LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

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\82N101221W.M
Title : SW846 8260

Signal : TIC: VN068895.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.314	83	121	130	rBV	157016	631284	26.09%	1.996%
2	4.285	832	856	919	rBV	643110	1984093	81.99%	6.273%
3	4.572	940	963	997	rVB2	102311	330229	13.65%	1.044%
4	5.363	1235	1258	1288	rVB2	11697	42165	1.74%	0.133%
5	7.072	1874	1895	1915	rBV6	12555	38996	1.61%	0.123%
6	7.335	1967	1993	2036	rBV	190767	534423	22.08%	1.690%
7	7.649	2089	2110	2135	rBV2	28350	80578	3.33%	0.255%
8	8.024	2226	2250	2261	rBV2	277197	665235	27.49%	2.103%
9	8.088	2262	2274	2306	rVB	537122	1224018	50.58%	3.870%
10	8.440	2385	2405	2431	rBV	297779	689448	28.49%	2.180%
11	8.652	2450	2484	2486	rBV3	12611	43901	1.81%	0.139%
12	8.839	2539	2554	2573	rVB2	27902	60156	2.49%	0.190%
13	8.971	2584	2603	2634	rBV	741424	1551025	64.09%	4.904%
14	9.158	2658	2673	2694	rBV3	16259	37033	1.53%	0.117%
15	9.274	2702	2716	2726	rBV3	18880	35707	1.48%	0.113%
16	9.413	2750	2768	2785	rBV	55103	110249	4.56%	0.349%
17	9.789	2892	2908	2925	rBV3	56716	115499	4.77%	0.365%
18	10.333	3096	3111	3127	rBV2	83656	159671	6.60%	0.505%
19	10.443	3135	3152	3175	rBV	1146224	2143948	88.59%	6.779%
20	10.856	3299	3306	3320	rVB4	15251	25998	1.07%	0.082%
21	10.950	3328	3341	3350	rBV3	23672	51980	2.15%	0.164%
22	11.087	3366	3392	3417	rBV3	103173	204327	8.44%	0.646%
23	11.186	3420	3429	3441	rVV3	19305	30365	1.25%	0.096%
24	11.747	3619	3638	3662	rBV	1018015	1913059	79.05%	6.049%
25	12.101	3759	3770	3778	rBV	39090	66443	2.75%	0.210%
26	12.272	3823	3834	3850	rVB2	22872	39954	1.65%	0.126%
27	12.353	3850	3864	3886	rBV	153439	260788	10.78%	0.825%
28	12.455	3887	3902	3913	rBV5	15743	33222	1.37%	0.105%
29	12.734	3991	4006	4029	rBV	809709	1415767	58.50%	4.476%
