LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

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\82N051022W.M
Title : SW846 8260

Signal : TIC: VN072440.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	37	43	53	rBV3	11835	33749	2.54%	0.358%
2	2.440	73	77	83	rVB4	10150	15612	1.18%	0.166%
3	2.758	123	131	135	rVB3	7269	14428	1.09%	0.153%
4	3.128	186	194	207	rVB	128533	294217	22.18%	3.121%
5	4.252	374	385	403	rBV5	15490	59359	4.48%	0.630%
6	5.081	513	526	534	rBV2	43479	166727	12.57%	1.769%
7	5.622	605	618	631	rBV2	78764	270215	20.37%	2.867%
8	7.051	851	861	868	rBV3	12840	37231	2.81%	0.395%
9	7.146	868	877	887	rVB5	11206	32845	2.48%	0.348%
10	7.828	984	993	1006	rVB5	8982	29758	2.24%	0.316%
11	8.022	1016	1026	1031	rBV	161209	403672	30.44%	4.283%
12	8.087	1031	1037	1045	rVV	280520	642902	48.48%	6.821%
13	8.175	1045	1052	1061	rVB2	43205	108058	8.15%	1.146%
14	8.434	1088	1096	1108	rVV	178747	433576	32.69%	4.600%
15	8.569	1109	1119	1122	rVV6	29605	70425	5.31%	0.747%
16	8.628	1123	1129	1137	rVV6	35261	114243	8.61%	1.212%
17	8.710	1137	1143	1151	rVB7	10039	24010	1.81%	0.255%
18	8.963	1178	1186	1197	rBV	444289	910606	68.66%	9.661%
19	9.422	1257	1264	1266	rBV6	8702	15208	1.15%	0.161%
20	9.881	1336	1342	1350	rVB4	15479	30667	2.31%	0.325%
21	10.010	1359	1364	1373	rVB3	25689	54131	4.08%	0.574%
22	10.192	1391	1395	1398	rBV5	8233	13716	1.03%	0.146%
23	10.222	1398	1400	1411	rVB4	6022	14113	1.06%	0.150%
24	10.440	1428	1437	1449	rBV	700485	1292619	97.46%	13.714%
25	10.545	1451	1455	1460	rVB7	7419	13376	1.01%	0.142%
26	10.857	1502	1508	1517	rVB5	10253	25177	1.90%	0.267%
27	11.739	1650	1658	1672	rBV	757147	1326243	100.00%	14.070%
28	12.575	1793	1800	1808	rVB	56440	94070	7.09%	0.998%
29	12.728	1818	1826	1836	rBV	606365	1030365	77.69%	10.931%
30	13.216	1904	1909	1916	rVB3	9308	13681	1.03%	0.145%
31	13.492	1948	1956	1962	rVB4	11097	24573	1.85%	0.261%
32	13.669	1979	1986	1999	rBV	677809	1165737	87.90%	12.368%
33	13.833	2007	2014	2017	rBV3	23232	39482	2.98%	0.419%
34	13.875	2017	2021	2026	rVV2	43481	73216	5.52%	0.777%
35	13.939	2026	2032	2037	rVV5	7605	16000	1.21%	0.170%
36	13.998	2037	2042	2048	rVB3	10760	15810	1.19%	0.168%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

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\82N051022W.M
Title : SW846 8260

37	14.128	2059	2064	2073	rVB3	9774	16580	1.25%	0.176%
38	14.210	2073	2078	2084	rBV3	27734	42604	3.21%	0.452%
39	14.327	2092	2098	2107	rVB	89690	152169	11.47%	1.614%
40	14.539	2125	2134	2137	rBV5	9125	14801	1.12%	0.157%
41	14.804	2174	2179	2184	rBV3	15695	25291	1.91%	0.268%
42	14.927	2193	2200	2206	rBV3	76969	149626	11.28%	1.587%
43	15.192	2235	2245	2249	rBV5	11645	26644	2.01%	0.283%
44	15.304	2255	2264	2270	rVB5	15318	34949	2.64%	0.371%
45	15.498	2291	2297	2306	rBV2	23253	43315	3.27%	0.460%

