LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

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\82N091620W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.547	833	873	927	rVB2	832028	4172995	3.17%	0.775%
2	5.007	983	1016	1045	rBV2	683441	2466636	1.87%	0.458%
3	6.582	1487	1506	1526	rBV	1547950	4745921	3.61%	0.882%
4	7.614	1788	1827	1843	rBV7	1726214	5788268	4.40%	1.075%
5	7.708	1844	1856	1878	rVB2	498360	1382708	1.05%	0.257%
6	7.839	1878	1897	1909	rBV	794070	1948107	1.48%	0.362%
7	8.126	1969	1986	1993	rBV5	583834	1483913	1.13%	0.276%
8	8.267	2020	2030	2051	rVB	721989	1721400	1.31%	0.320%
9	8.547	2099	2117	2142	rBV3	1039128	2911352	2.21%	0.541%
10	9.048	2243	2273	2286	rBV	3659090	8926620	6.78%	1.658%
11	9.582	2427	2439	2447	rBV	979644	1938444	1.47%	0.360%
12	9.939	2537	2550	2561	rBV	1069242	1989446	1.51%	0.370%
13	10.058	2574	2587	2604	rBV3	1441659	3236316	2.46%	0.601%
14	10.257	2632	2649	2662	rVB7	433994	1340645	1.02%	0.249%
15	10.492	2710	2722	2739	rVB5	643221	1371434	1.04%	0.255%
16	11.383	2987	2999	3010	rBV2	916103	1692736	1.29%	0.314%
17	11.486	3011	3031	3049	rVV	29381432	53602965	40.73%	9.958%
18	11.589	3051	3063	3087	rVB	2136407	4203022	3.19%	0.781%
19	12.225	3249	3261	3272	rBV	4899225	8001487	6.08%	1.486%
20	12.566	3351	3367	3380	rBV	10974579	18785005	14.27%	3.490%
21	12.662	3380	3397	3403	rVV	4002541	6737773	5.12%	1.252%
22	12.711	3403	3412	3436	rVB	21496561	36472314	27.71%	6.775%
23	12.868	3446	3461	3476	rBV	10699718	18355688	13.95%	3.410%
24	13.019	3493	3508	3532	rVB	68875220	131621205	100.00%	24.451%
25	13.145	3533	3547	3557	rBV3	846328	1916711	1.46%	0.356%
26	13.351	3592	3611	3626	rBV	25634512	45338461	34.45%	8.422%
27	13.518	3642	3663	3671	rBV2	18039045	37296657	28.34%	6.928%
28	13.560	3671	3676	3694	rVV2	7959724	13943976	10.59%	2.590%
29	13.714	3712	3724	3733	rBV	2212615	3513867	2.67%	0.653%
30	13.778	3733	3744	3748	rVV	4823995	7455683	5.66%	1.385%
31	13.807	3749	3753	3761	rVV	4472819	6119407	4.65%	1.137%
32	13.865	3761	3771	3781	rVV	7059451	11079426	8.42%	2.058%
33	13.920	3781	3788	3794	rVV	1081813	1608006	1.22%	0.299%
34	13.968	3794	3803	3815	rVB2	4917011	7975619	6.06%	1.482%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

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\82N091620W.M
Title : SW846 8260

35	14.103	3834	3845	3855	rBV	2109685	3262910	2.48%	0.606%
36	14.183	3856	3870	3876	rBV	3645865	5897909	4.48%	1.096%
37	14.222	3876	3882	3891	rVB	5303541	7874175	5.98%	1.463%
38	14.450	3943	3953	3963	rBV	3992340	6108319	4.64%	1.135%
39	14.566	3975	3989	4001	rBV3	7990905	15751207	11.97%	2.926%
40	14.714	4024	4035	4051	rBV	1560509	2610688	1.98%	0.485%
41	14.823	4052	4069	4076	rBV4	744406	1692238	1.29%	0.314%
42	14.929	4090	4102	4115	rVB3	746029	1555094	1.18%	0.289%
43	15.103	4136	4156	4170	rBV	11414154	21018104	15.97%	3.904%
44	16.122	4459	4473	4499	rVB	3804477	7667717	5.83%	1.424%
45	16.309	4517	4531	4561	rVB	1748233	3728829	2.83%	0.693%

Sum of corrected areas: 538311403

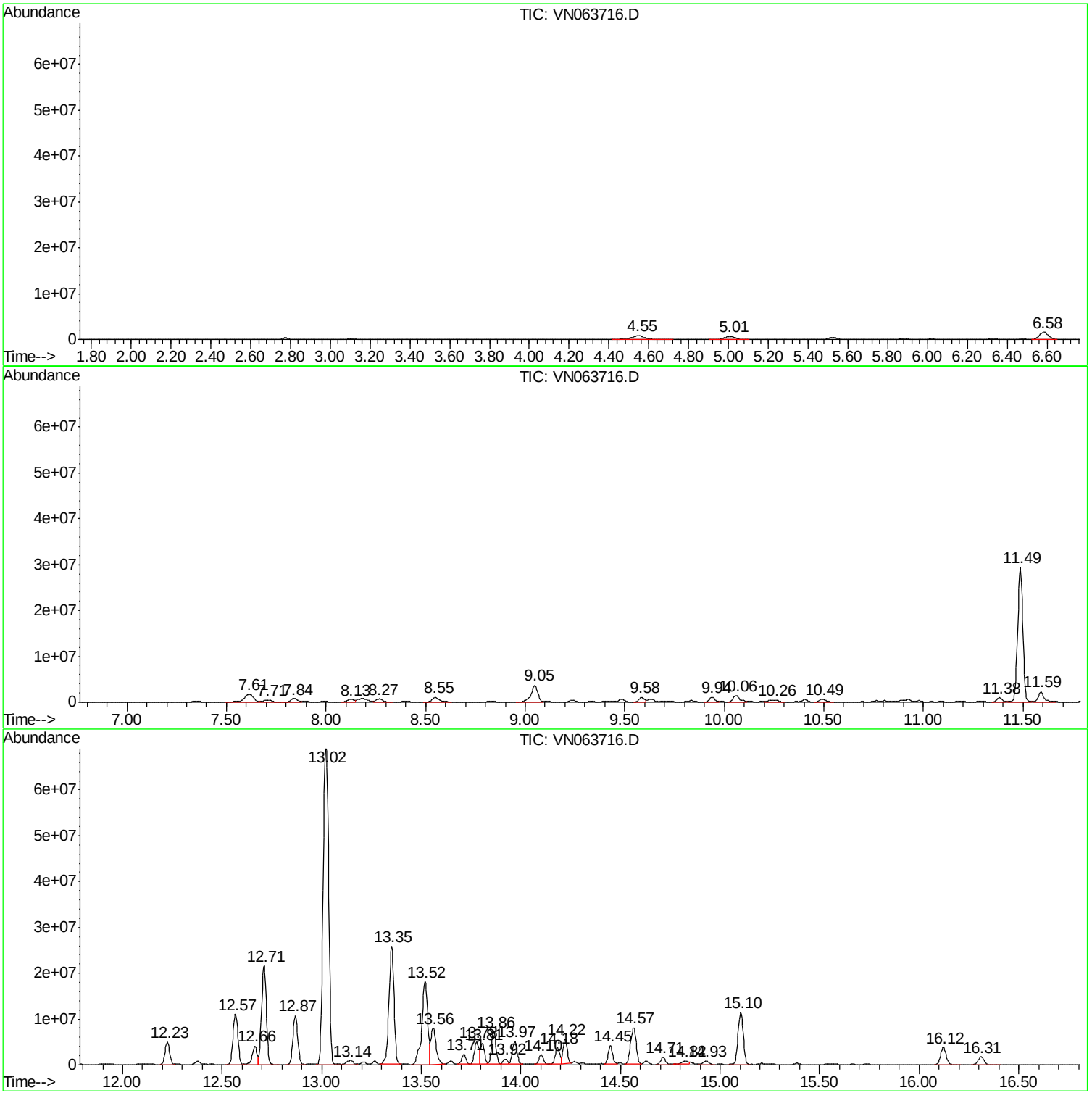
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

