LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TRE-1125

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82N012521W.M
Title : SW846 8260

Signal : TIC: VN065636.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.782	616	635	667	rBV	574183	1484429	17.63%	3.404%
2	5.692	1211	1229	1260	rBV4	27751	93867	1.12%	0.215%
3	7.550	1787	1807	1817	rBV	136726	340596	4.05%	0.781%
4	7.624	1818	1830	1851	rVB	274018	657538	7.81%	1.508%
5	7.994	1926	1945	1972	rBV3	300190	774389	9.20%	1.776%
6	8.550	2102	2118	2136	rBV	420015	877275	10.42%	2.012%
7	9.235	2317	2331	2362	rBV	875410	1621375	19.26%	3.718%
8	9.872	2507	2529	2543	rBV	100170	183615	2.18%	0.421%
9	10.058	2573	2587	2595	rBV	671005	1220804	14.50%	2.800%
10	10.122	2595	2607	2638	rVB	4390979	8109441	96.34%	18.598%
11	10.325	2660	2670	2700	rVB	60226	121274	1.44%	0.278%
12	10.608	2739	2758	2772	rVB2	62089	108791	1.29%	0.250%
13	10.733	2785	2797	2815	rBV	852436	1372249	16.30%	3.147%
14	10.823	2815	2825	2852	rVB	132958	232431	2.76%	0.533%
15	11.138	2909	2923	2938	rBV	262620	421512	5.01%	0.967%
16	11.376	2985	2997	3016	rVB	576351	1003376	11.92%	2.301%
17	11.479	3016	3029	3047	rVB	680263	1131661	13.44%	2.595%
18	11.589	3047	3063	3088	rBV	2277415	4288028	50.94%	9.834%
19	11.917	3152	3165	3183	rBV	1543753	2549715	30.29%	5.847%
20	12.373	3295	3307	3328	rVB	434255	728529	8.65%	1.671%
21	12.563	3356	3366	3375	rBV	112076	177144	2.10%	0.406%
22	12.627	3375	3386	3392	rBV	523662	856500	10.17%	1.964%
23	12.704	3403	3410	3429	rVB	229161	367329	4.36%	0.842%
24	12.862	3447	3459	3474	rBV	251555	403059	4.79%	0.924%
25	13.010	3492	3505	3518	rBV	945441	1500733	17.83%	3.442%
26	13.093	3519	3531	3546	rBV2	122383	248568	2.95%	0.570%
27	13.312	3588	3599	3605	rBV	525675	913094	10.85%	2.094%
28	13.418	3620	3632	3644	rBV	5404366	8417855	100.00%	19.305%
29	13.489	3644	3654	3655	rBV3	255848	327889	3.90%	0.752%
30	13.560	3671	3676	3696	rVB4	123983	267561	3.18%	0.614%
31	13.859	3760	3769	3778	rVB	73740	111689	1.33%	0.256%
32	13.965	3793	3802	3820	rVB2	79495	144207	1.71%	0.331%
33	14.216	3874	3880	3890	rVB	80400	122013	1.45%	0.280%
34	14.444	3943	3951	3960	rBV	73194	111888	1.33%	0.257%
35	14.560	3974	3987	3998	rBV3	167611	340225	4.04%	0.780%
36	14.711	4027	4034	4043	rBV	61870	86079	1.02%	0.197%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TRE-1125

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82N012521W.M
Title : SW846 8260

37	14.920	4089	4099	4104	rBV6	52517	95824	1.14%	0.220%
38	14.968	4105	4114	4128	rVB	649719	988385	11.74%	2.267%
39	15.100	4145	4155	4165	rVB	282797	480984	5.71%	1.103%
40	16.113	4460	4470	4487	rVB	91896	187517	2.23%	0.430%
41	16.305	4517	4530	4545	rBV2	62930	134072	1.59%	0.307%