30	12.935	4071	4081	4093	rBV4	15248	28682	1.19%	0.091%
31	13.055	4120	4126	4138	rVB3	19967	30682	1.27%	0.097%
32	13.195	4162	4178	4194	rBV3	107882	192227	7.94%	0.608%
33	13.334	4208	4230	4243	rBV2	149211	257784	10.65%	0.815%
34	13.412	4245	4259	4271	rBV	1464220	2316585	95.72%	7.325%
35	13.517	4289	4298	4311	rVB5	25588	40643	1.68%	0.129%
36	13.675	4343	4357	4369	rBV	980846	1658858	68.55%	5.245%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

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\82N101221W.M
Title : SW846 8260

37	13.739	4369	4381	4407	rVB3	1119007	2164952	89.46%	6.845%
38	13.946	4447	4458	4472	rVB2	129777	208702	8.62%	0.660%
39	14.072	4495	4505	4520	rBV3	75450	133008	5.50%	0.421%
40	14.142	4520	4531	4557	rVB6	100884	262933	10.86%	0.831%
41	14.268	4566	4578	4590	rBV3	96044	154108	6.37%	0.487%
42	14.348	4592	4608	4626	rBV	1239128	1963139	81.12%	6.207%
43	14.418	4628	4634	4641	rBV4	19626	24919	1.03%	0.079%
44	14.528	4662	4675	4694	rBV	668493	1074644	44.41%	3.398%
45	14.635	4702	4715	4719	rBV	770725	1138949	47.06%	3.601%
46	14.665	4720	4726	4749	rVV	1566883	2420042	100.00%	7.652%
47	14.753	4751	4759	4776	rVB4	89150	164675	6.80%	0.521%
48	14.887	4795	4809	4821	rBV8	49637	96006	3.97%	0.304%
49	14.962	4825	4837	4844	rBV4	23321	46184	1.91%	0.146%
50	15.131	4892	4900	4908	rBV2	19236	30341	1.25%	0.096%
51	15.204	4911	4927	4945	rVB3	776144	1389990	57.44%	4.395%
52	15.322	4958	4971	4973	rBV4	129351	183567	7.59%	0.580%
53	15.348	4975	4981	4996	rVB2	239071	379961	15.70%	1.201%
54	15.480	5017	5030	5037	rBV	171534	317530	13.12%	1.004%
55	15.517	5038	5044	5080	rVB4	208598	428458	17.70%	1.355%

Sum of corrected areas: 31627130

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Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