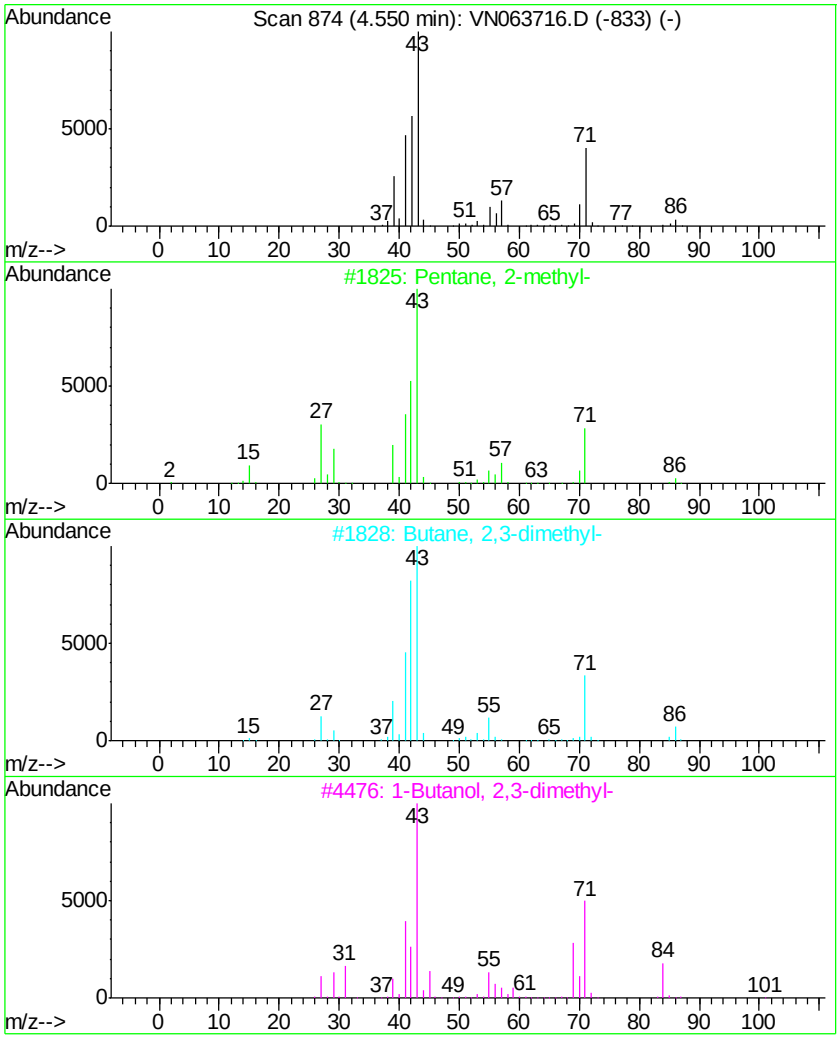
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

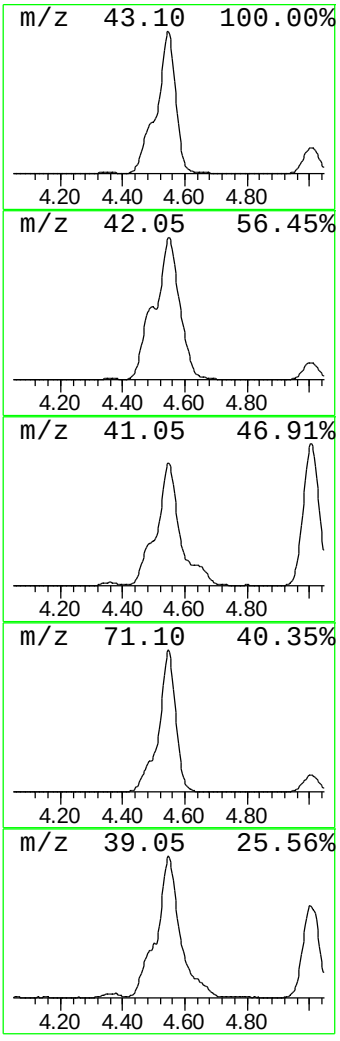
****

Peak Number 1 Pentane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	36.05 ug/l	4173000	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	49
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	42
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38
5	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	36





