LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

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\82N032521W.M
Title : SW846 8260

Signal : TIC: VN066445.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.982	97	109	121	rBV	246801	328411	7.96%	0.802%
2	2.143	152	169	183	rBV	699272	988072	23.95%	2.413%
3	2.223	189	199	211	rVB	45519	69049	1.67%	0.169%
4	2.757	379	398	422	rBV	2087021	4106876	99.56%	10.030%
5	3.081	504	519	543	rVB3	385480	849504	20.59%	2.075%
6	3.258	576	585	598	rVB	28676	55029	1.33%	0.134%
7	3.494	657	673	701	rVB2	291939	687460	16.67%	1.679%
8	3.720	739	757	781	rVB2	181062	530109	12.85%	1.295%
9	3.985	847	856	883	rVB2	42613	116137	2.82%	0.284%
10	4.430	999	1022	1038	rBV3	402347	1401164	33.97%	3.422%
11	4.943	1186	1213	1241	rVB4	113391	405772	9.84%	0.991%
12	5.460	1388	1406	1424	rVB4	18663	54042	1.31%	0.132%
13	5.820	1518	1540	1567	rVB3	58536	180195	4.37%	0.440%
14	5.962	1571	1593	1612	rBV4	31601	100004	2.42%	0.244%
15	6.273	1683	1709	1730	rBV5	37622	119291	2.89%	0.291%
16	6.418	1739	1763	1782	rBV5	46051	147239	3.57%	0.360%
17	6.525	1782	1803	1824	rBV4	215165	651740	15.80%	1.592%
18	6.745	1859	1885	1909	rVB7	17327	73067	1.77%	0.178%
19	7.303	2077	2093	2114	rVB5	54504	148085	3.59%	0.362%
20	7.507	2145	2169	2181	rBV	267852	691665	16.77%	1.689%
21	7.582	2182	2197	2214	rVV3	631251	1656555	40.16%	4.046%
22	7.662	2216	2227	2254	rVB3	116150	300735	7.29%	0.734%
23	7.794	2262	2276	2287	rBV4	18521	41733	1.01%	0.102%
24	7.957	2314	2337	2365	rBV3	1160160	2922432	70.85%	7.137%
25	8.129	2366	2401	2425	rVV2	260116	891971	21.62%	2.178%
26	8.223	2427	2436	2459	rVB5	29174	69237	1.68%	0.169%
27	8.512	2525	2544	2570	rBV	763781	1649315	39.98%	4.028%
28	8.751	2619	2633	2642	rBV5	19399	42870	1.04%	0.105%
29	9.011	2700	2730	2745	rBV7	70153	231088	5.60%	0.564%
30	9.151	2768	2782	2794	rBV3	20364	43068	1.04%	0.105%
31	9.454	2881	2895	2916	rVB	127061	255497	6.19%	0.624%
32	9.588	2916	2945	2971	rBV2	231519	644277	15.62%	1.573%
33	9.910	3050	3065	3079	rBV4	38025	89956	2.18%	0.220%
34	10.028	3092	3109	3123	rBV	1188611	2157398	52.30%	5.269%
35	10.092	3123	3133	3148	rVB	288570	505070	12.24%	1.233%
36	10.457	3257	3269	3292	rVB5	27893	58550	1.42%	0.143%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

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\82N032521W.M
Title : SW846 8260

37	11.347	3585	3601	3624	rBV	994886	1759608	42.66%	4.297%
38	11.452	3625	3640	3665	rVV	2485128	4124916	100.00%	10.074%
39	11.567	3667	3683	3708	rVB	913763	1748632	42.39%	4.270%
40	11.889	3790	3803	3820	rBV	64625	115846	2.81%	0.283%
41	12.192	3902	3916	3930	rBV	217100	357510	8.67%	0.873%
42	12.345	3956	3973	3997	rBV	703629	1240154	30.06%	3.029%
43	12.535	4031	4044	4062	rBV	290905	477986	11.59%	1.167%
44	12.635	4069	4081	4088	rBV	124822	195979	4.75%	0.479%
45	12.678	4088	4097	4110	rVB2	201941	323755	7.85%	0.791%
46	12.836	4143	4156	4178	rBV	189970	318671	7.73%	0.778%
47	12.983	4197	4211	4241	rVB	1004460	1661486	40.28%	4.058%
48	13.115	4246	4260	4274	rVB4	28708	61224	1.48%	0.150%
49	13.286	4311	4324	4332	rBV	804827	1472958	35.71%	3.597%
50	13.485	4378	4398	4412	rBV	1232586	2139748	51.87%	5.226%
51	13.683	4463	4472	4485	rVB4	34103	59501	1.44%	0.145%
52	13.748	4486	4496	4516	rBV2	53701	120119	2.91%	0.293%
53	13.833	4517	4528	4541	rBV	145255	247951	6.01%	0.606%
54	13.938	4557	4567	4582	rVB4	111774	194384	4.71%	0.475%
55	14.153	4636	4647	4656	rBV	134236	224681	5.45%	0.549%
56	14.421	4737	4747	4760	rBV2	71569	119552	2.90%	0.292%
57	14.536	4776	4790	4806	rBV4	240121	458653	11.12%	1.120%
58	15.073	4979	4990	5004	rBV	140348	261684	6.34%	0.639%