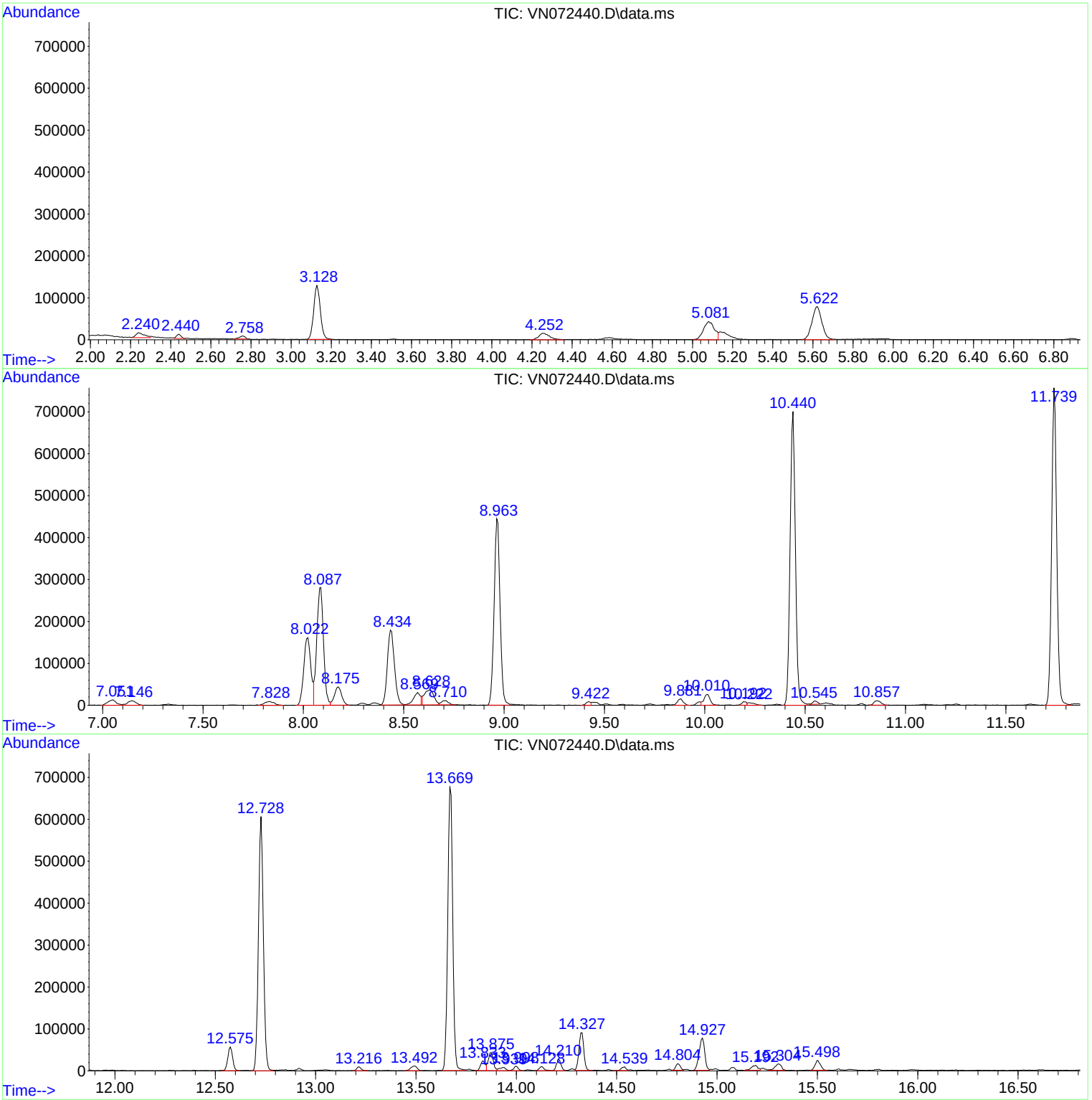
Sum of corrected areas: 9425796

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

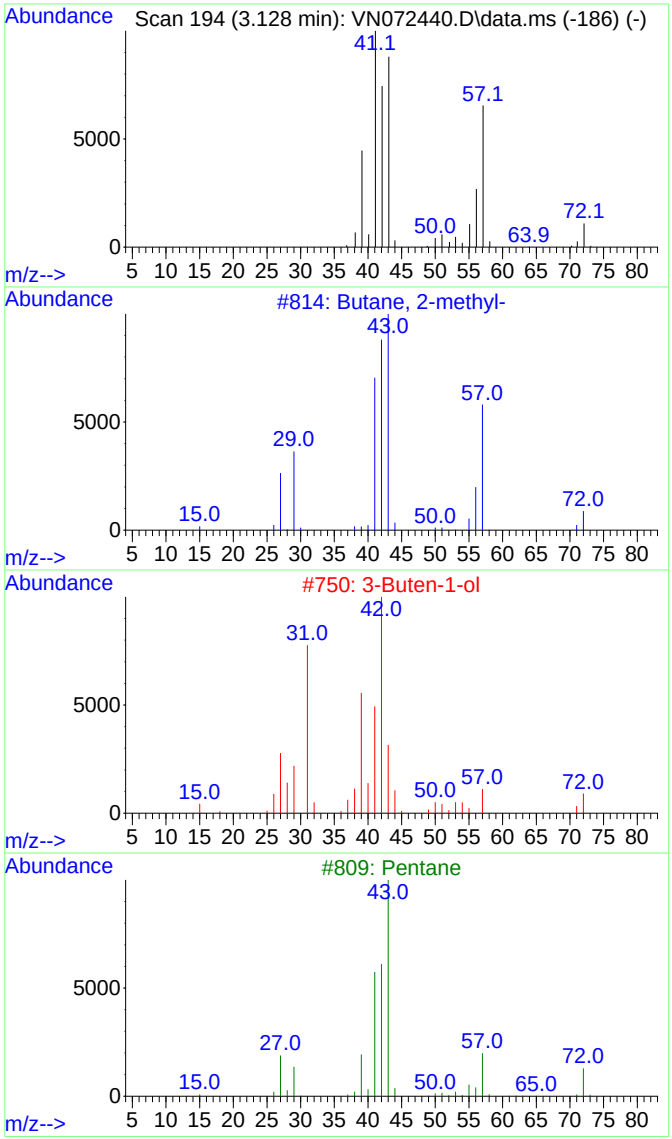
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

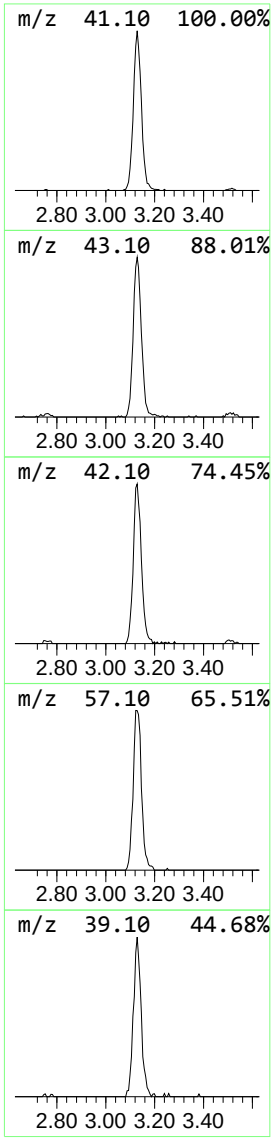
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	22.88 ug/l	294217	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	50