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

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

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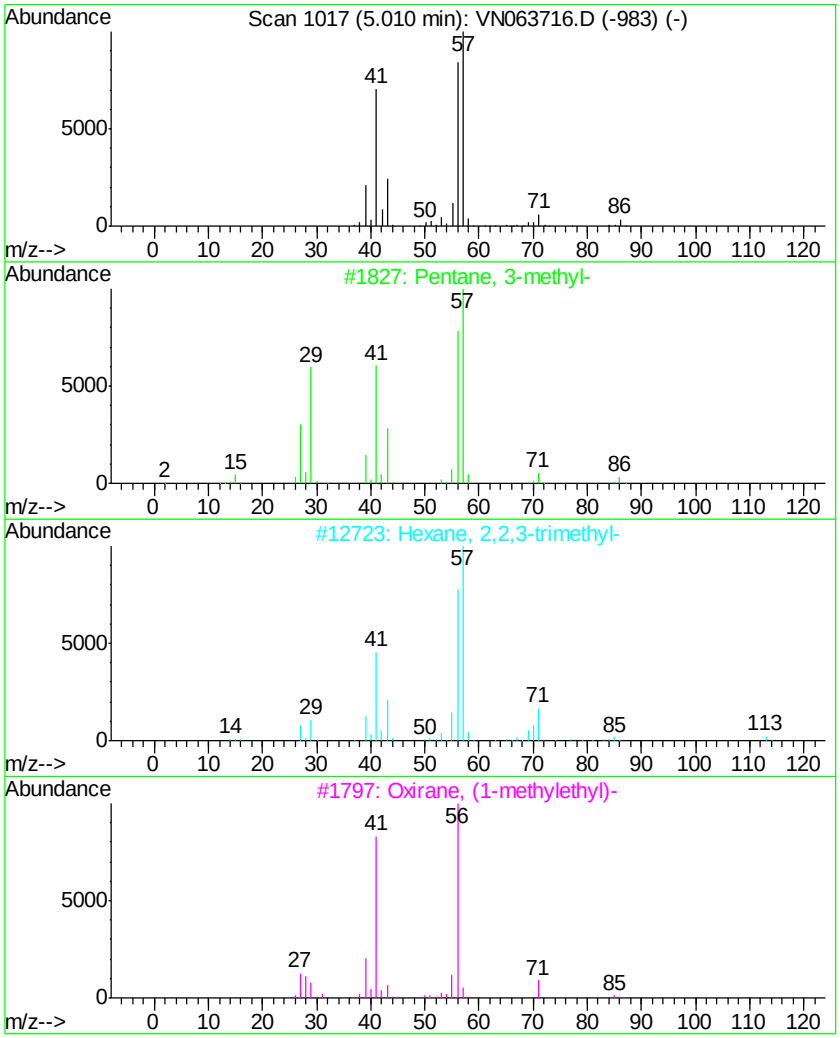
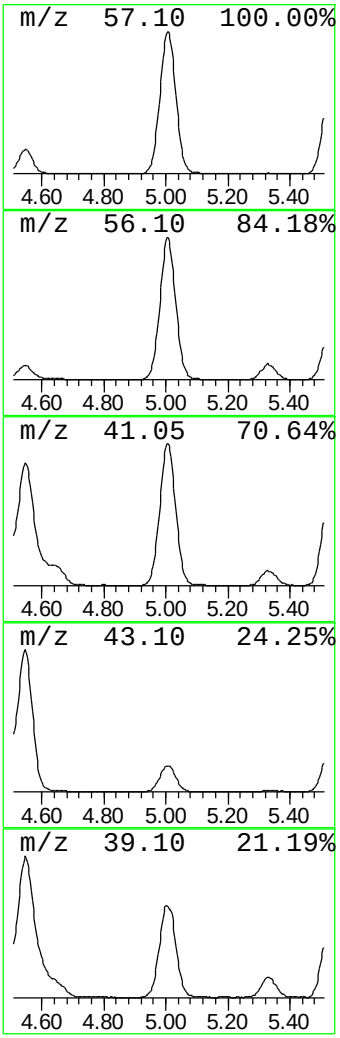
Peak Number 2 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	21.31 ug/l	2466640	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

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

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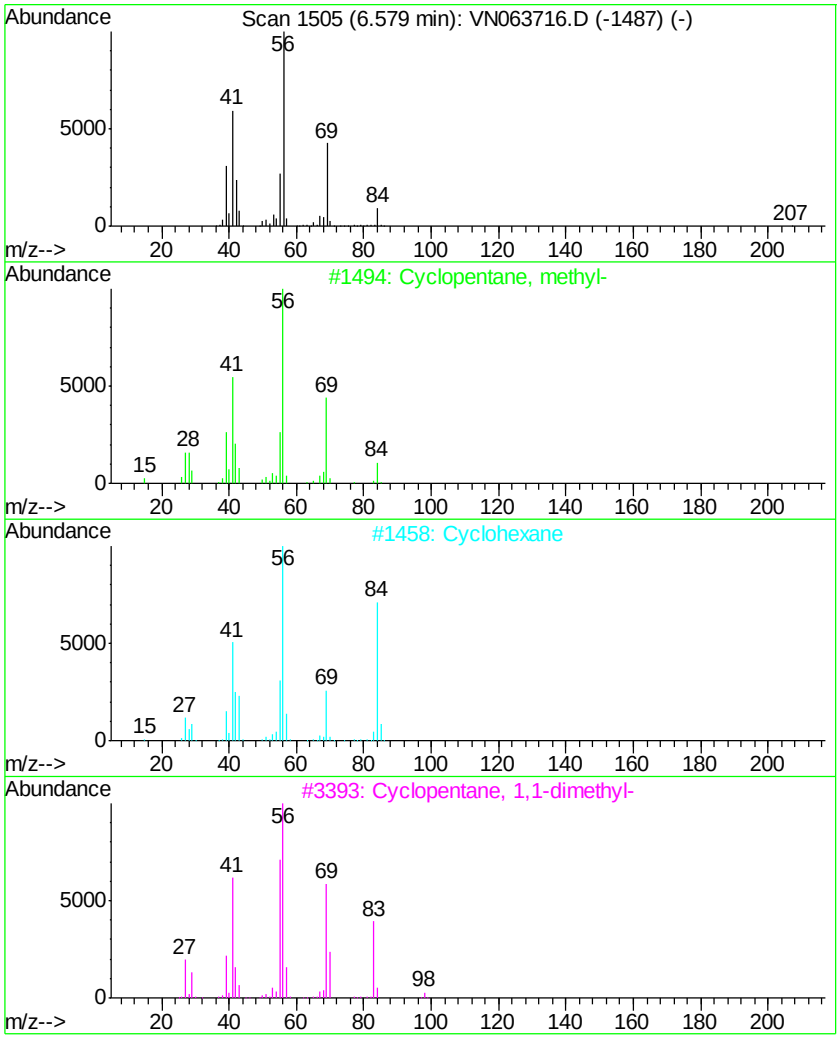
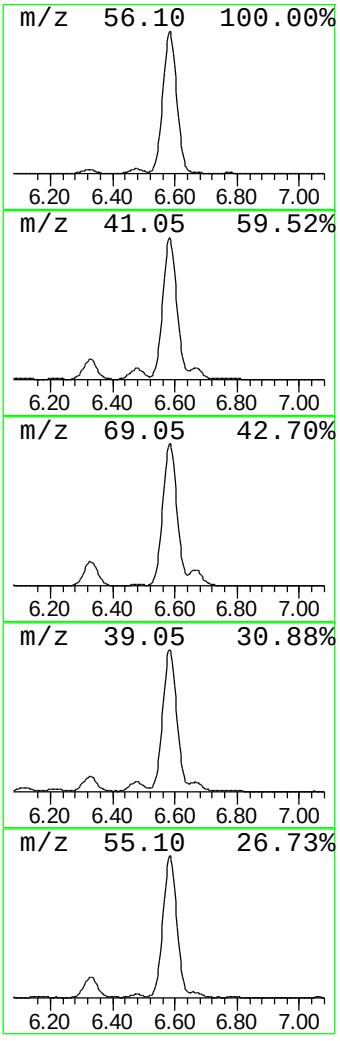
Peak Number 3 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	41.00 ug/l	4745920	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