Sum of corrected areas: 40947661

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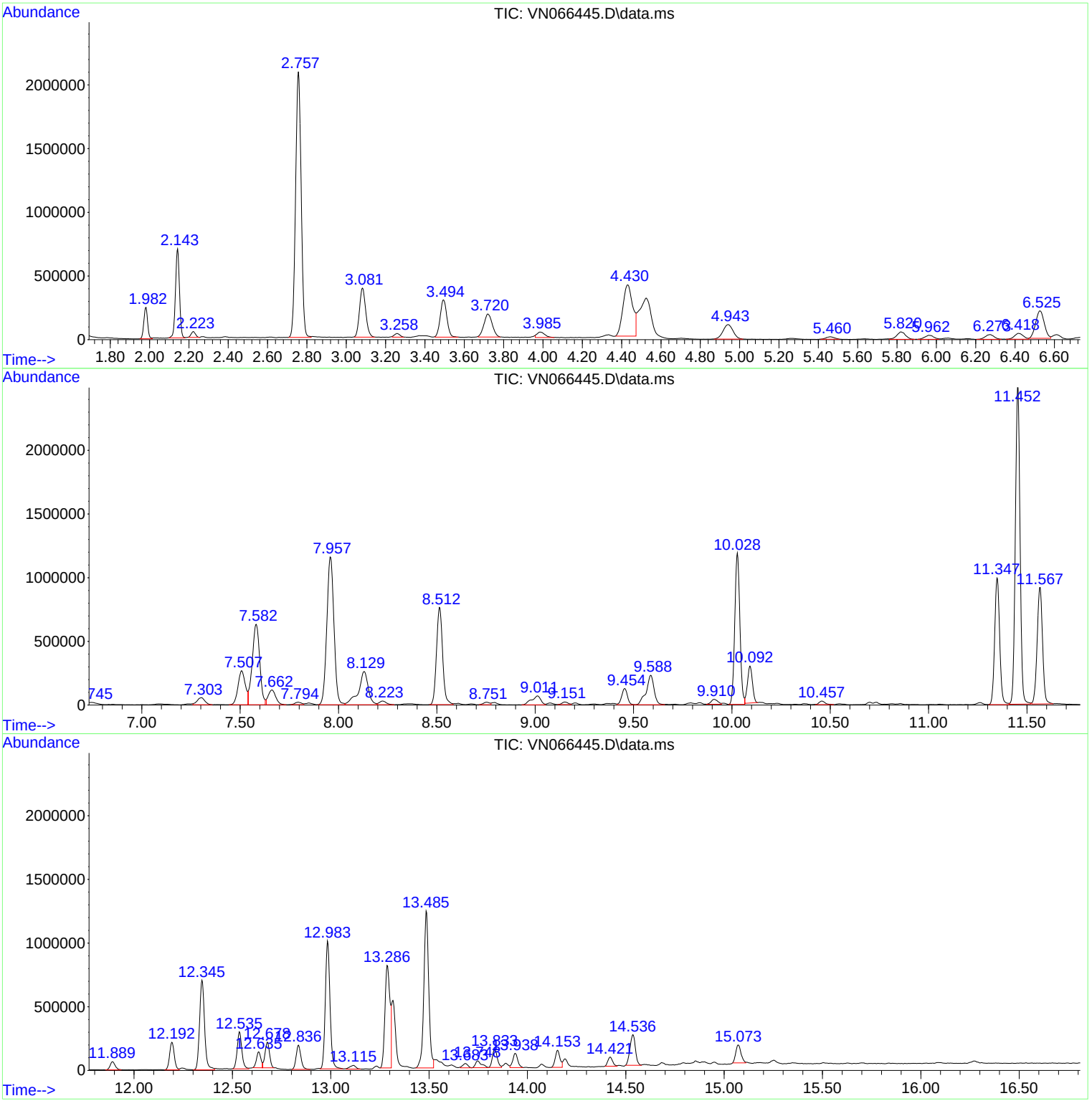
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

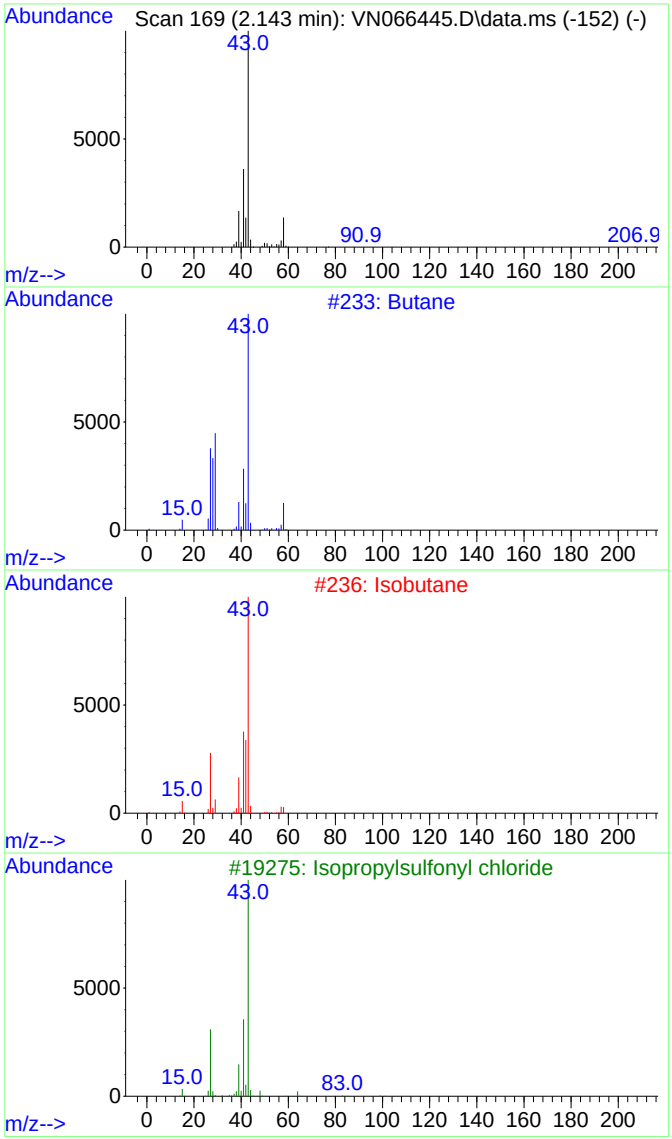
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