2	3-Buten-1-ol	72	C4H8O	000627-27-0	50
3	Pentane	72	C5H12	000109-66-0	47
4	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	23
5	2-Butene, (Z)-	56	C4H8	000590-18-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

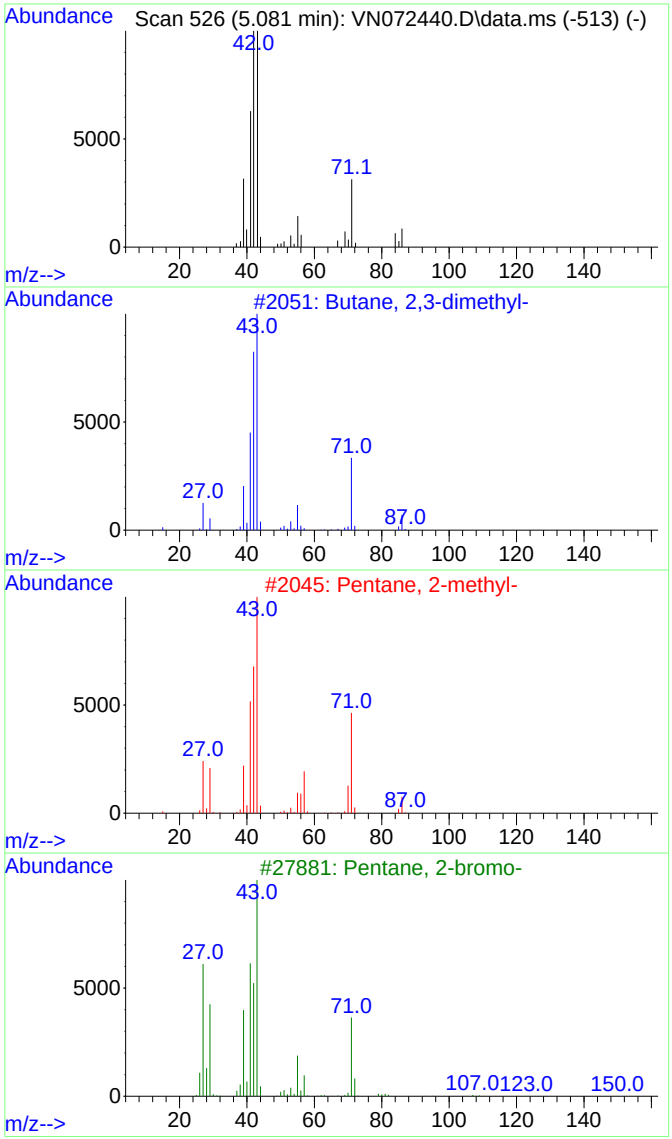
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

