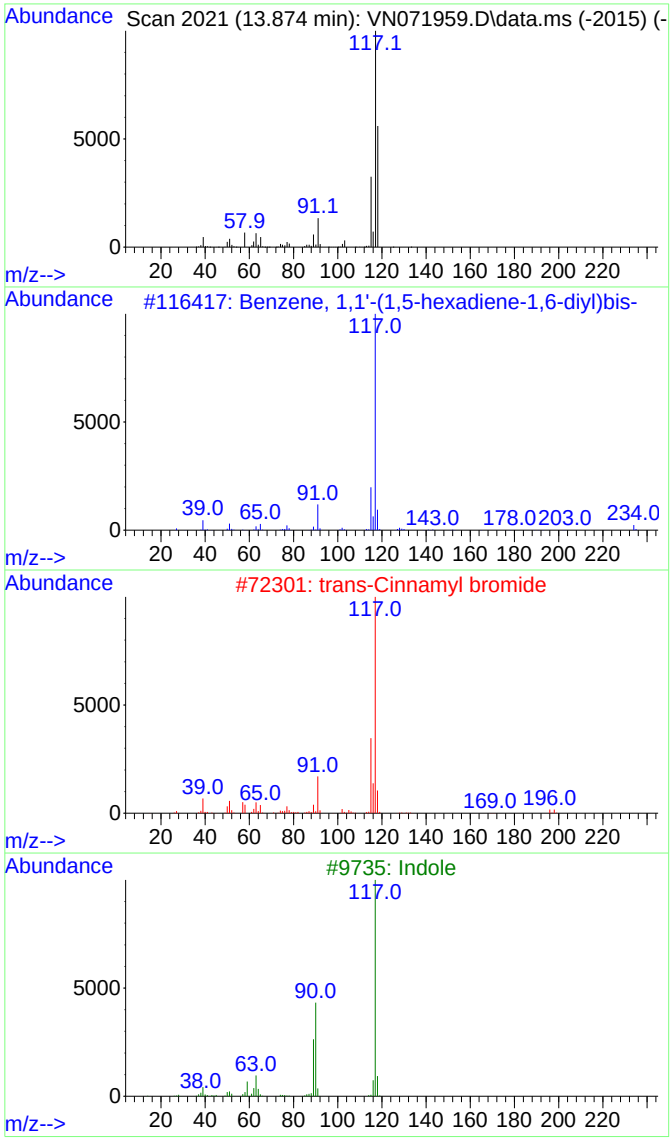
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

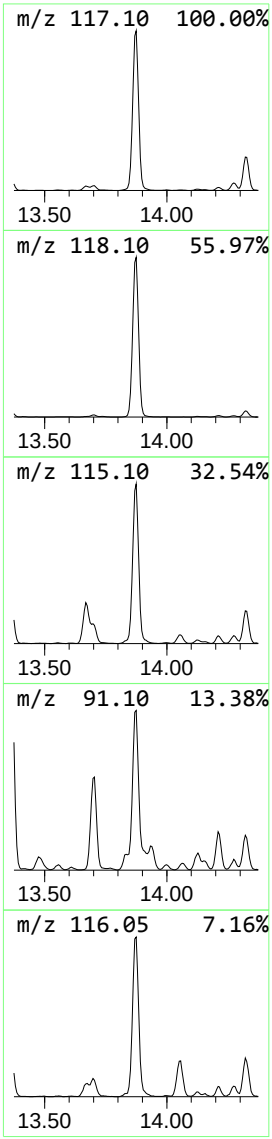
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	65.35 ug/l	11377000	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
3	Indole	117	C8H7N	000120-72-9	46
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
5	m-Aminophenylacetylene	117	C8H7N	054060-30-9	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