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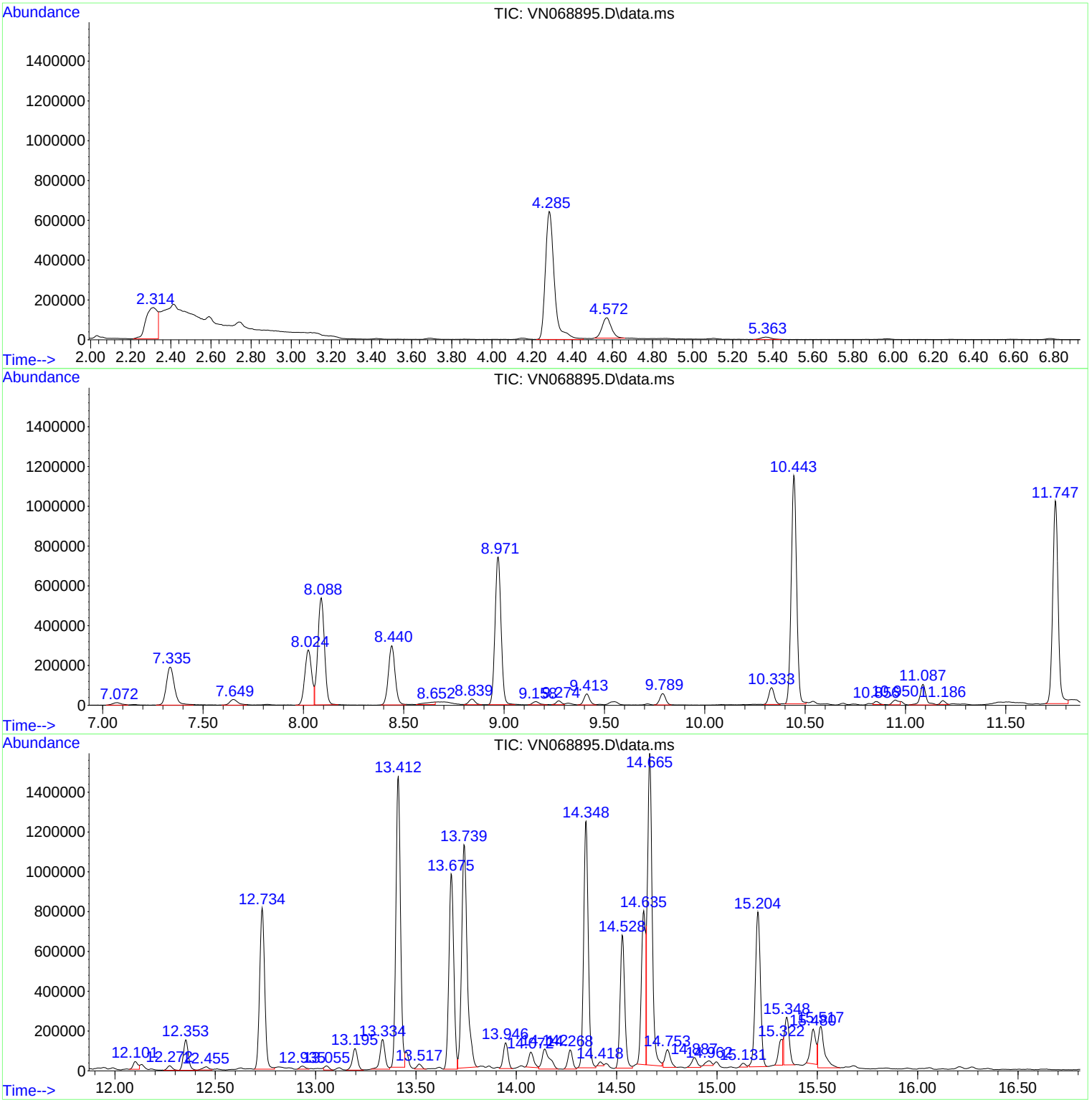
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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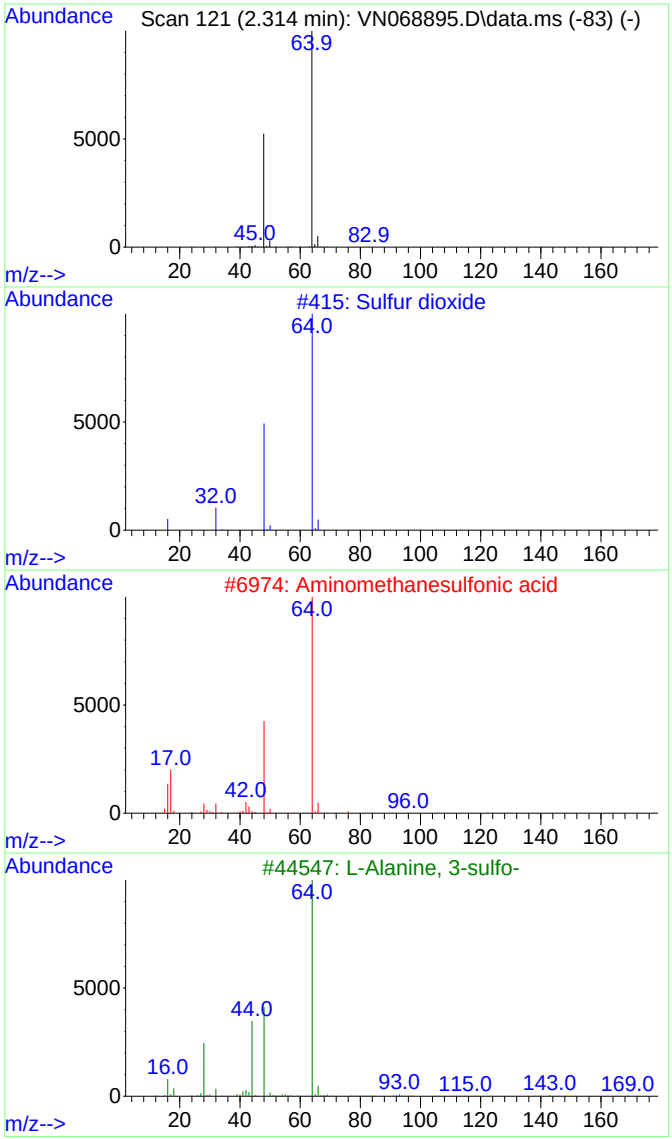
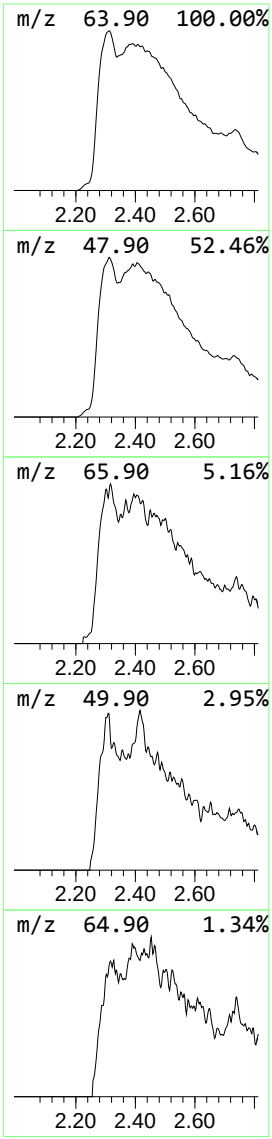
Peak Number 1 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.314	25.79 ug/l	631284	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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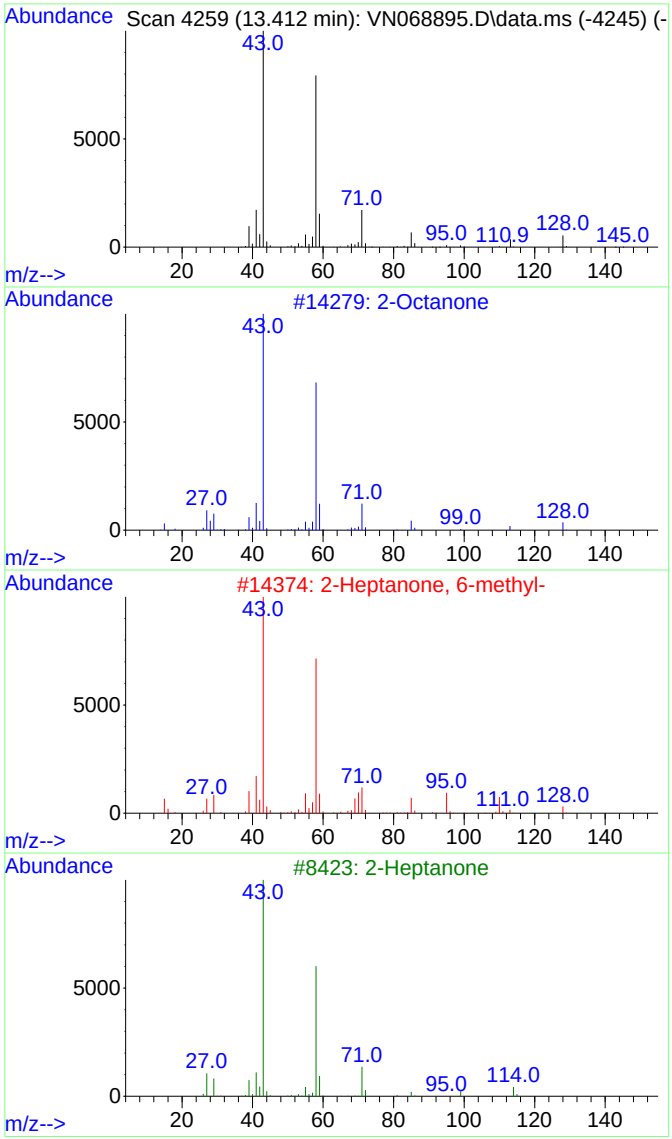
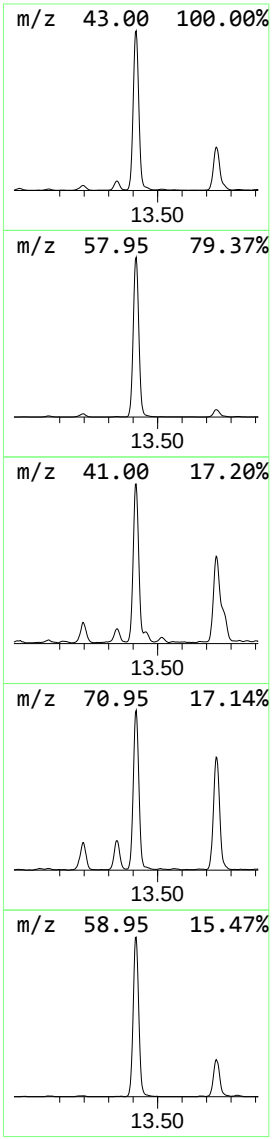
Peak Number 2 2-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.412	69.82 ug/l	2316590	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	94
2	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	90
3	2-Heptanone	114	C7H14O	000110-43-0	72
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72