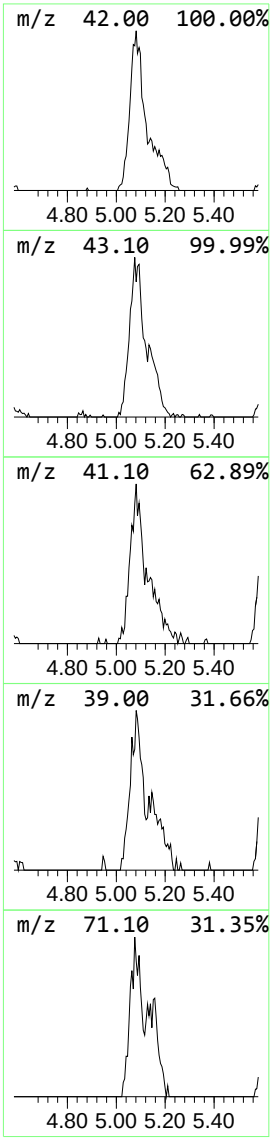
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	12.97 ug/l	166727	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
3	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	37
4	1,2,4,5-Tetrazine, 1,4-dihydro-3...	112	C4H8N4	037454-64-1	33
5	1-Pentene	70	C5H10	000109-67-1	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

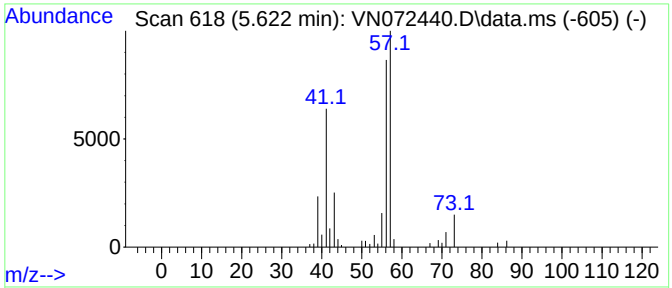
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

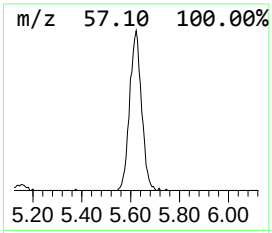
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

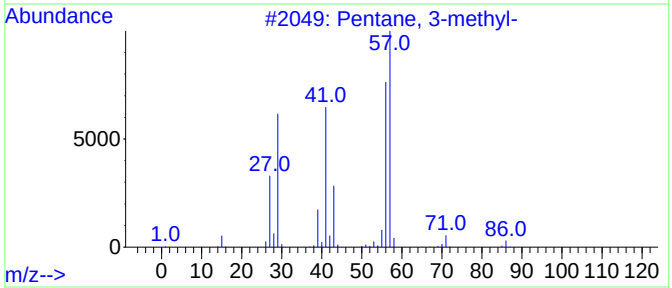
****
Peak Number 3 Pentane, 3-methyl- Concentration Rank 2

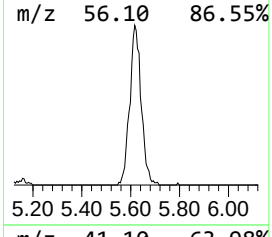
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	21.02 ug/l	270215	Pentafluorobenzene	8.081

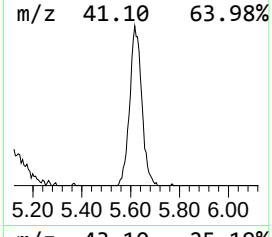
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	80
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	56
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	52