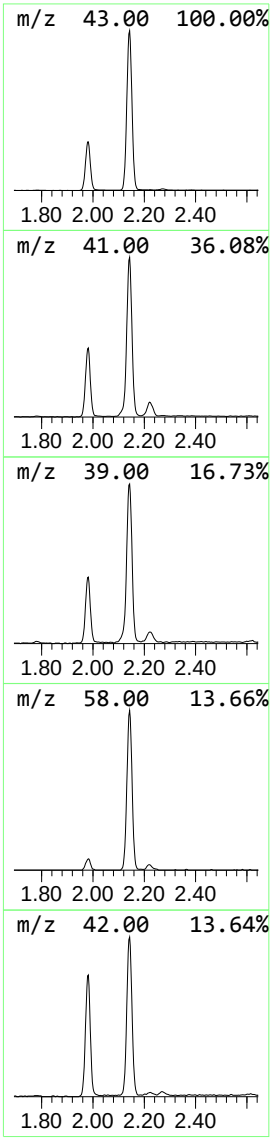
****

Peak Number 1 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.143	29.82 ug/l	988072	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Isobutane	58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

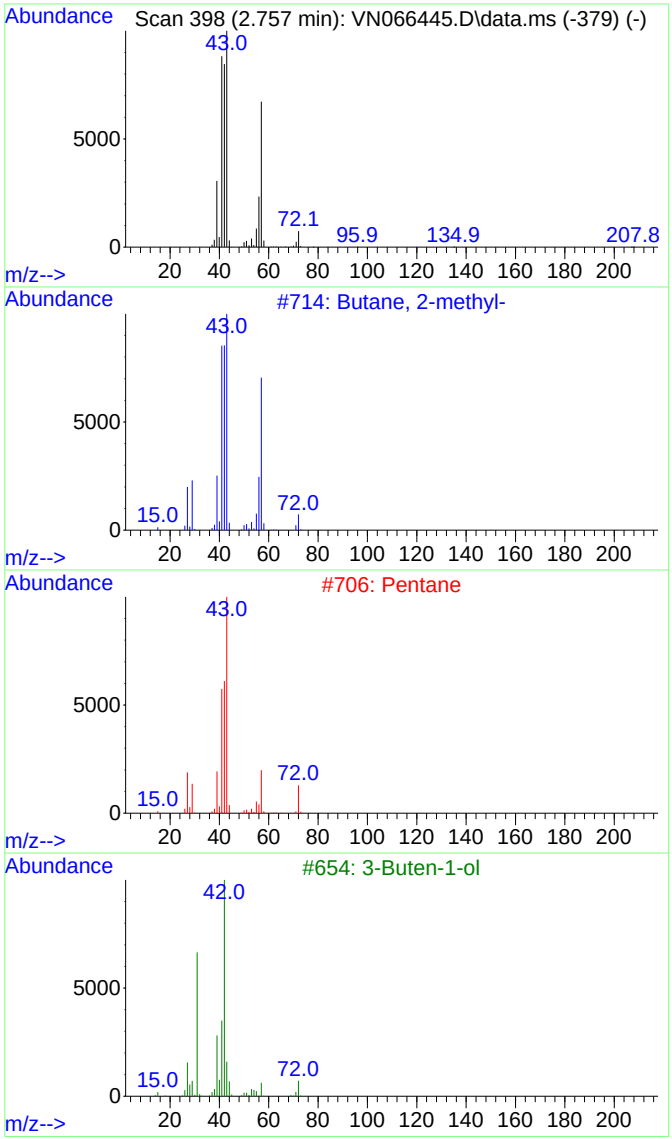
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

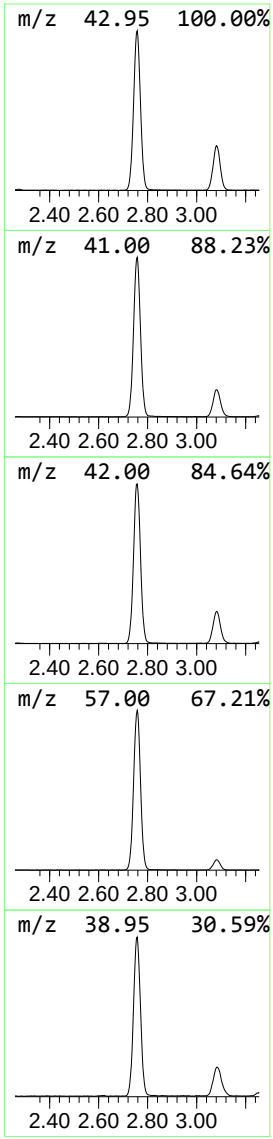
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.757	123.96 ug/l	4106880	Pentafluorobenzene	7.584

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	64
3	3-Buten-1-ol	72	C4H8O	000627-27-0	47
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

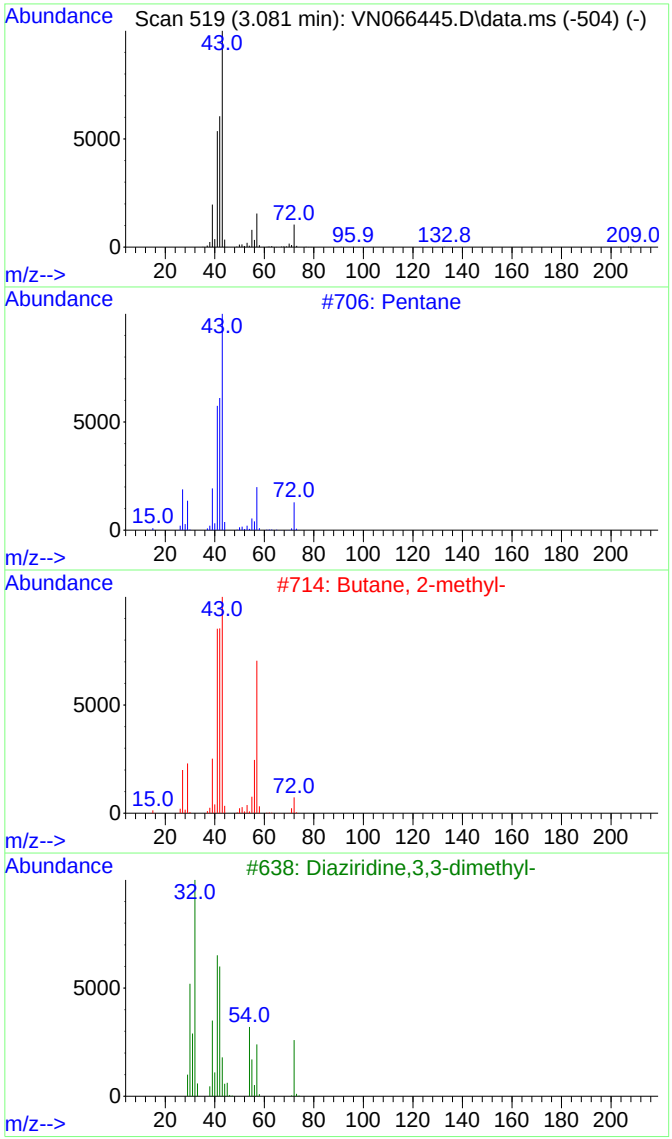
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