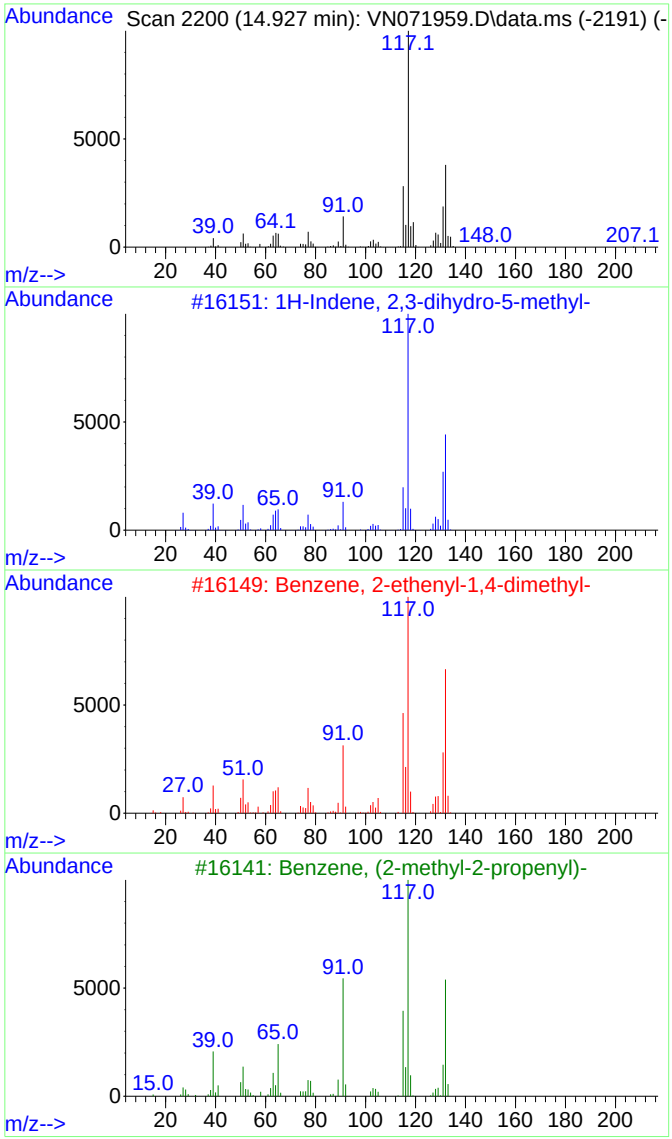
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

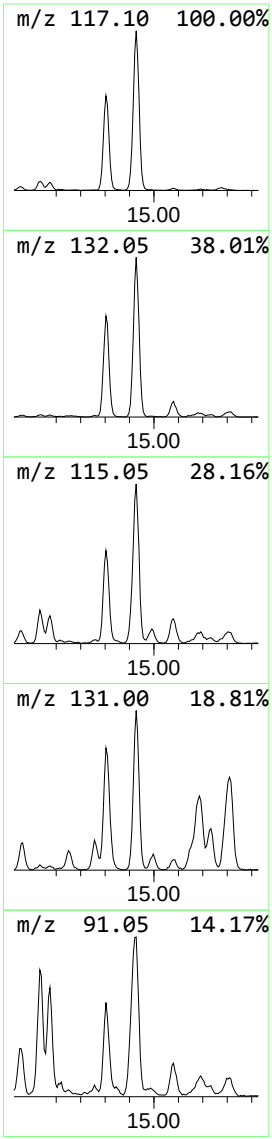
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	16.60 ug/l	2889680	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	90
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041222\
Data File : VN071959.D
Acq On : 12 Apr 2022 17:25
Operator : JC\MD
Sample : N2308-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
INF0422

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.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-methyl-	3.134	66.6	ug/l	5191470	1	8.080	3896690	50.0
Pentane	3.516	32.3	ug/l	2515980	1	8.080	3896690	50.0
Butane, 2,3-dim...	5.081	15.2	ug/l	1187030	1	8.080	3896690	50.0
Cyclobutane, me...	5.181	58.7	ug/l	4576870	1	8.080	3896690	50.0
Pentane, 3-methyl-	5.616	23.3	ug/l	1814290	1	8.080	3896690	50.0
Cyclopentane, m...	7.145	68.1	ug/l	5306180	1	8.080	3896690	50.0
Benzene, 1-ethy...	12.980	18.0	ug/l	3140490	4	13.668	8704410	50.0
Benzene, 1-ethy...	13.215	32.5	ug/l	5665110	4	13.668	8704410	50.0
Benzene, 1,1'-(...	13.874	65.3	ug/l	11377000	4	13.668	8704410	50.0
1H-Indene, 2,3-...	14.927	16.6	ug/l	2889680	4	13.668	8704410	50.0