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

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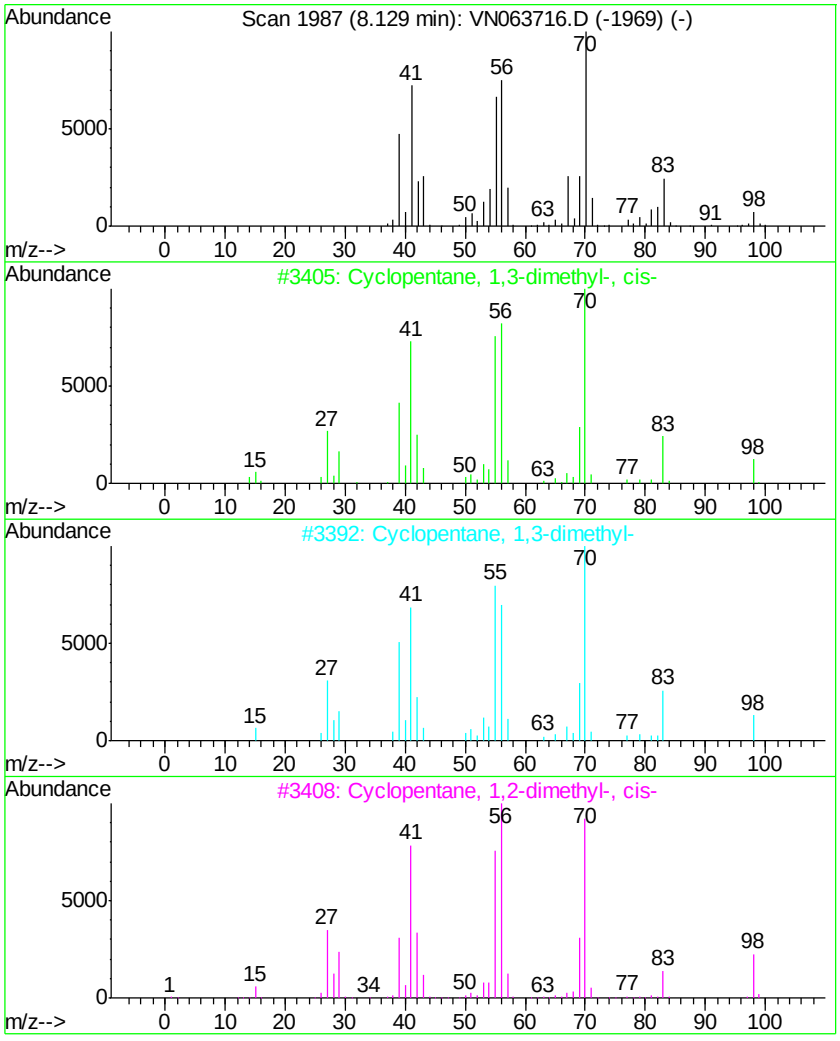
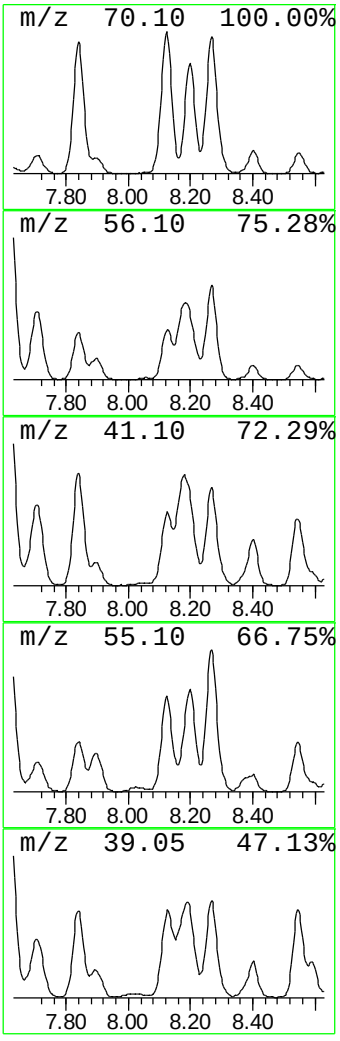
Peak Number 4 Cyclopentane, 1,3-dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	25.48 ug/l	1483910	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	64
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	59
3	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	50
4	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	43
5	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