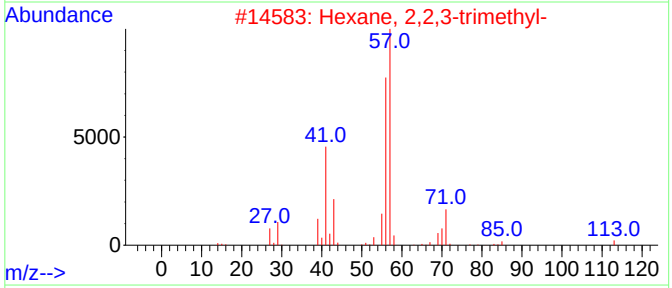


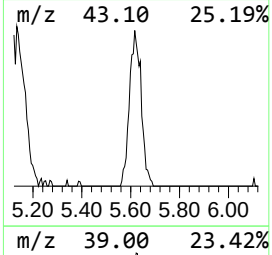


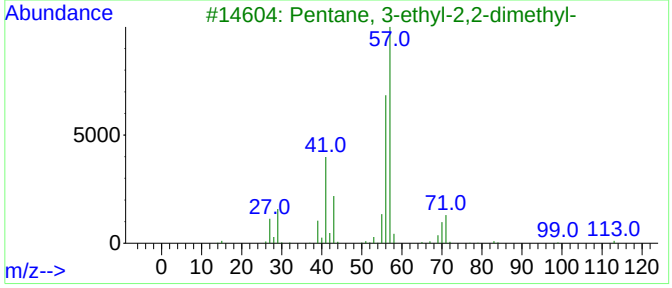


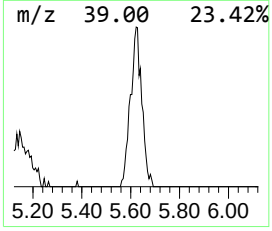












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

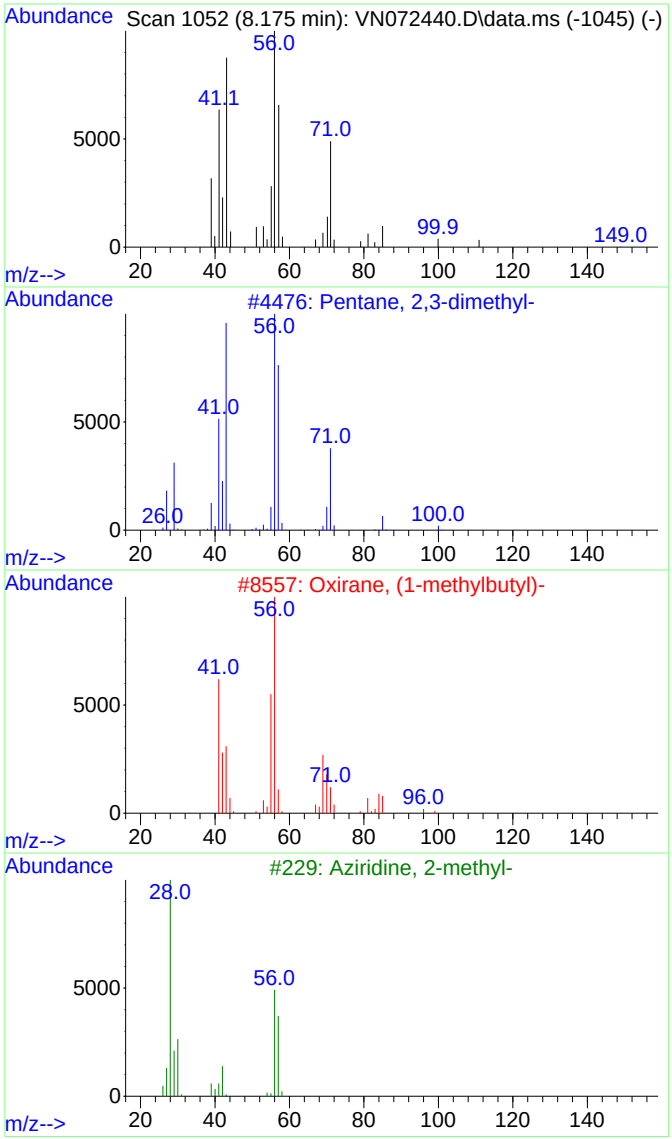
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