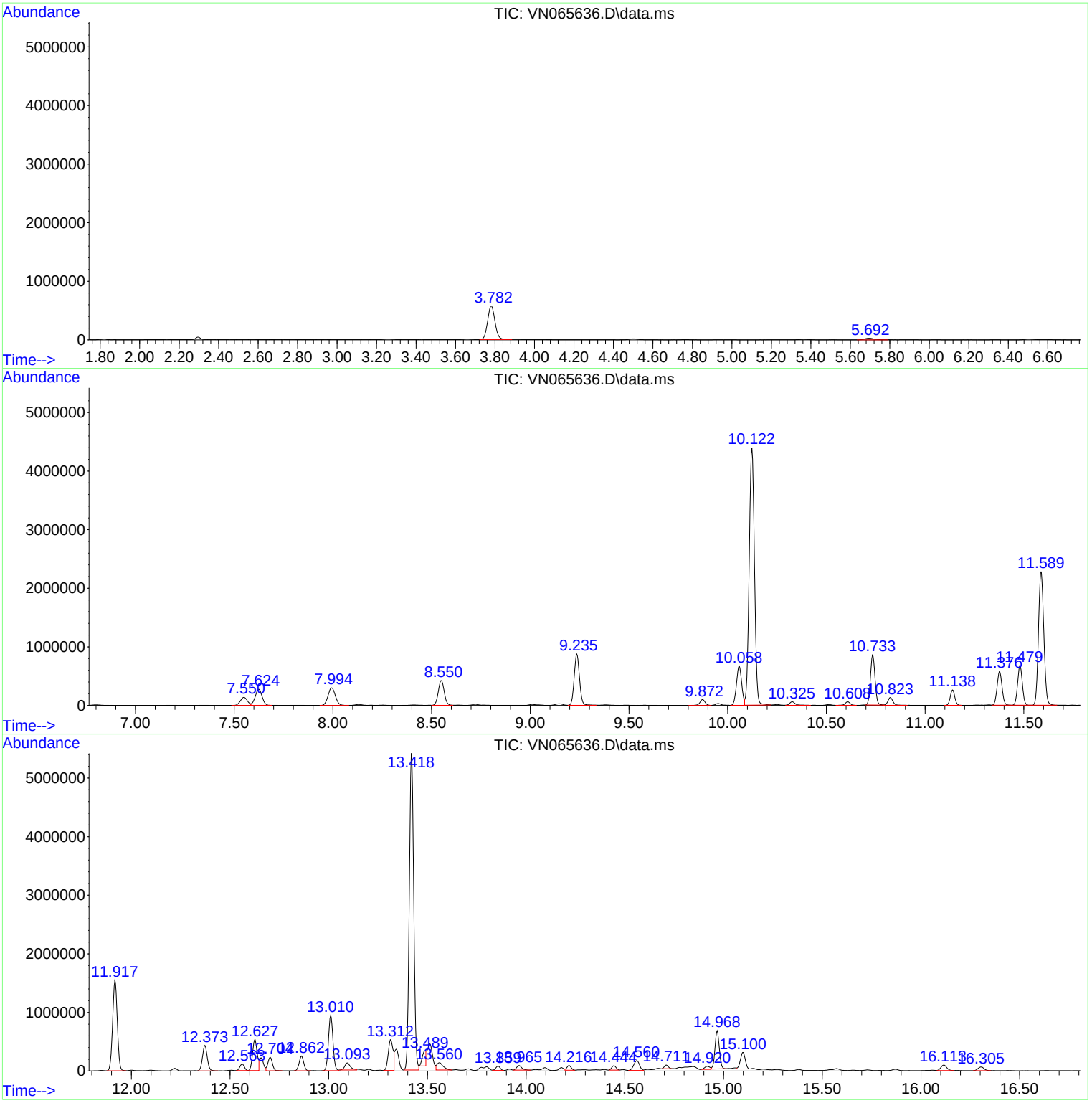
Sum of corrected areas: 43603510

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

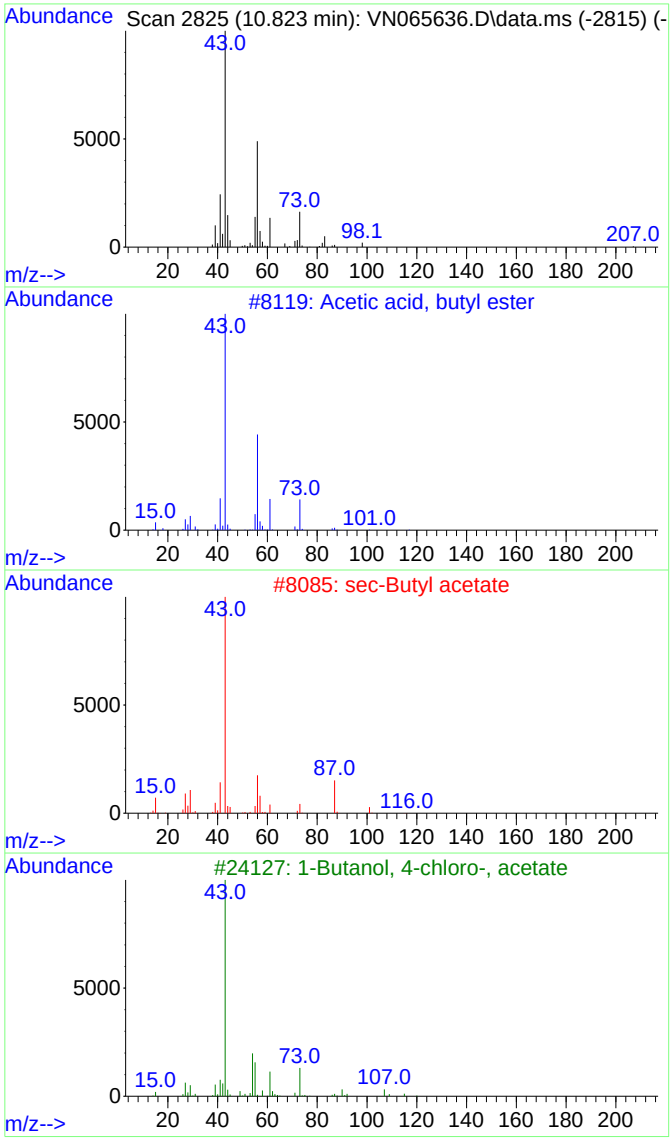
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

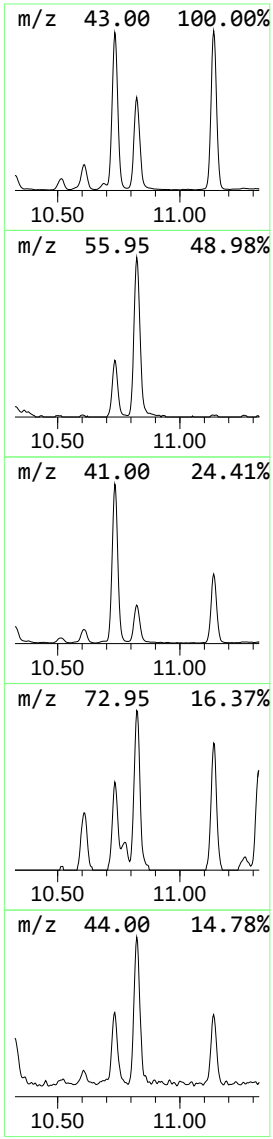
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.823	11.58 ug/l	232431	Chlorobenzene-d5	11.376