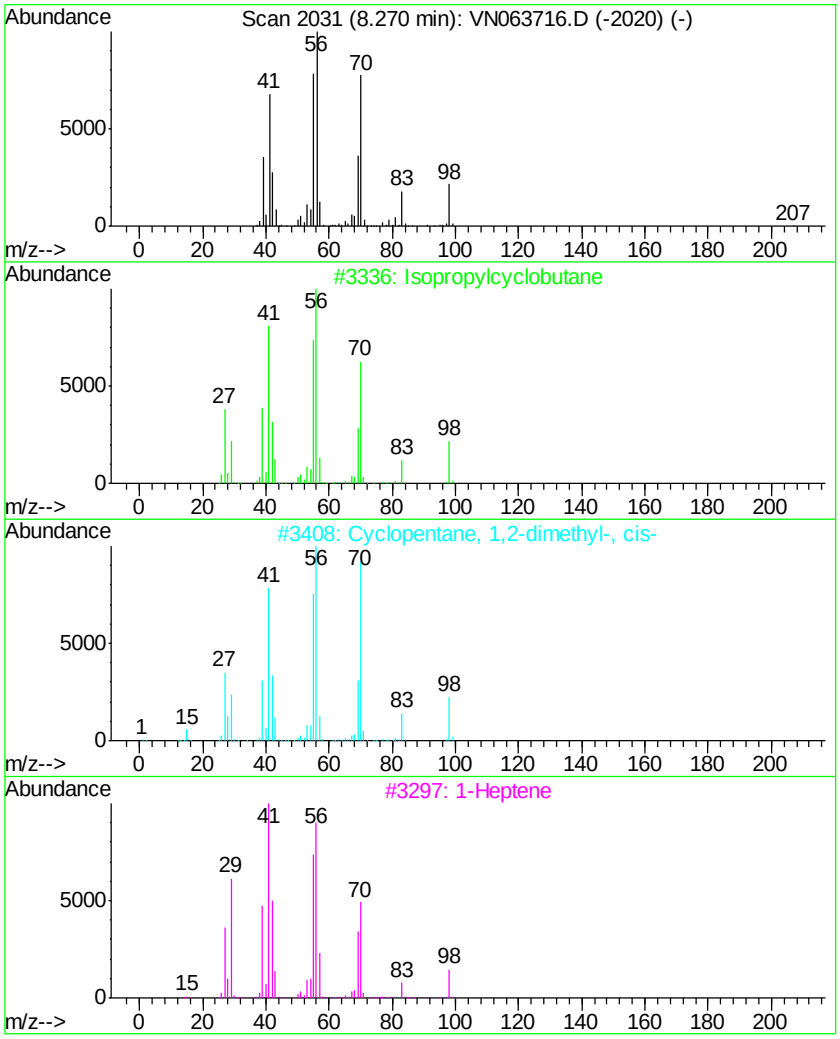
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

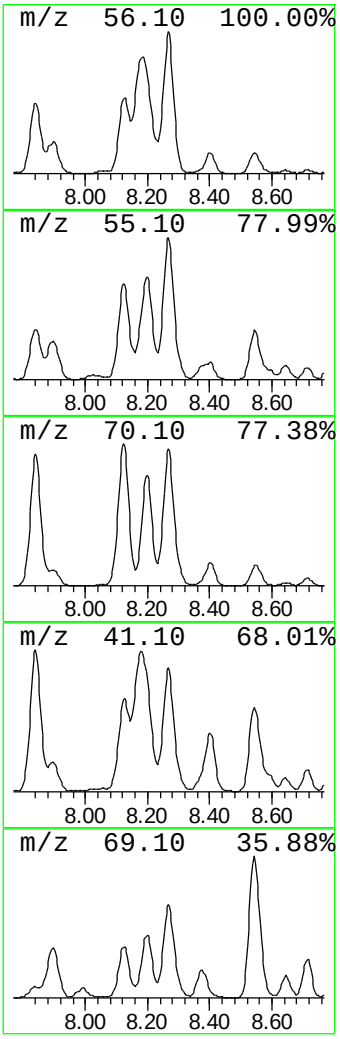
****

Peak Number 5 Isopropylcyclobutane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.27	29.56 ug/l	1721400	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	97
2	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	91
3	1-Heptene	98	C7H14	000592-76-7	91
4	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	91
5	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	87





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

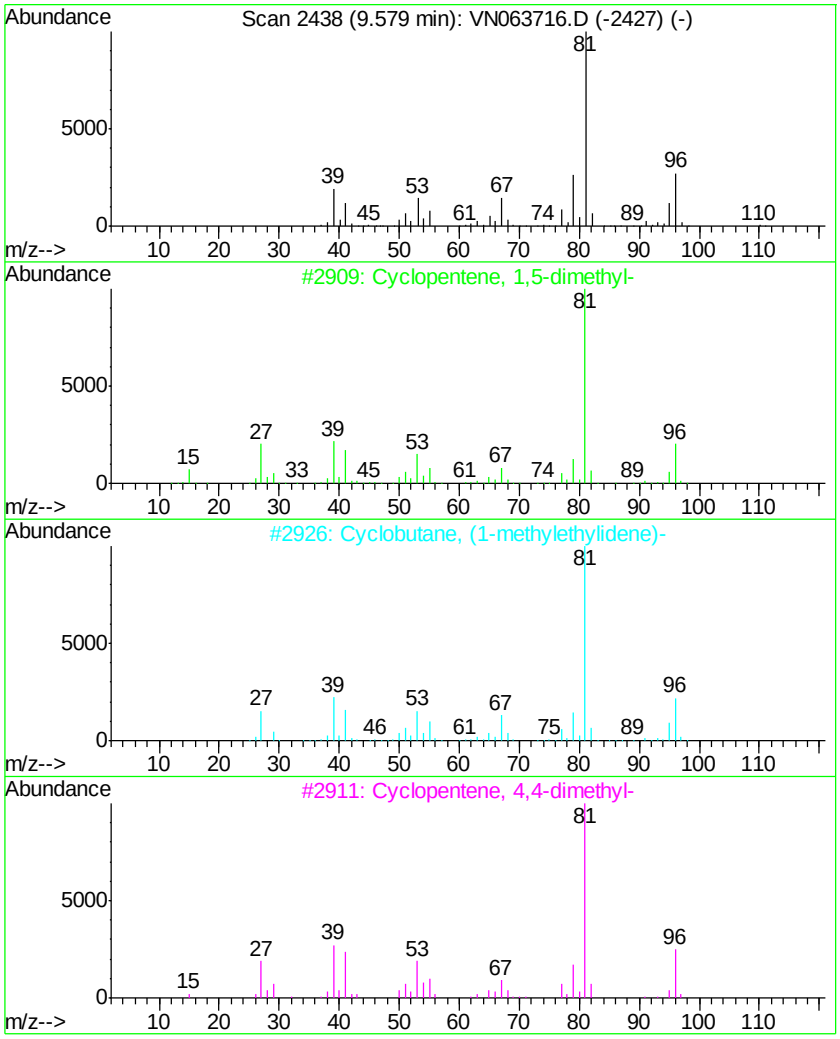
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