5	2-Hexanone	100	C6H12O	000591-78-6	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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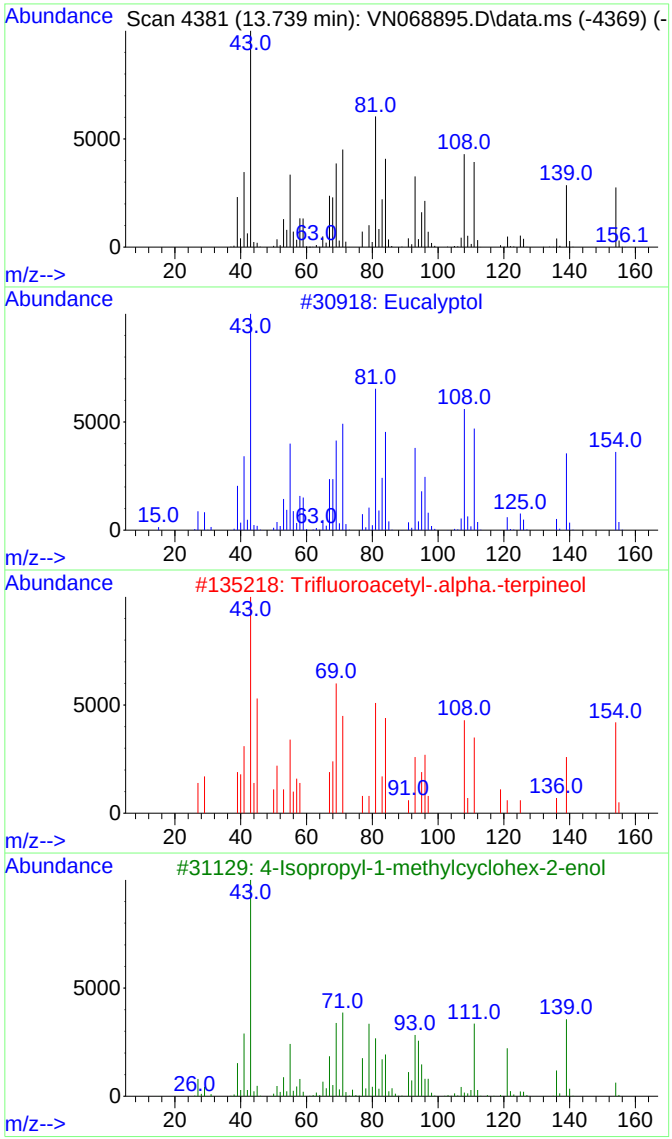
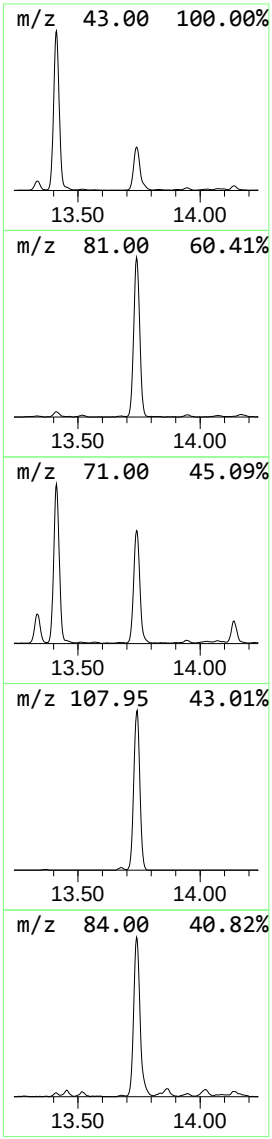
Peak Number 3 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	65.25 ug/l	2164950	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	38
3	4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	32
4	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	25
5	2-(3'-Oxo-butyl)-cyclopentanone	154	C9H14O2	1010143-37-2	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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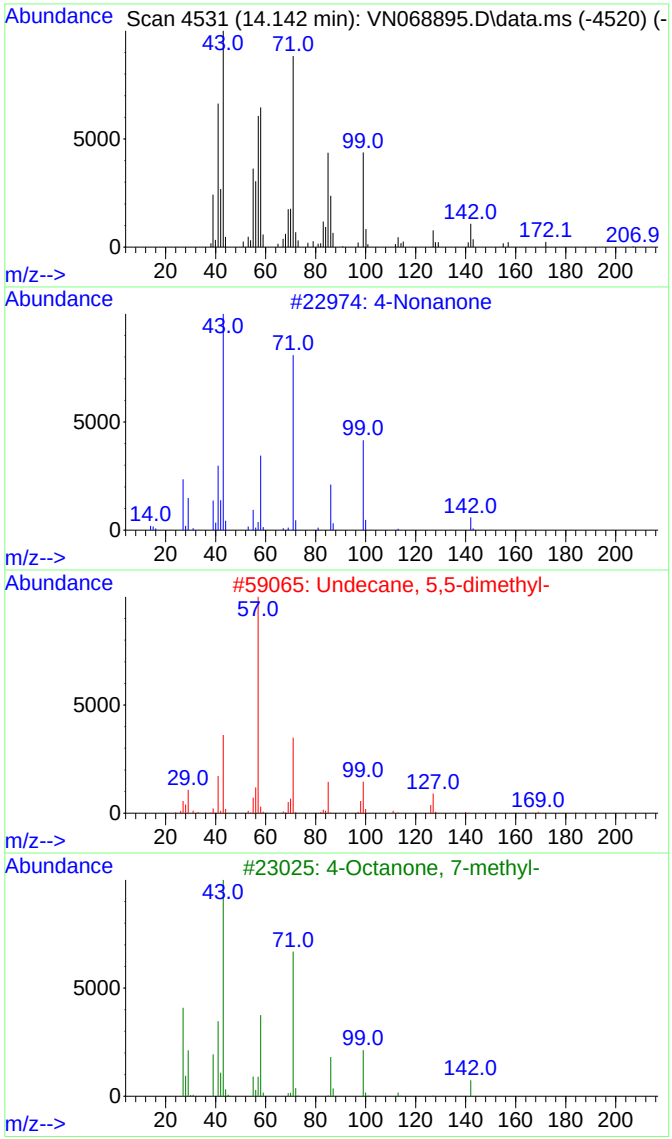
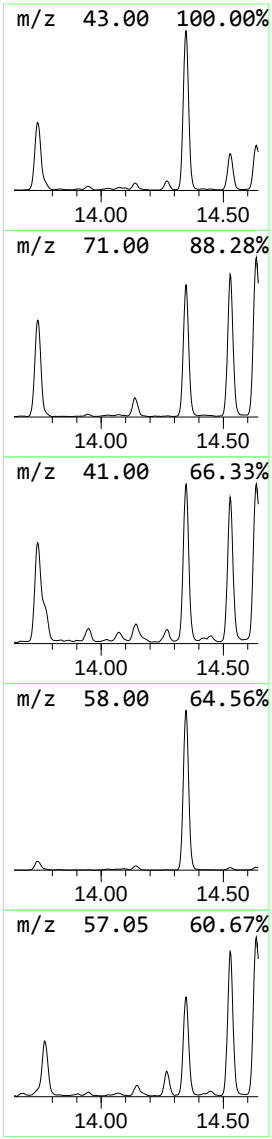
Peak Number 4 4-Nonanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.142	7.93 ug/l	262933	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nonanone	142	C9H18O	004485-09-0	60