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
2	sec-Butyl acetate	116	C6H12O2	000105-46-4	33
3	1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	12
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10
5	Isopropyl acetate	102	C5H10O2	000108-21-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

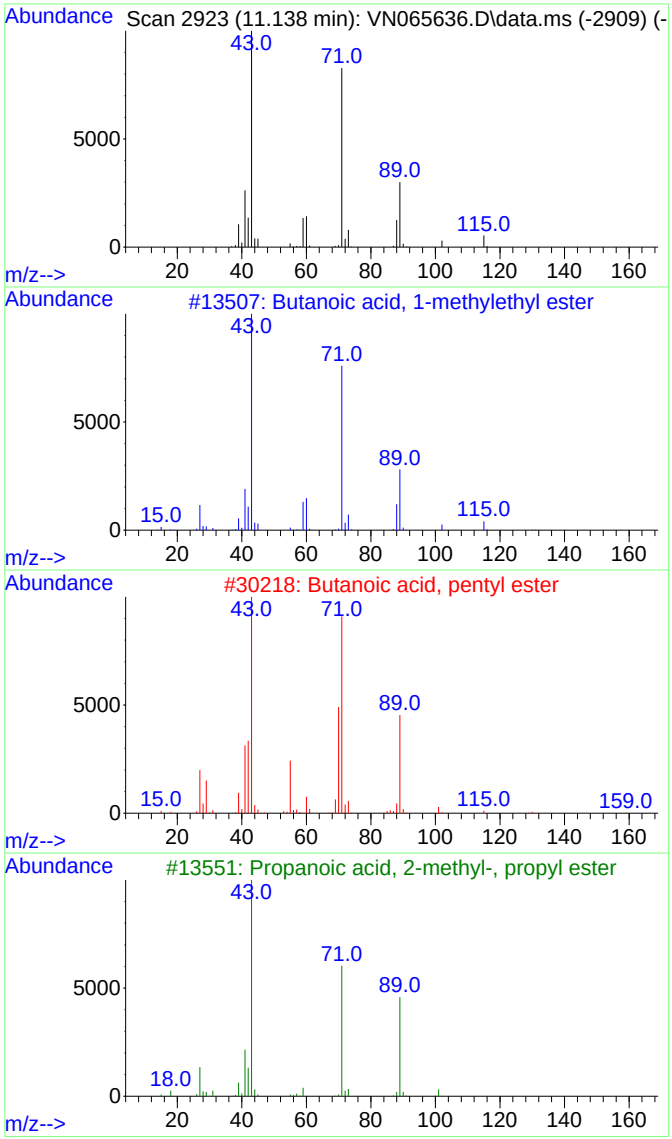
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

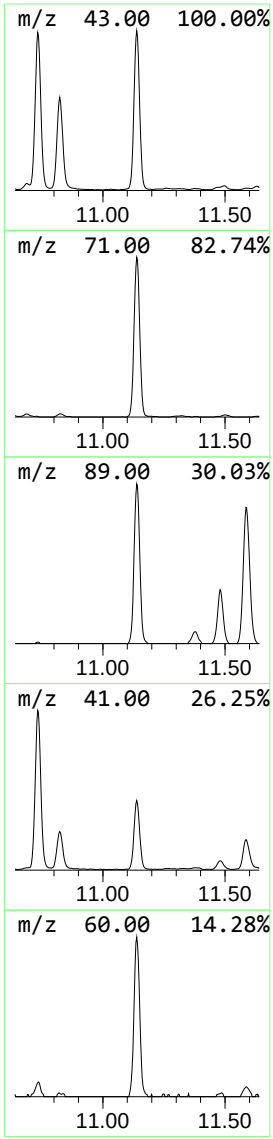
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanoic acid, 1-methylethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	21.00 ug/l	421512	Chlorobenzene-d5	11.376

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	47
5	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

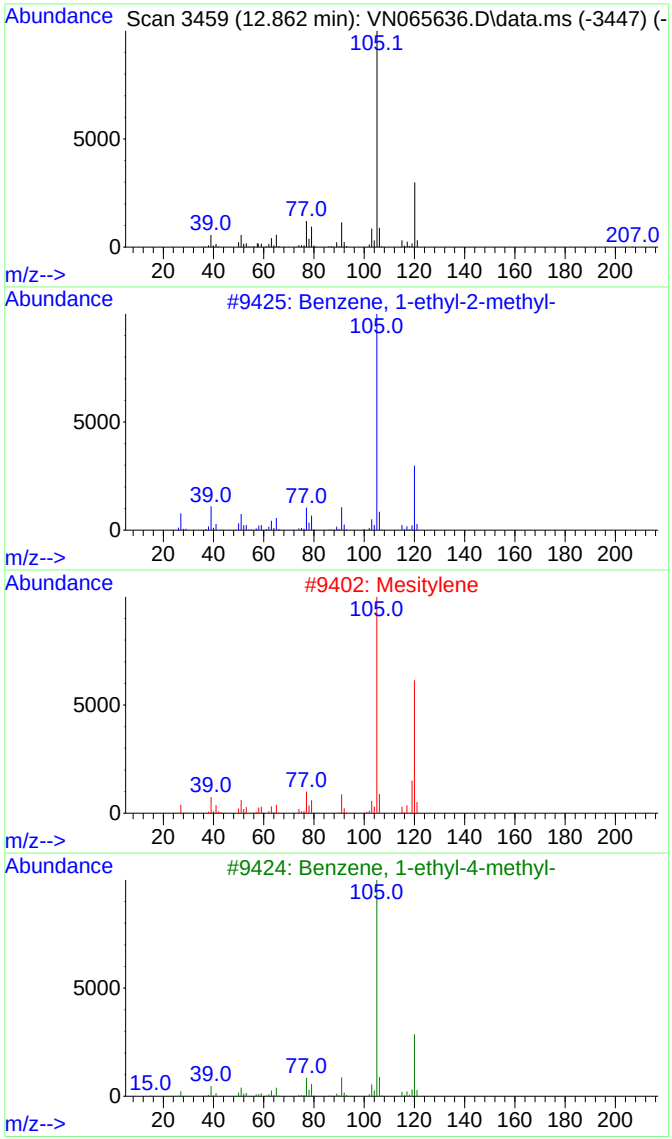
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