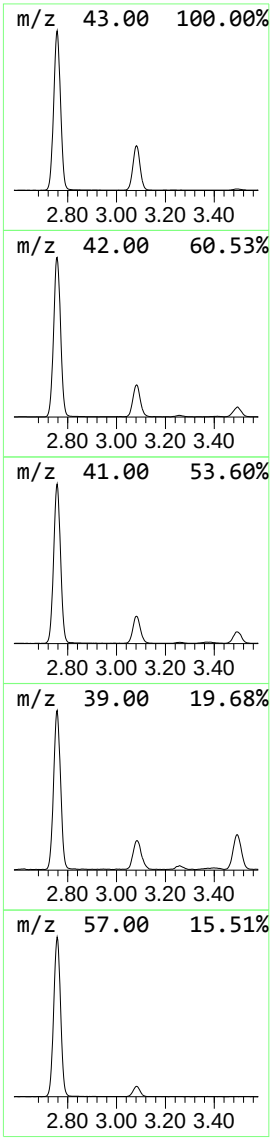
****

Peak Number 3 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	25.64 ug/l	849504	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	45
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	5,9-Dodecadien-2-one, 6,10-dimet...	208	C14H24O	1000132-10-9	9
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

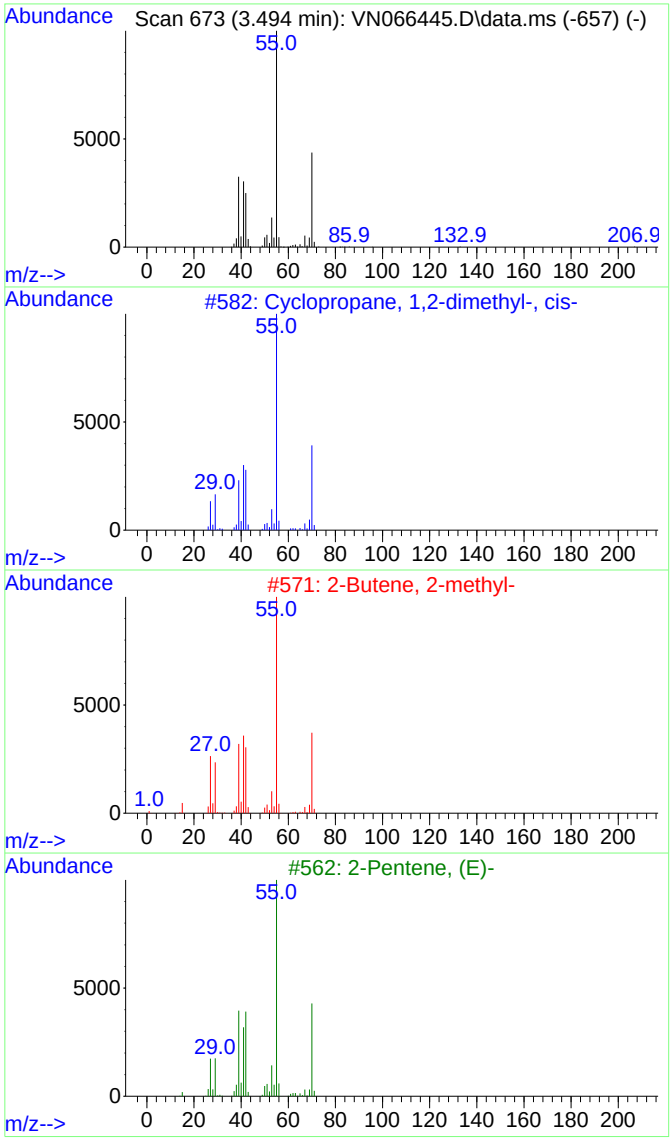
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

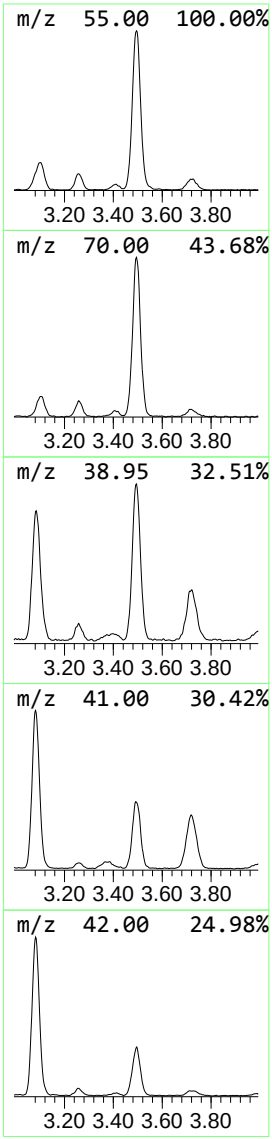
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.494	20.75 ug/l	687460	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3	2-Pentene, (E)-	70	C5H10	000646-04-8	86
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR12