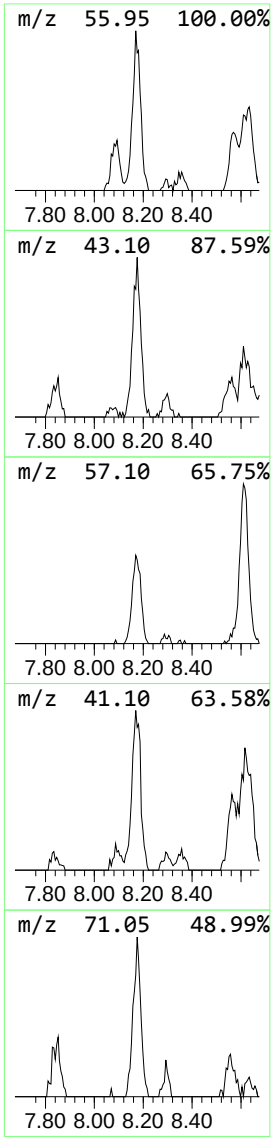
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	8.40 ug/l	108058	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	87
2	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	45
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	38
5	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

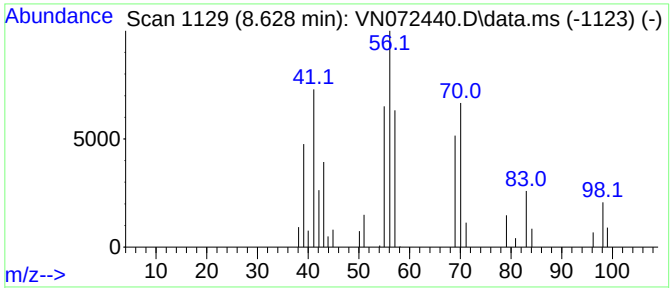
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

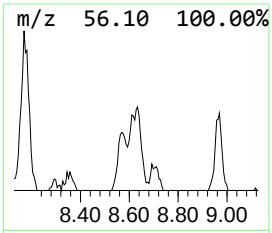
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

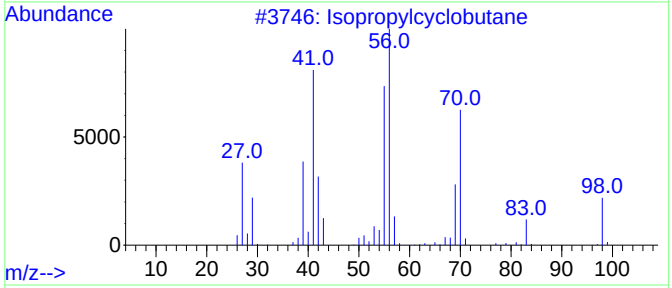
****
Peak Number 5 Isopropylcyclobutane Concentration Rank 7

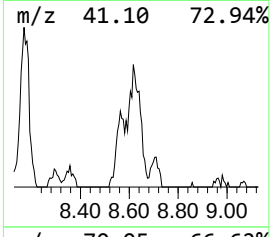
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.628	6.27 ug/l	114243	1,4-Difluorobenzene	8.963

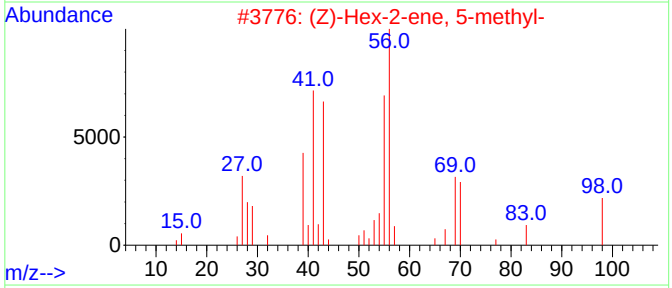
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	80
2	(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	53
3	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	52
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	52
5	1-Nonanol	144	C9H20O	000143-08-8	50