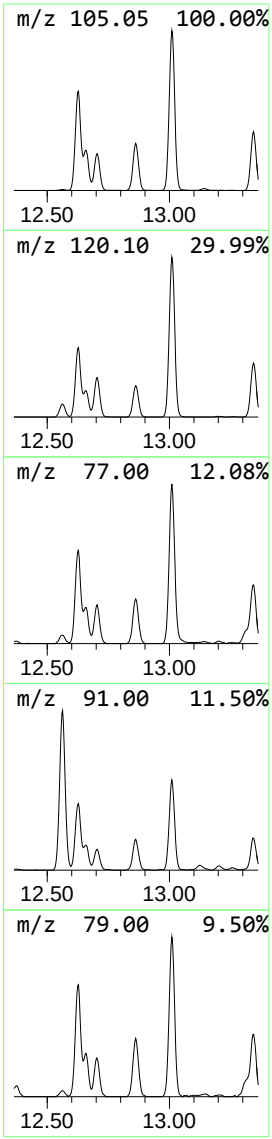
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.862	22.07 ug/l	403059	1,4-Dichlorobenzene-d4	13.315

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

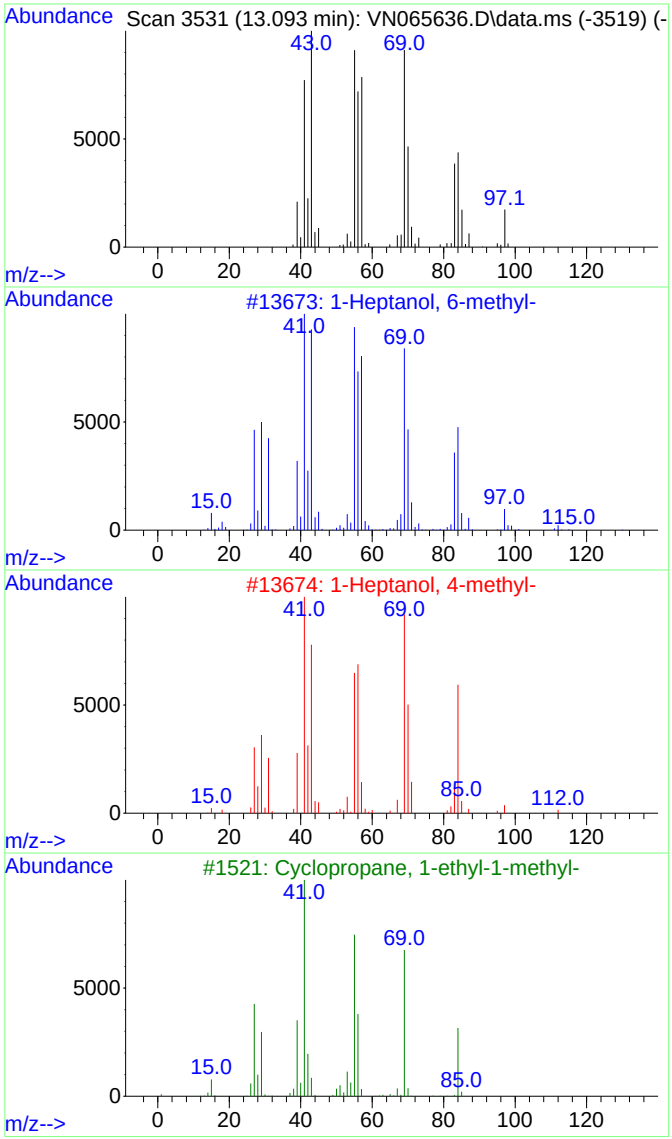
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

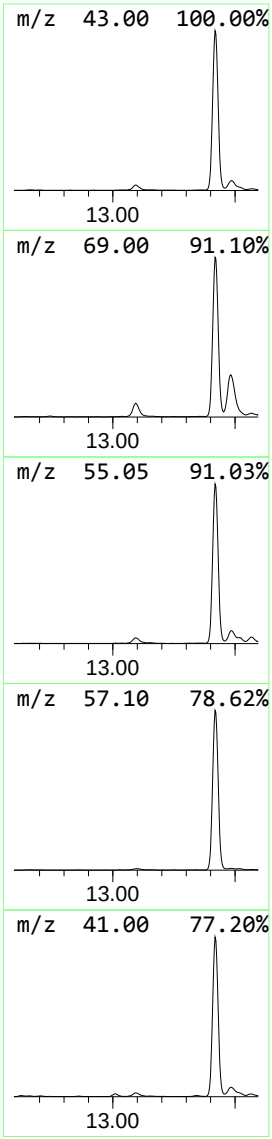
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heptanol, 6-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.093	13.61 ug/l	248568	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	90
2	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	53
3	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	50
4	1-Octanol	130	C8H18O	000111-87-5	50
5	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