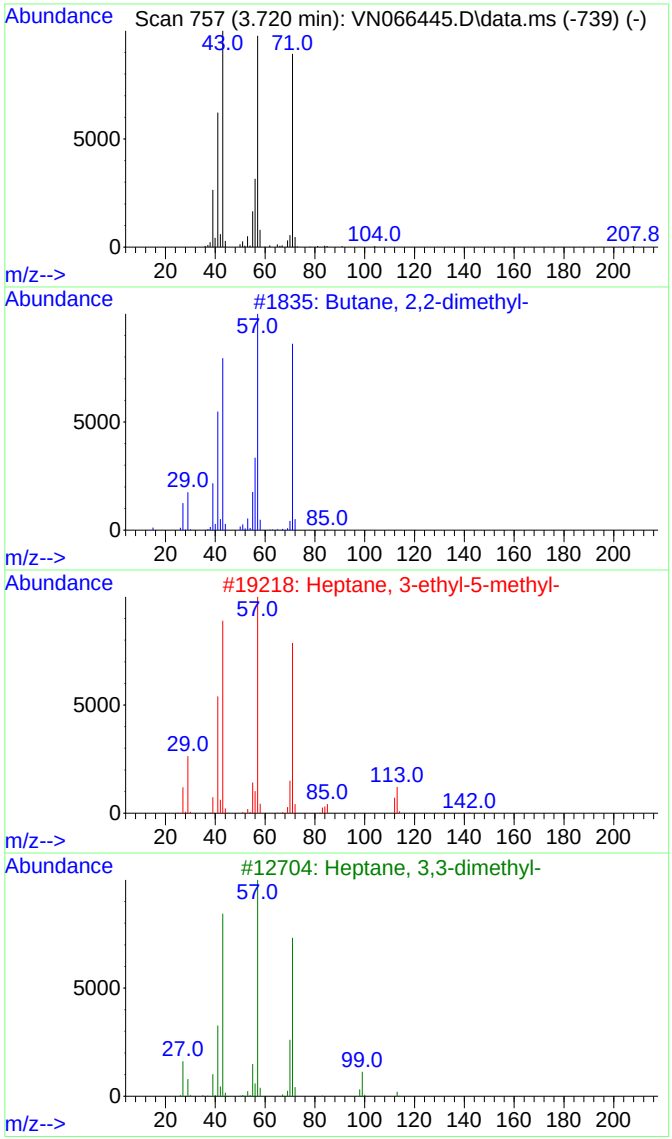
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

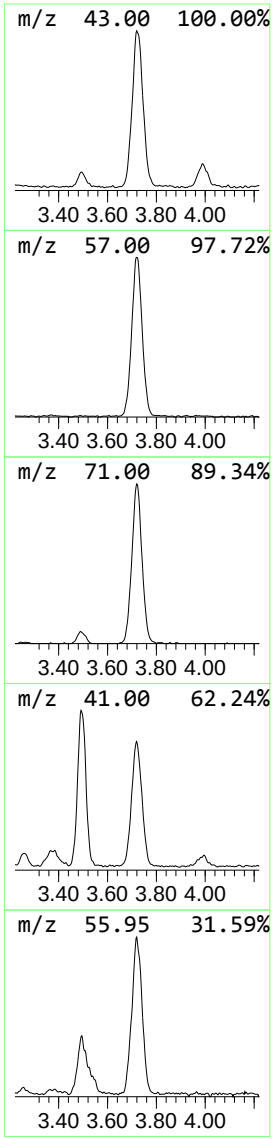
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.720	16.00 ug/l	530109	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	86
2	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	72
3	Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	64
4	3-Hexanone, 4-ethyl-	128	C8H16O	006137-12-8	50
5	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	47





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Operator : JC/MD
Sample : M1835-05
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

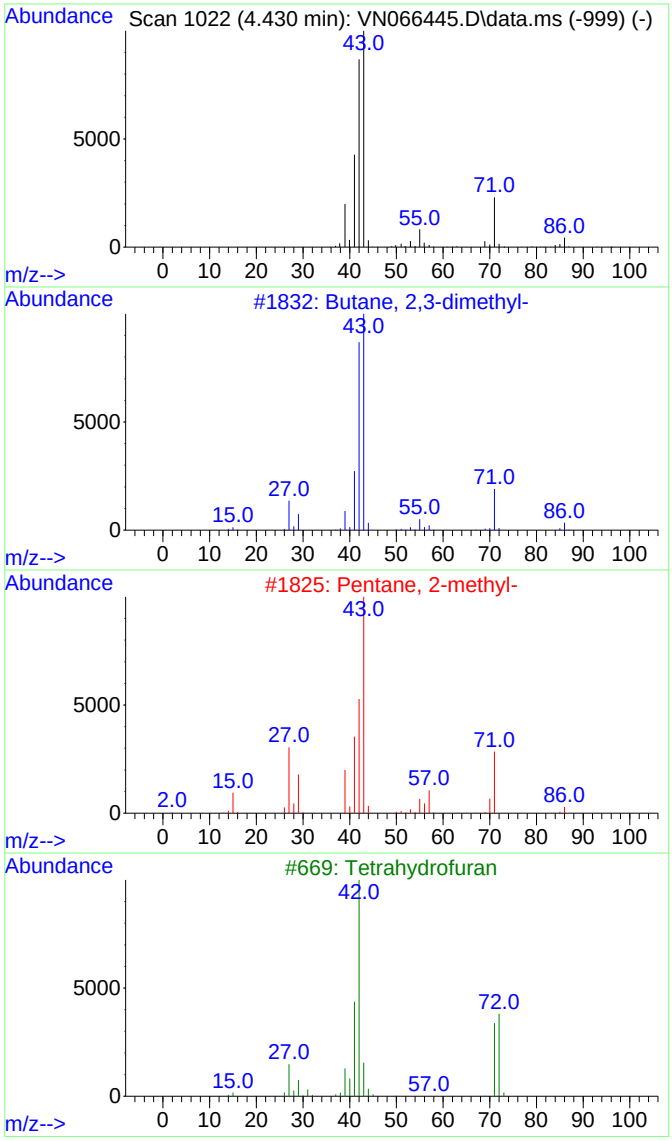
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