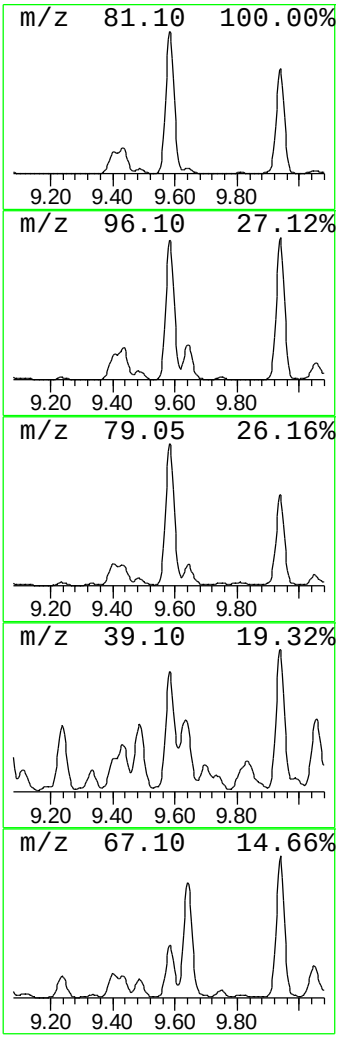
****

Peak Number 6 Cyclopentene, 1,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.58	33.29 ug/l	1938440	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	90
2	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
3	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	83
4	3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	78
5	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	72





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

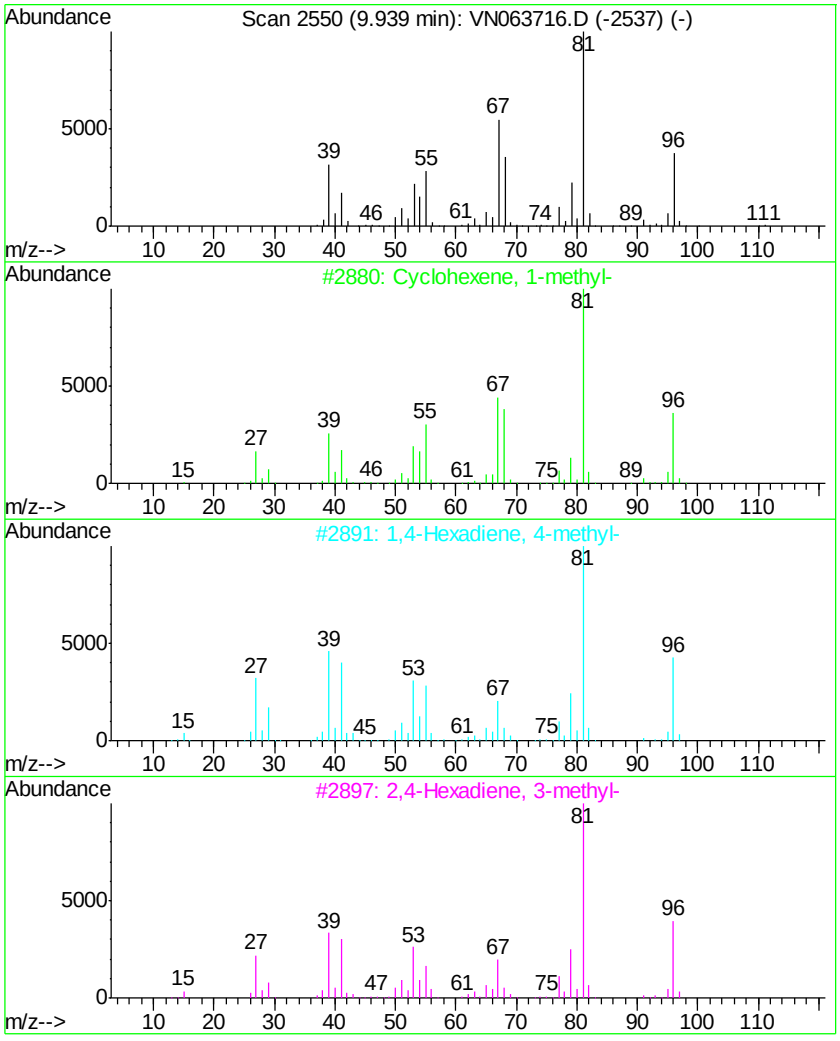
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

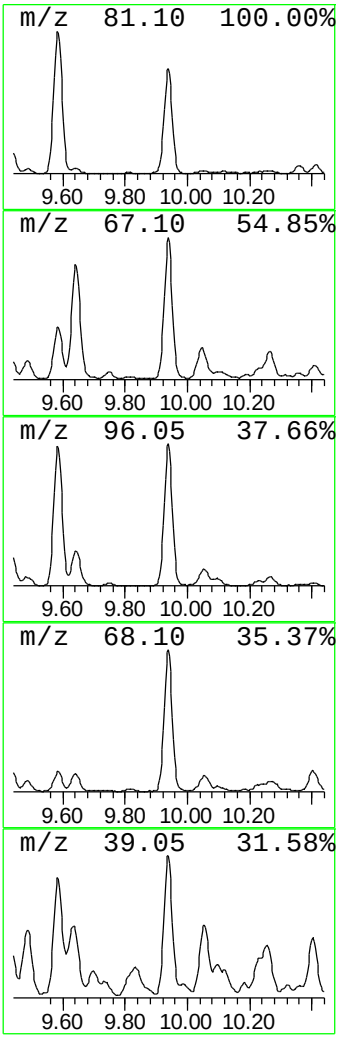
****

Peak Number 7 Cyclohexene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.94	34.17 ug/l	1989450	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	95
2	1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	95
3	2,4-Hexadiene, 3-methyl-	96	C7H12	028823-42-9	93
4	Cyclohexane, methylene-	96	C7H12	001192-37-6	87
5	Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	87