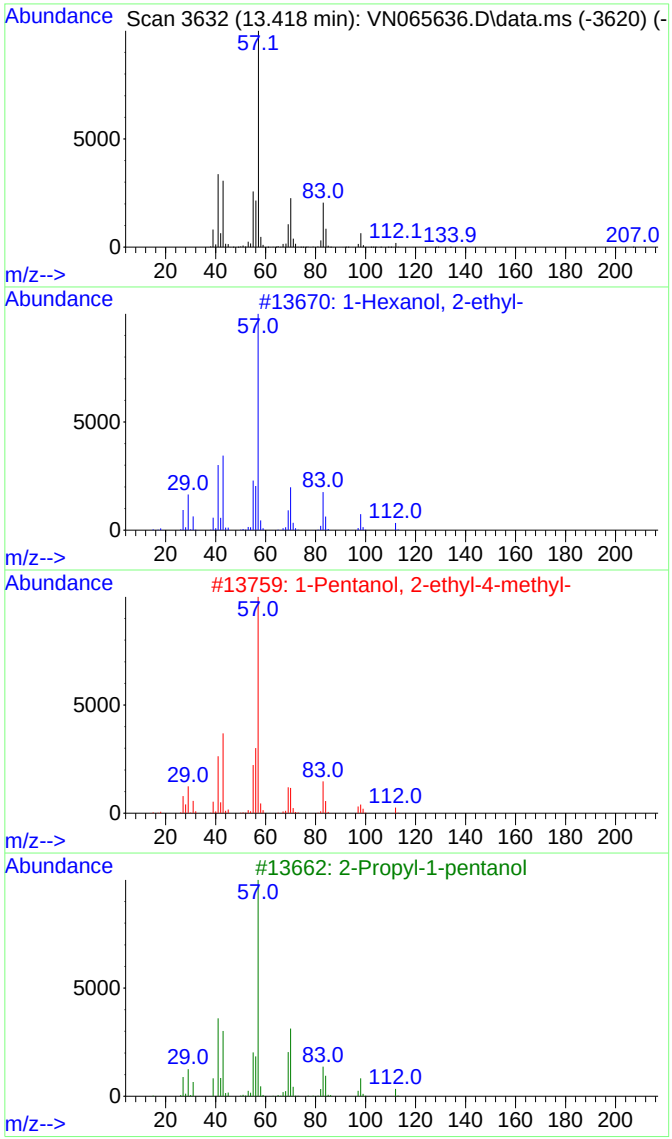
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

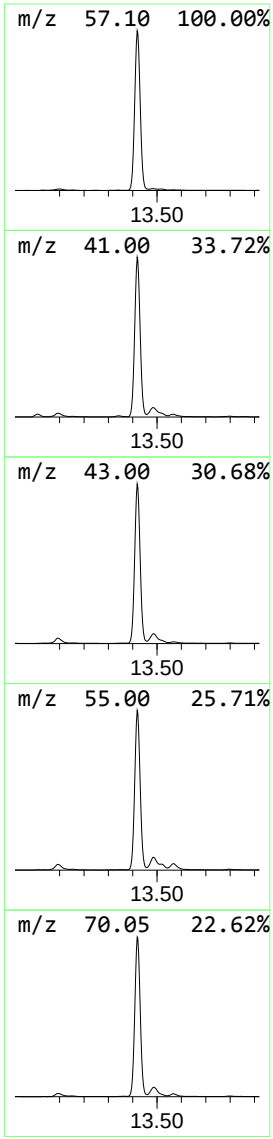
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.418	460.95 ug/l	8417860	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

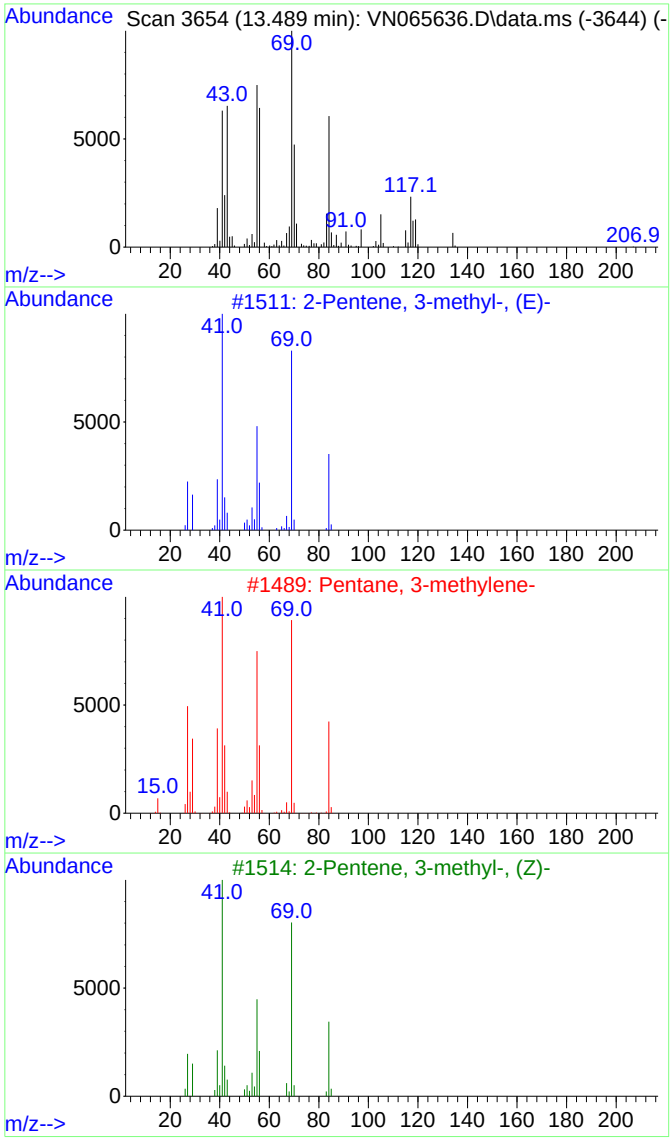
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