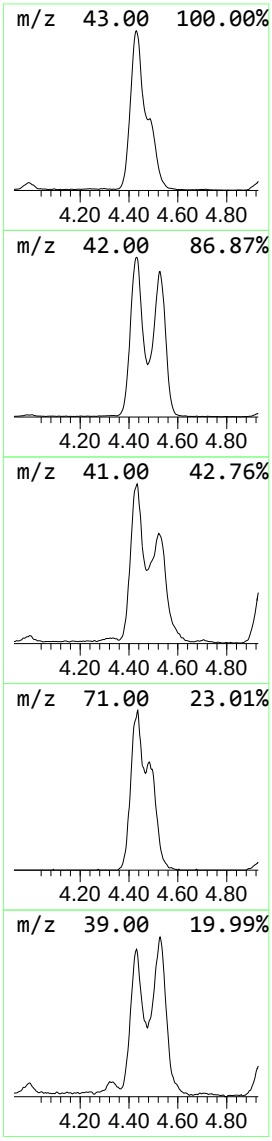
****

Peak Number 6 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.430	42.29 ug/l	1401160	Pentafluorobenzene	7.584

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Butane, 2-methyl-	72	C5H12	000078-78-4	36
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	33





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Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

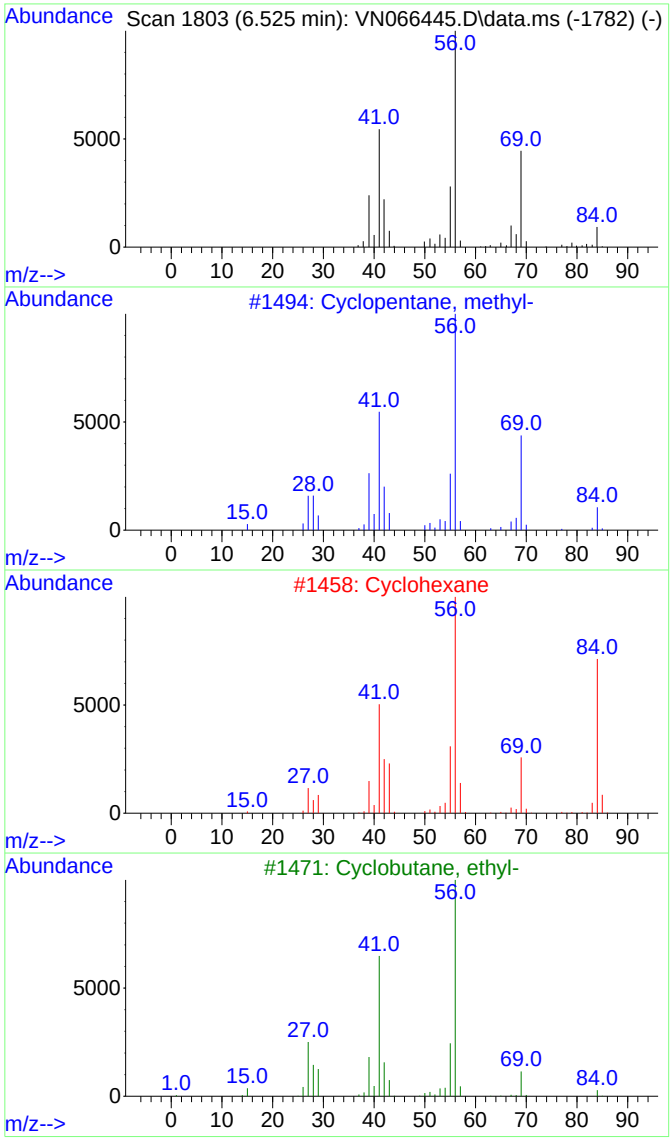
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

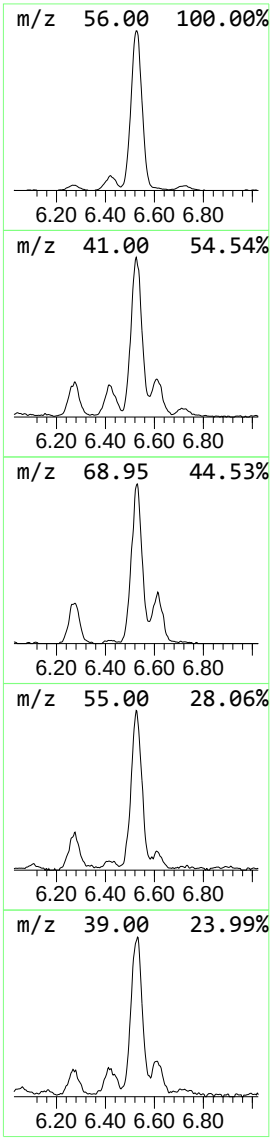
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.525	19.67 ug/l	651740	Pentafluorobenzene	7.584

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	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5	Cyclobutane	56	C4H8	000287-23-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ASR12