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

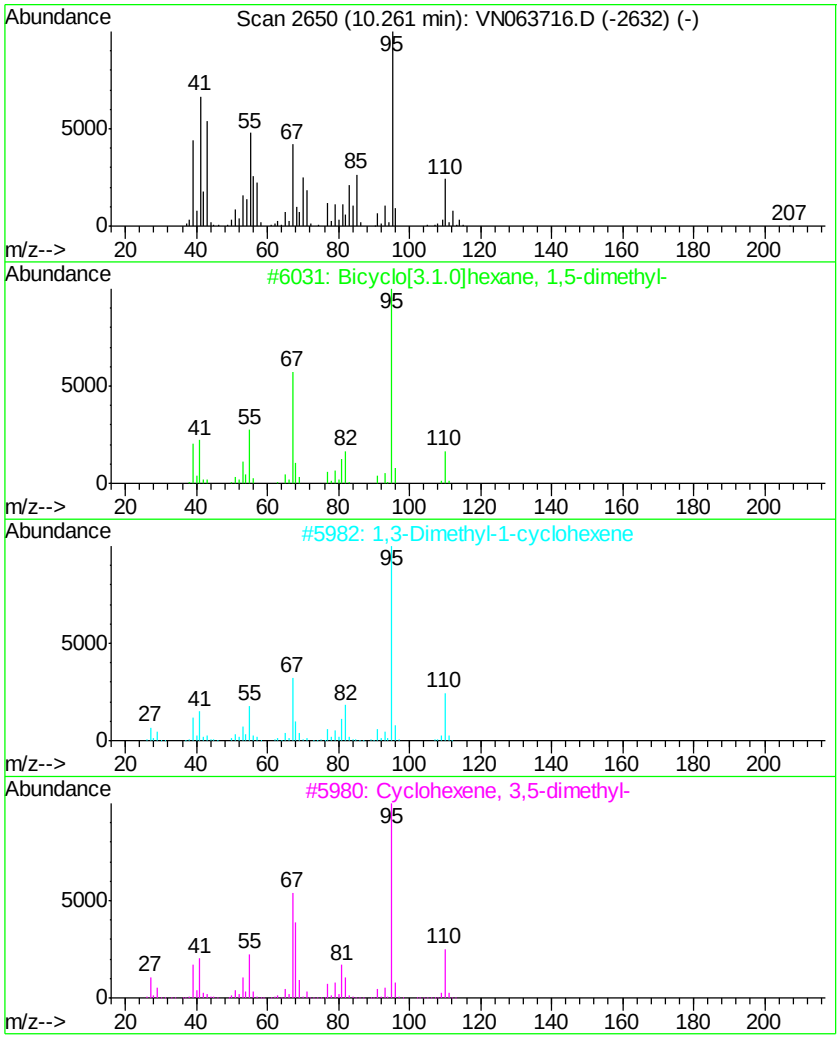
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

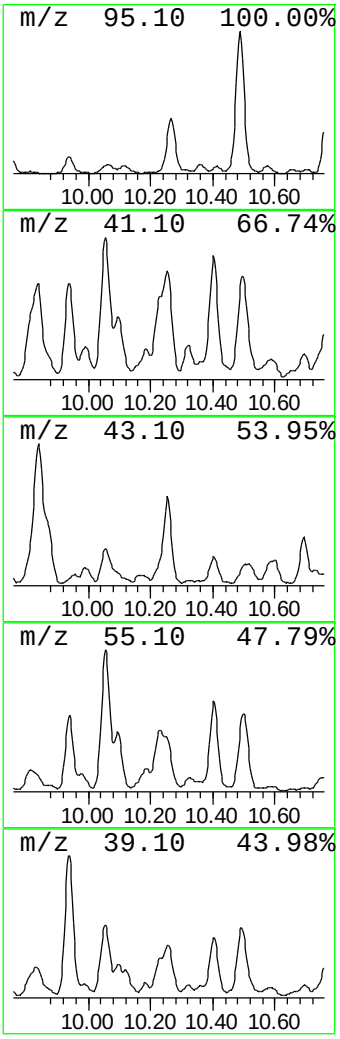
****

Peak Number 8 Bicyclo[3.1.0]hexane, 1,5-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	39.60 ug/l	1340650	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	55
2	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	55
3	Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	55
4	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	55
5	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	55





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

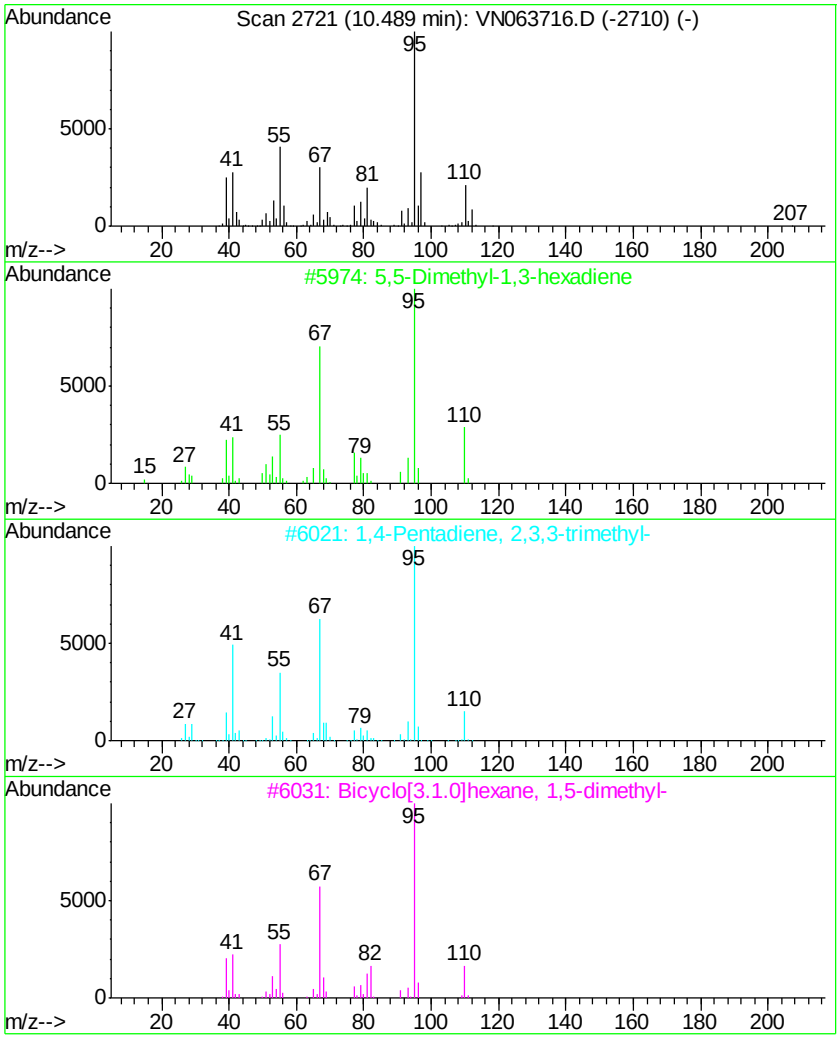
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