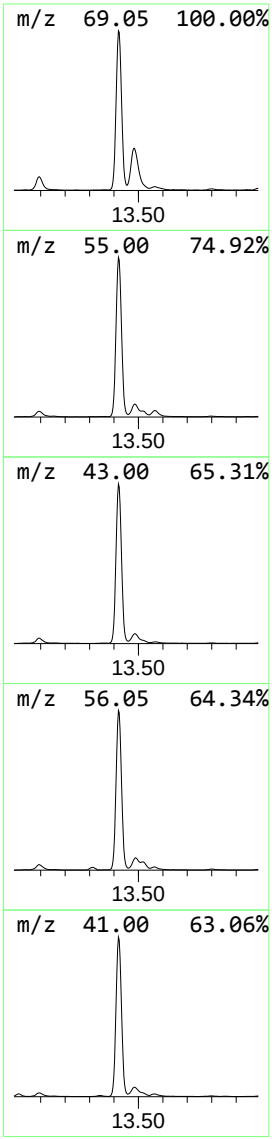
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Pentene, 3-methyl-, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.489	17.95 ug/l	327889	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	50
2	Pentane, 3-methylene-	84	C6H12	000760-21-4	50
3	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	50
4	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	43
5	1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

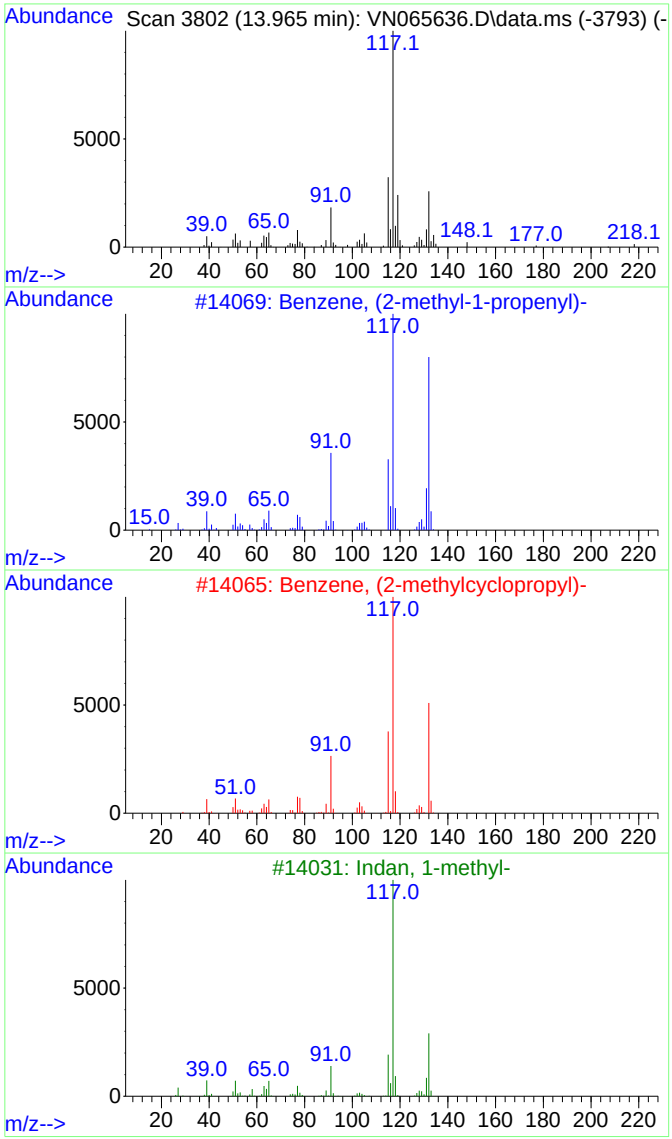
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

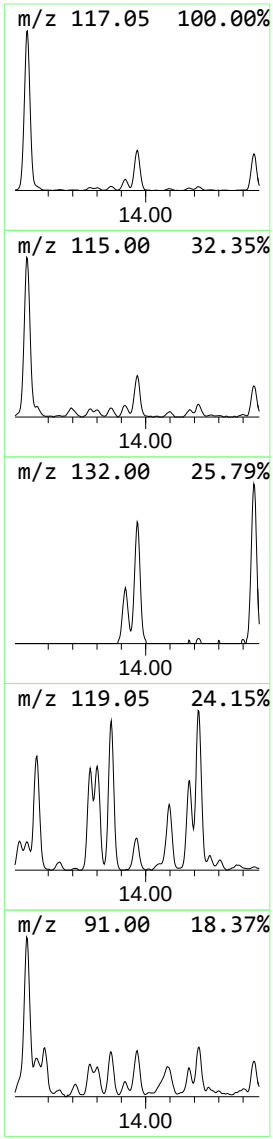
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, (2-methyl-1-propen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	7.90 ug/l	144207	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
2	Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	76
3	Indan, 1-methyl-	132	C10H12	000767-58-8	76
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	74
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