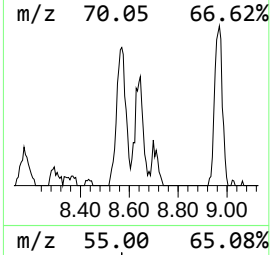


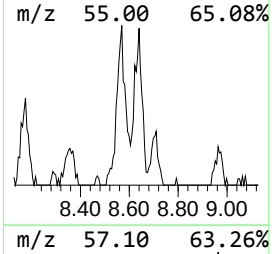


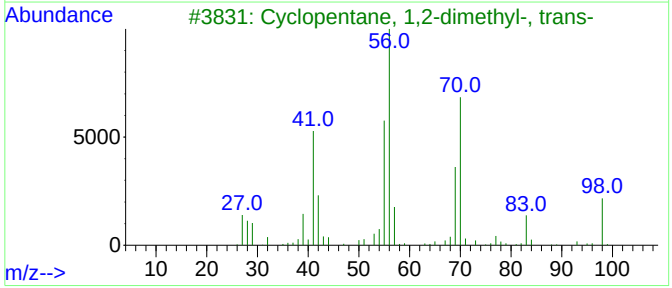


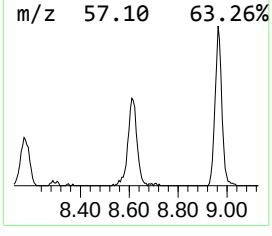












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

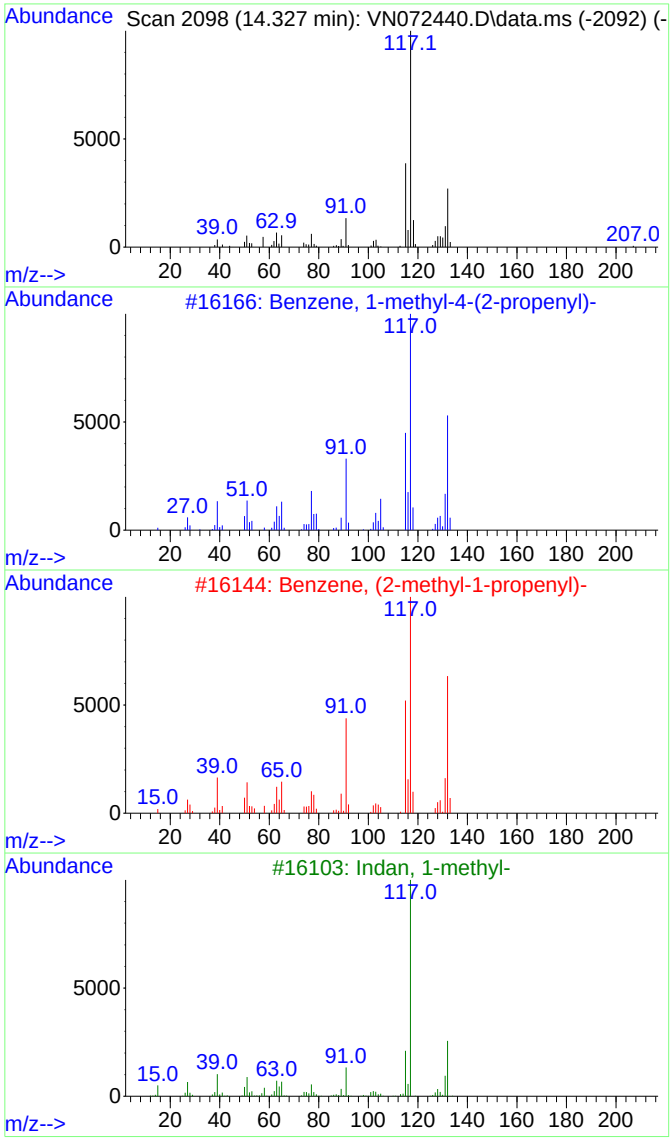
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

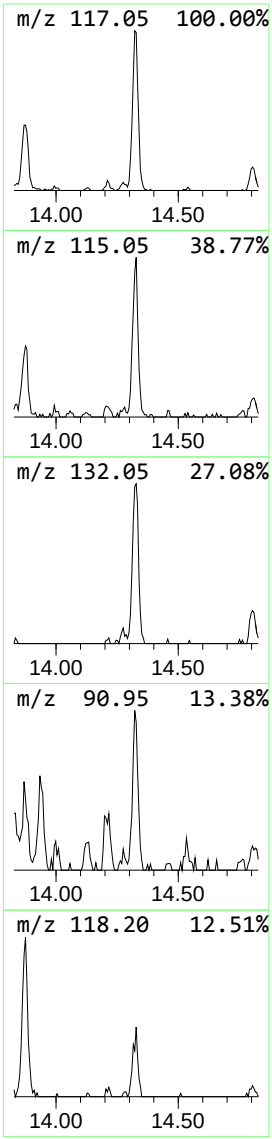
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-methyl-4-(2-prop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.328	6.53 ug/l	152169	1,4-Dichlorobenzene-d4	13.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	80
2	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	80
3	Indan, 1-methyl-	132	C10H12	000767-58-8	68
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	64
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	62