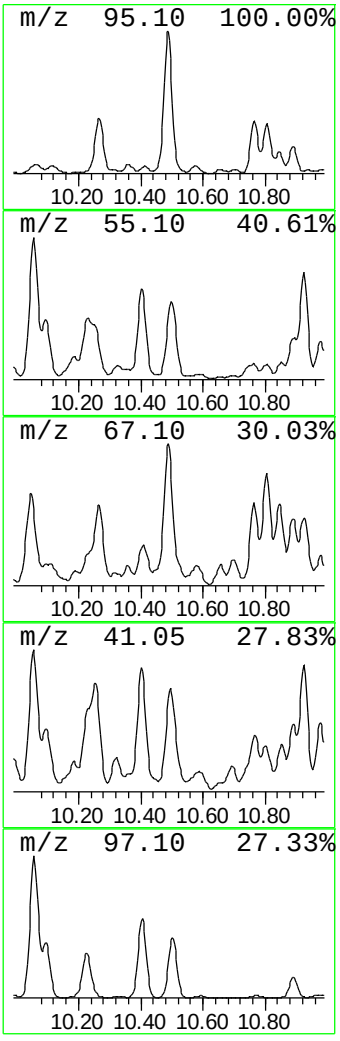
****

Peak Number 9 5,5-Dimethyl-1,3-hexadiene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.49	40.51 ug/l	1371430	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	87
2	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	76
3	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	76
4	trans-3,5-Dimethylcyclohexene	110	C8H14	056021-63-7	76
5	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	74





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.M
Quant Title : SW846 8260

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

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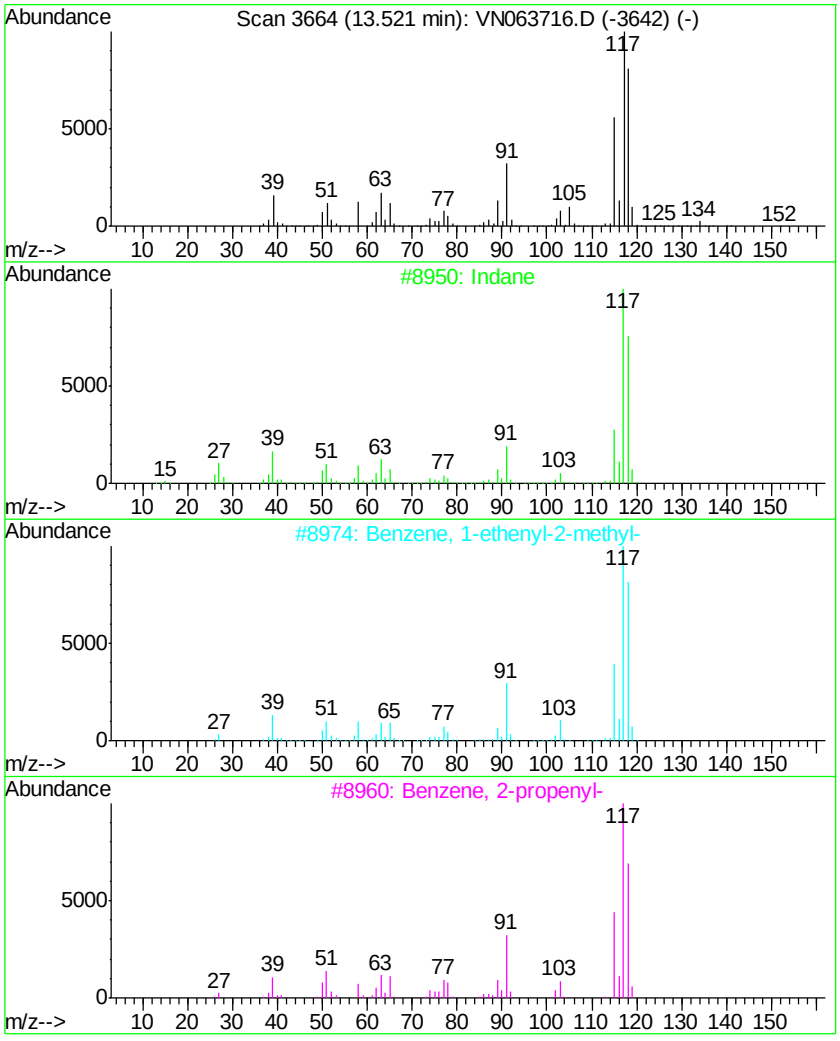
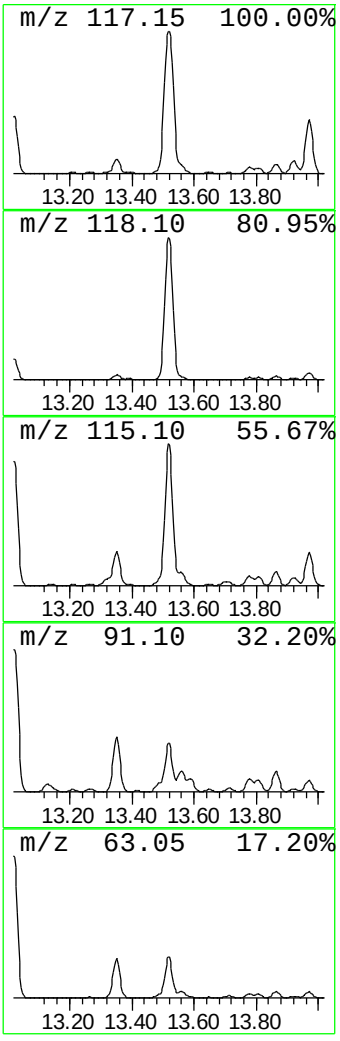
Peak Number 10 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	41.13 ug/l	37296700	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	90
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	89
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN092820\
Data File : VN063716.D
Acq On : 28 Sep 2020 19:32
Operator : JC/MD
Sample : L4178-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091620W.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
Pentane, 2-methyl-	4.55	36.0	ug/l	4173000	1	7.63	5788270	50.0
Pentane, 3-methyl-	5.01	21.3	ug/l	2466640	1	7.63	5788270	50.0
Cyclopentane, met...	6.58	41.0	ug/l	4745920	1	7.63	5788270	50.0
Cyclopentane, 1,3...	8.13	25.5	ug/l	1483910	2	8.55	2911350	50.0
Isopropylcyclobutane	8.27	29.6	ug/l	1721400	2	8.55	2911350	50.0
Cyclopentene, 1,5...	9.58	33.3	ug/l	1938440	2	8.55	2911350	50.0
Cyclohexene, 1-me...	9.94	34.2	ug/l	1989450	2	8.55	2911350	50.0
Bicyclo[3.1.0]hex...	10.26	39.6	ug/l	1340650	3	11.38	1692740	50.0
5,5-Dimethyl-1,3-...	10.49	40.5	ug/l	1371430	3	11.38	1692740	50.0
Indane	13.52	41.1	ug/l	37296700	4	13.32	45338500	50.0