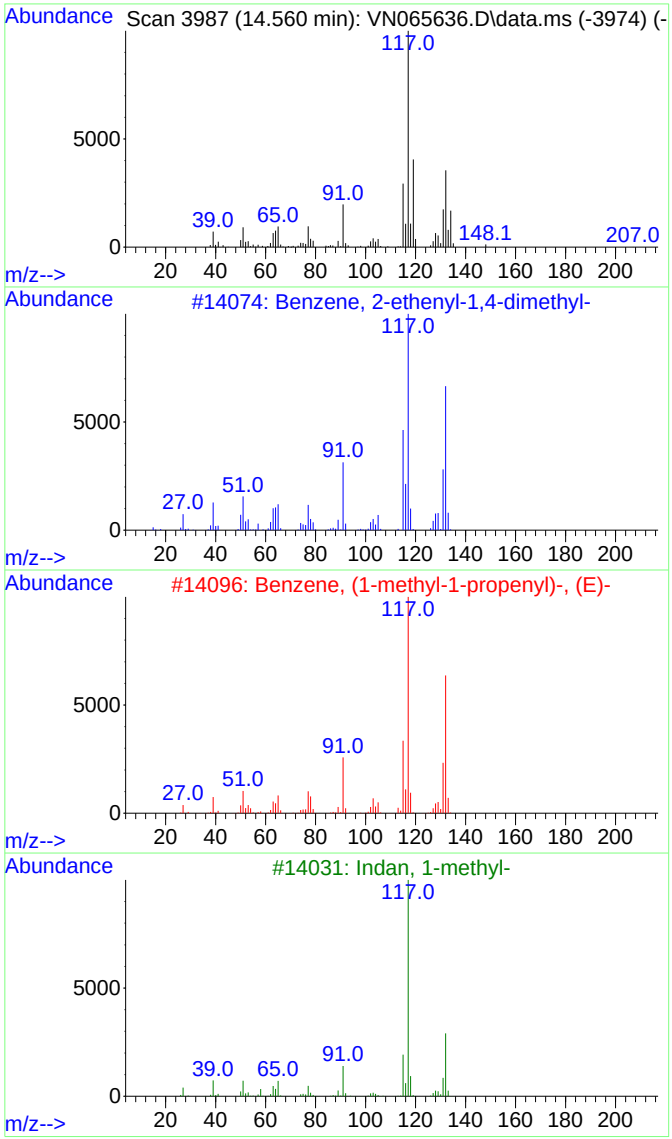
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

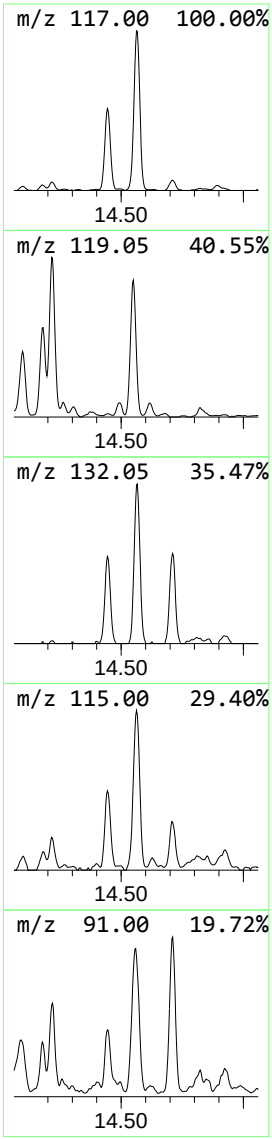
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.560	18.63 ug/l	340225	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	76
3	Indan, 1-methyl-	132	C10H12	000767-58-8	70
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70
5	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

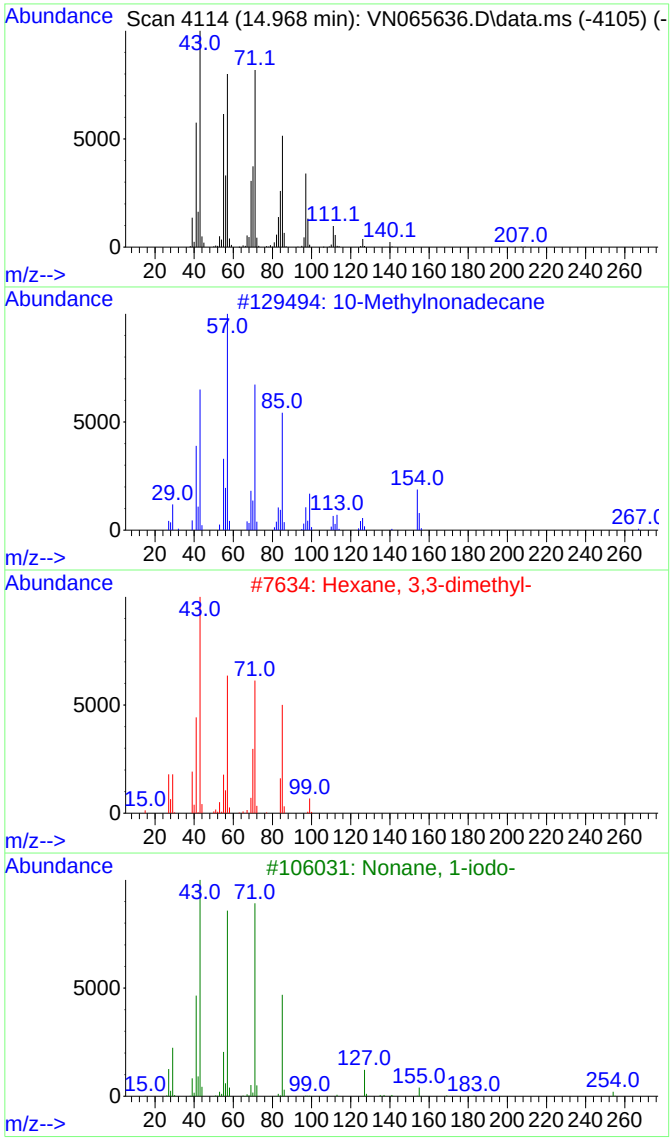
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