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

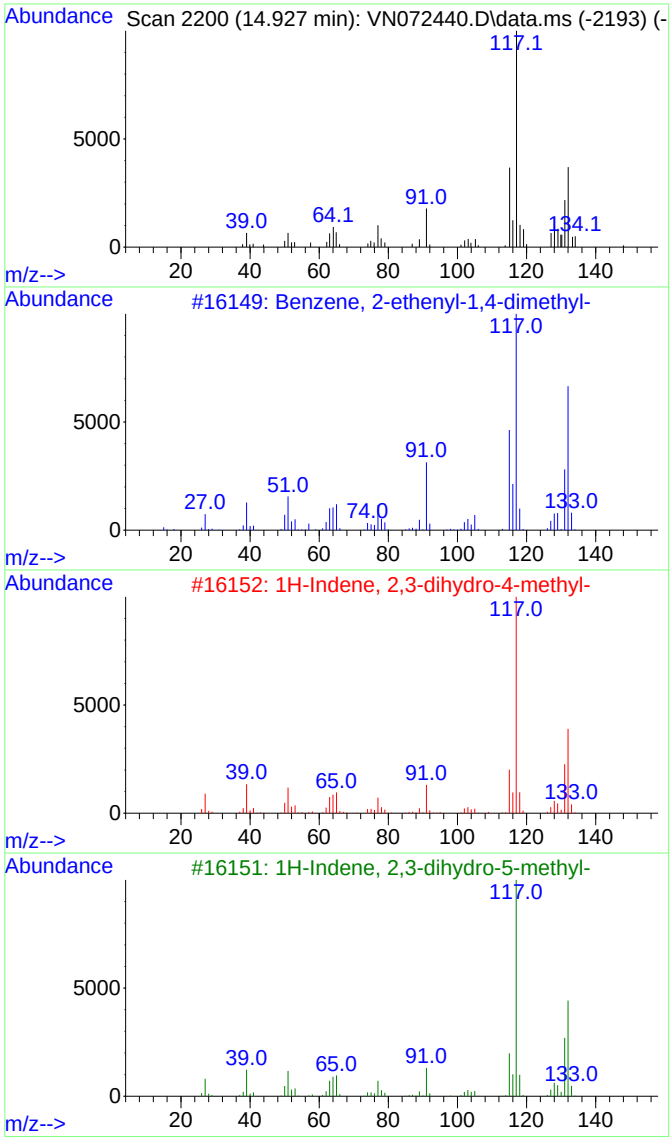
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

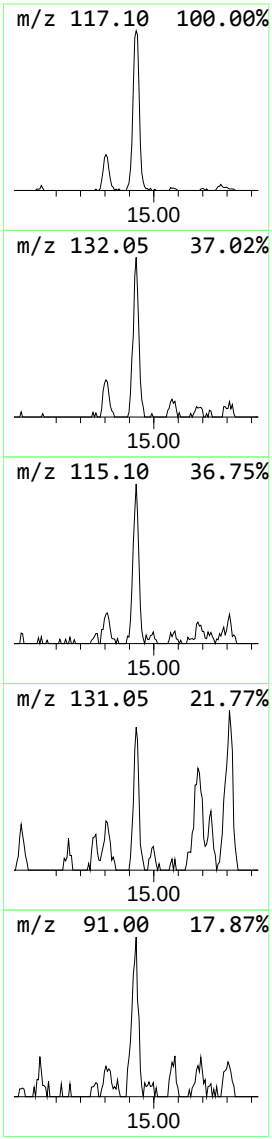
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.928	6.42 ug/l	149626	1,4-Dichlorobenzene-d4	13.669

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	87
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81
4	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	81
5	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051122\
Data File : VN072440.D
Acq On : 12 May 2022 01:43
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.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-	3.128	22.9	ug/l	294217	1	8.081	642902	50.0
Butane, 2,3-dim...	5.081	13.0	ug/l	166727	1	8.081	642902	50.0
Pentane, 3-methyl-	5.622	21.0	ug/l	270215	1	8.081	642902	50.0
Pentane, 2,3-di...	8.175	8.4	ug/l	108058	1	8.081	642902	50.0
Isopropylcyclob...	8.628	6.3	ug/l	114243	2	8.963	910606	50.0
Benzene, 1-meth...	14.328	6.5	ug/l	152169	4	13.669	1165740	50.0
Benzene, 2-ethe...	14.928	6.4	ug/l	149626	4	13.669	1165740	50.0