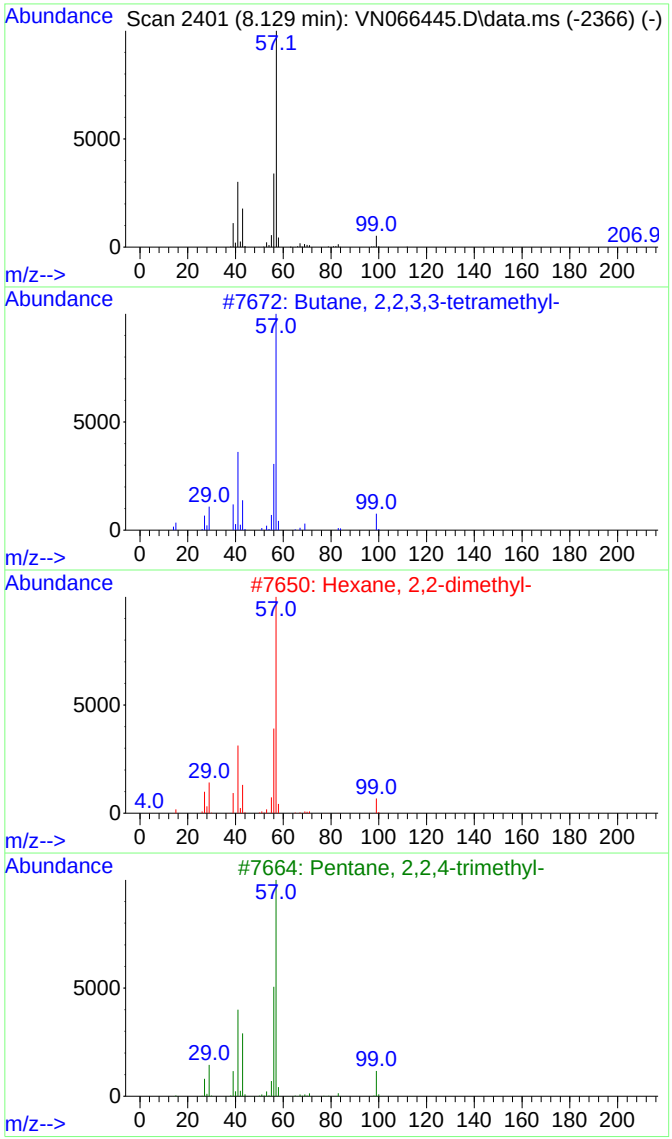
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

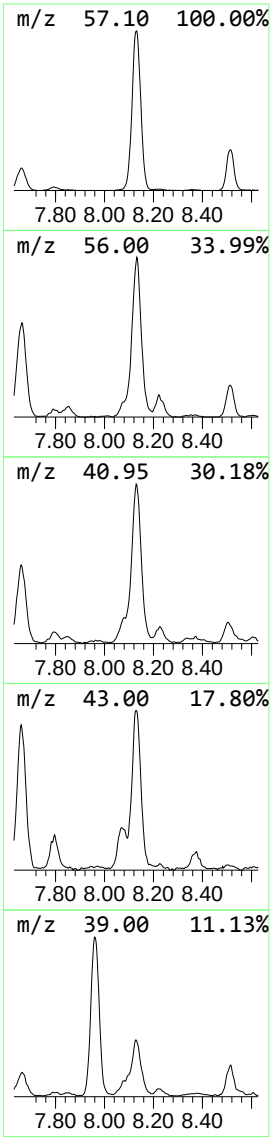
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butane, 2,2,3,3-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.129	27.04 ug/l	891971	1,4-Difluorobenzene	8.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

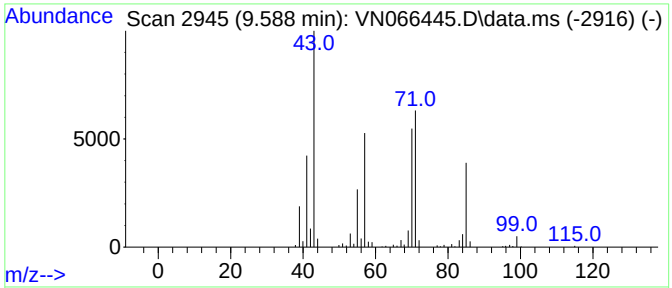
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

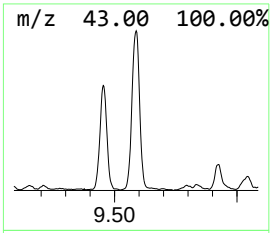
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

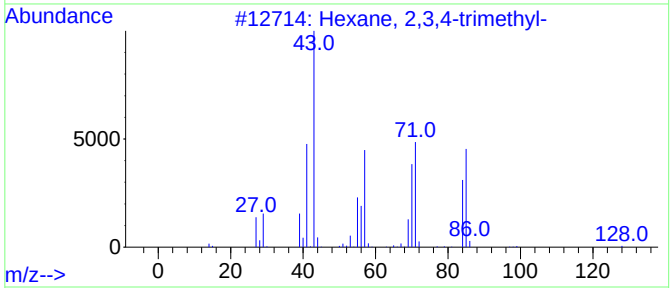
****
Peak Number 9 Hexane, 2,3,4-trimethyl- Concentration Rank 9

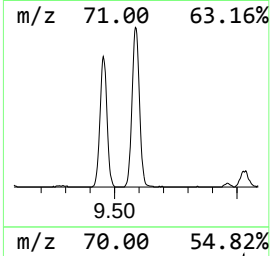
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.588	19.53 ug/l	644277	1,4-Difluorobenzene	8.515

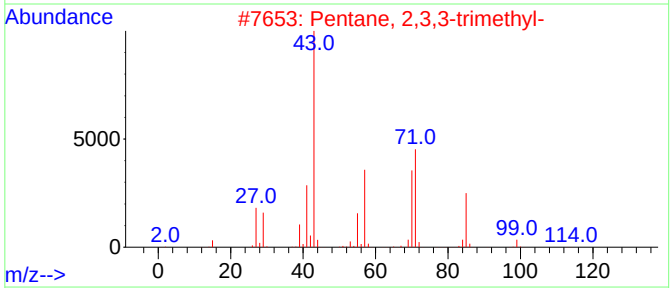
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	78
2	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5	Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	50