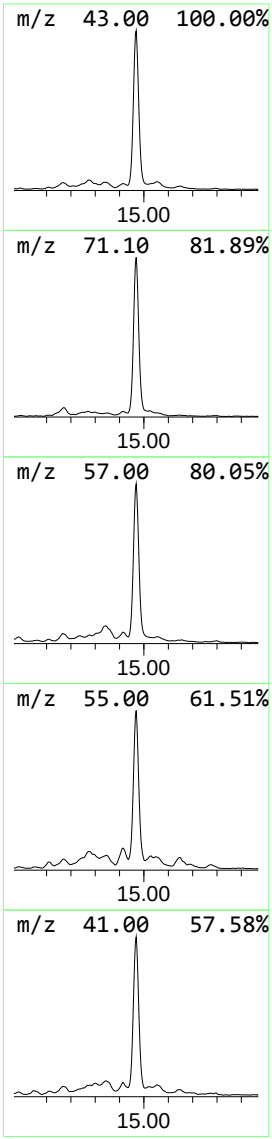
****

Peak Number 9 10-Methylnonadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	54.12 ug/l	988385	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	64
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	58
3	Nonane, 1-iodo-	254	C9H19I	004282-42-2	47
4	Octane, 4-methyl-	128	C9H20	002216-34-4	43
5	1-Tetradecene	196	C14H28	001120-36-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1125

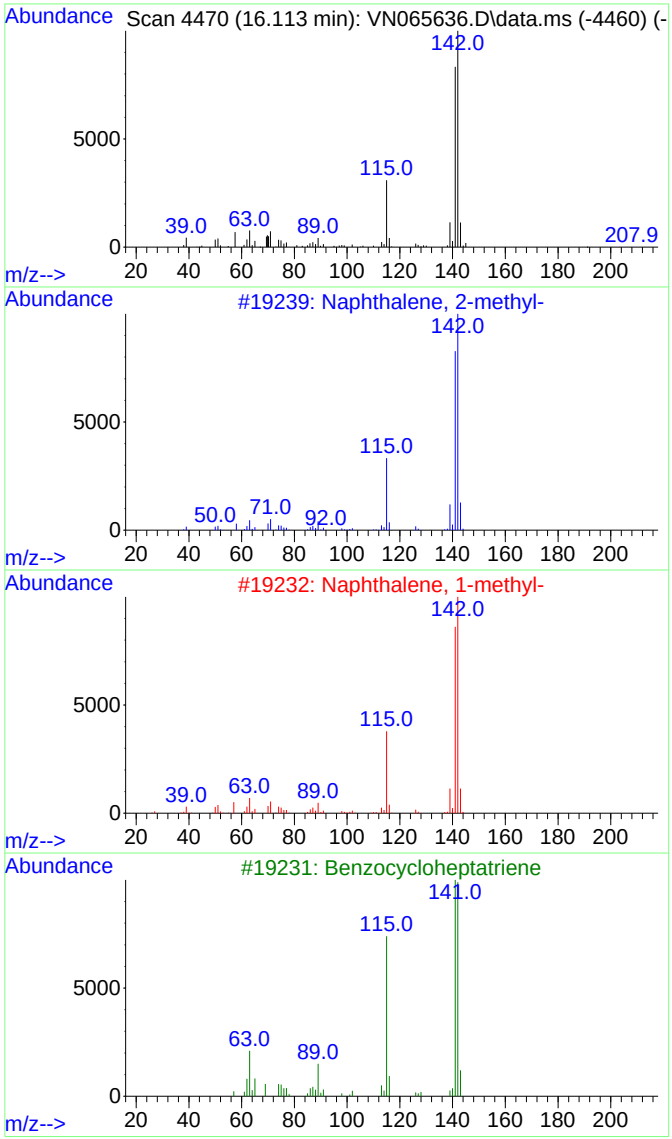
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

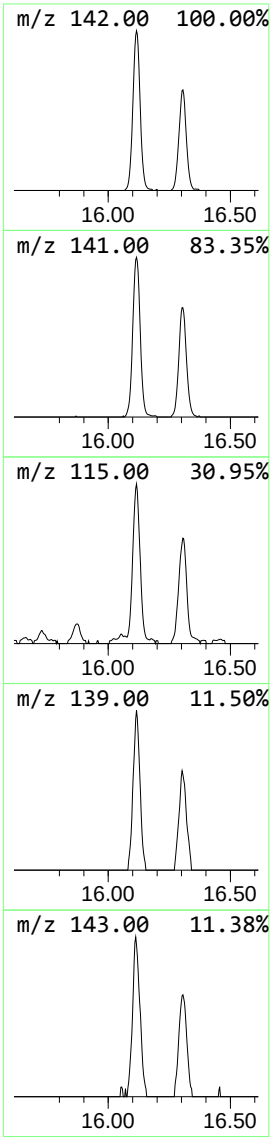
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.113	10.27 ug/l	187517	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	93
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065636.D
Acq On : 27 Jan 2021 17:50
Operator : JC/MD
Sample : M1229-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TRE-1125

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.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
Acetic acid, bu...	10.823	11.6	ug/l	232431	3	11.376	1003380	50.0
Butanoic acid, ...	11.139	21.0	ug/l	421512	3	11.376	1003380	50.0
Benzene, 1-ethy...	12.862	22.1	ug/l	403059	4	13.315	913094	50.0
1-Heptanol, 6-m...	13.093	13.6	ug/l	248568	4	13.315	913094	50.0
1-Hexanol, 2-et...	13.418	461.0	ug/l	8417860	4	13.315	913094	50.0
2-Pentene, 3-me...	13.489	18.0	ug/l	327889	4	13.315	913094	50.0
Benzene, (2-met...	13.965	7.9	ug/l	144207	4	13.315	913094	50.0
Benzene, 2-ethe...	14.560	18.6	ug/l	340225	4	13.315	913094	50.0
10-Methylnonade...	14.968	54.1	ug/l	988385	4	13.315	913094	50.0
Naphthalene, 2-...	16.113	10.3	ug/l	187517	4	13.315	913094	50.0