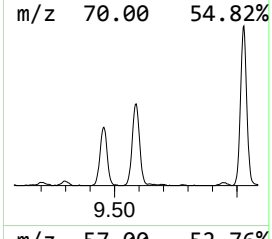


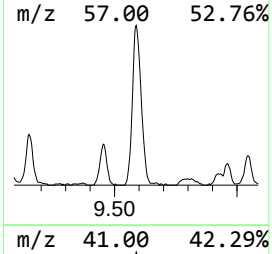


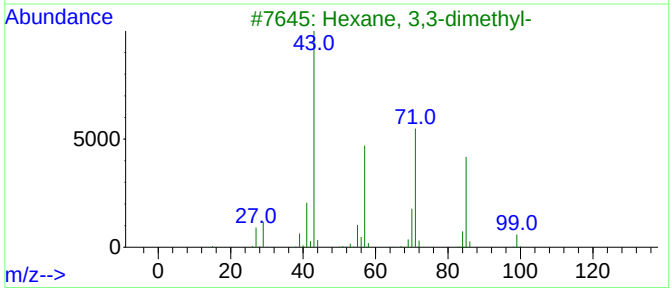


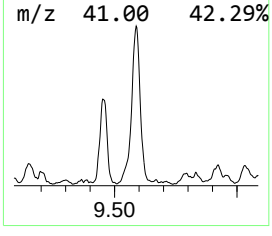












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

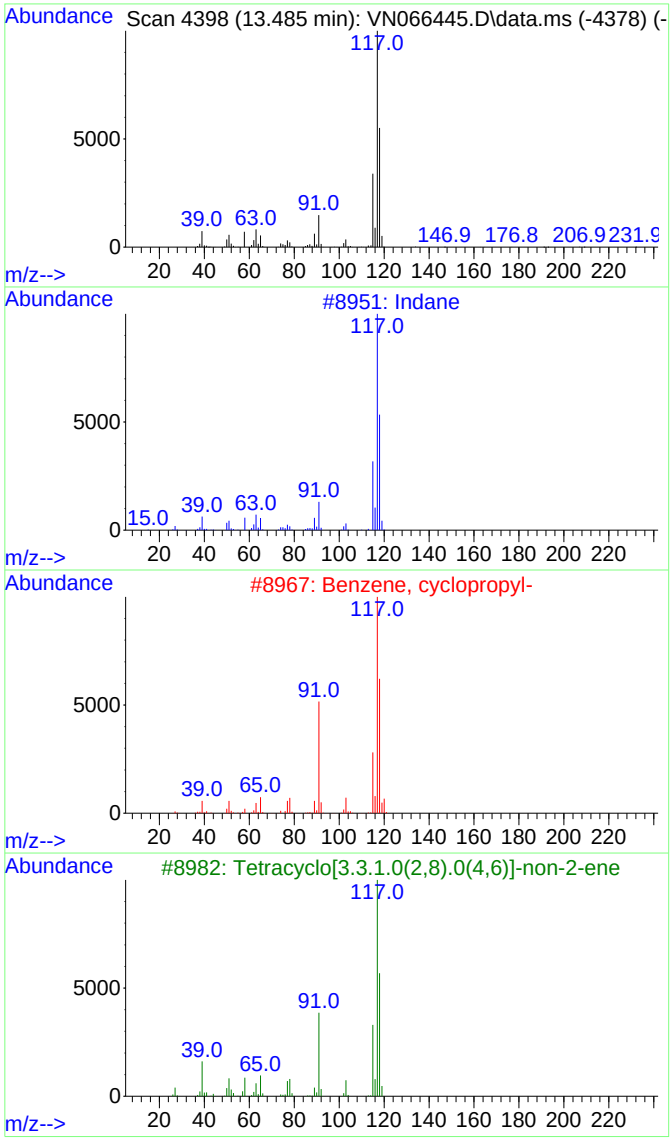
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

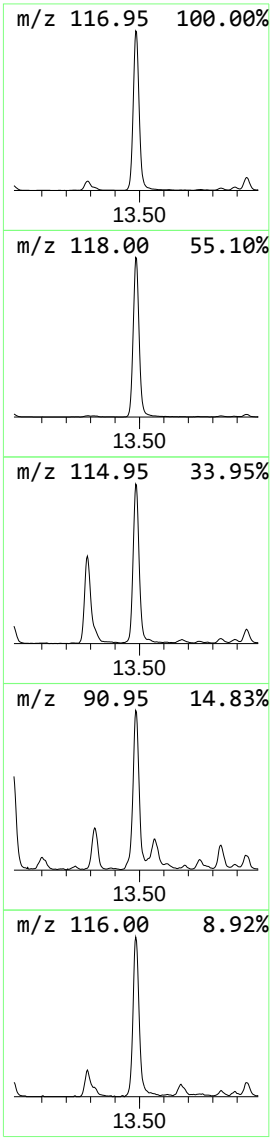
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.485	72.63 ug/l	2139750	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	95
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	74
5	Deltacyclene	118	C9H10	007785-10-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033121\
Data File : VN066445.D
Acq On : 31 Mar 2021 17:31
Operator : JC/MD
Sample : M1835-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : ASR12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane	2.143	29.8	ug/l	988072	1	7.584	1656560	50.0
Butane, 2-methyl-	2.757	124.0	ug/l	4106880	1	7.584	1656560	50.0
Pentane	3.081	25.6	ug/l	849504	1	7.584	1656560	50.0
Cyclopropane, 1...	3.494	20.8	ug/l	687460	1	7.584	1656560	50.0
Butane, 2,2-dim...	3.720	16.0	ug/l	530109	1	7.584	1656560	50.0
Butane, 2,3-dim...	4.430	42.3	ug/l	1401160	1	7.584	1656560	50.0
Cyclopentane, m...	6.525	19.7	ug/l	651740	1	7.584	1656560	50.0
Butane, 2,2,3,3...	8.129	27.0	ug/l	891971	2	8.515	1649320	50.0
Hexane, 2,3,4-t...	9.588	19.5	ug/l	644277	2	8.515	1649320	50.0
Indane	13.485	72.6	ug/l	2139750	4	13.286	1472960	50.0