2	Undecane, 5,5-dimethyl-	184	C13H28	017312-73-1	47
3	4-Octanone, 7-methyl-	142	C9H18O	020809-46-5	47
4	2-Bromononane	206	C9H19Br	002216-35-5	43
5	Octane, 2-methyl-	128	C9H20	003221-61-2	43





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Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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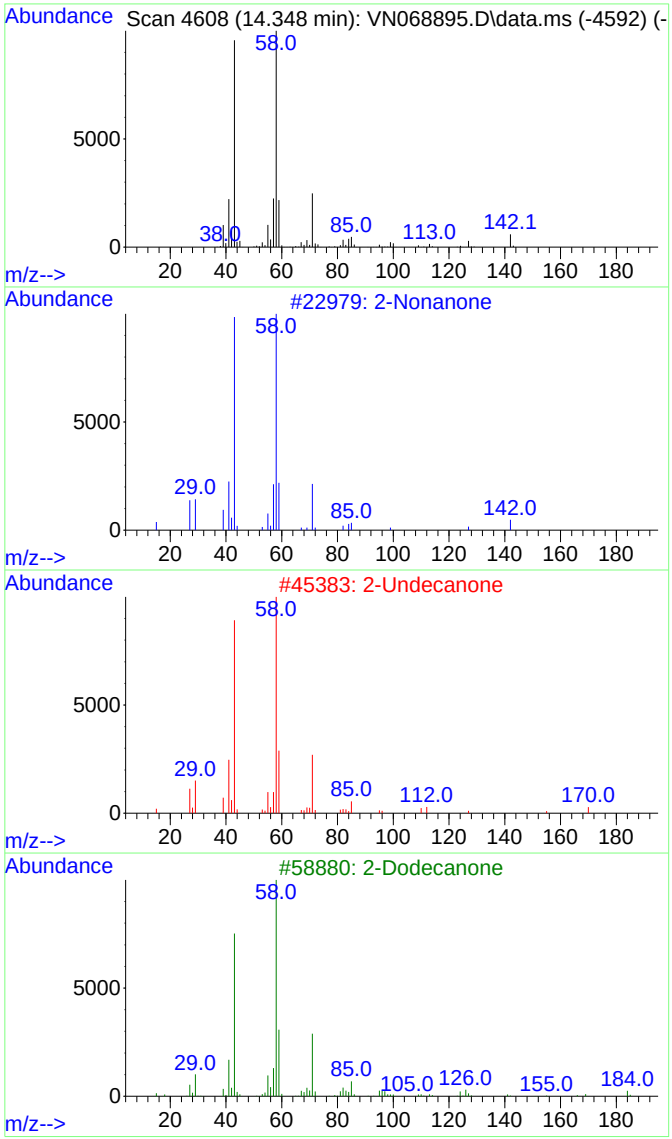
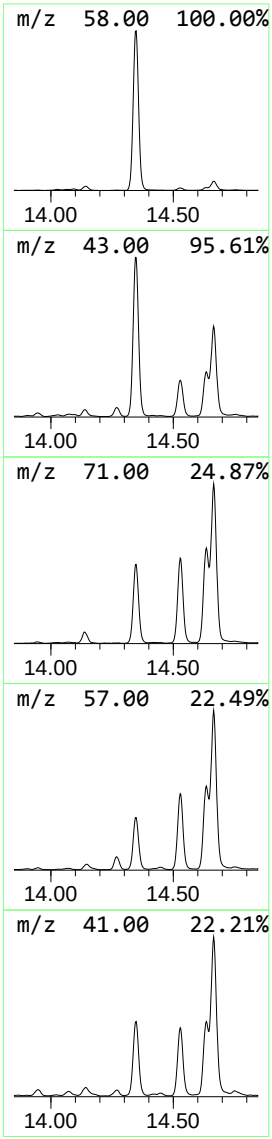
Peak Number 5 2-Nonanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.348	59.17 ug/l	1963140	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	94
2	2-Undecanone	170	C11H22O	000112-12-9	78
3	2-Dodecanone	184	C12H24O	006175-49-1	72
4	2-Heptanone	114	C7H14O	000110-43-0	64
5	2,4(3H,5H)-Furandione, 5-hexyl-5...	198	C11H18O3	054852-79-8	64





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Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

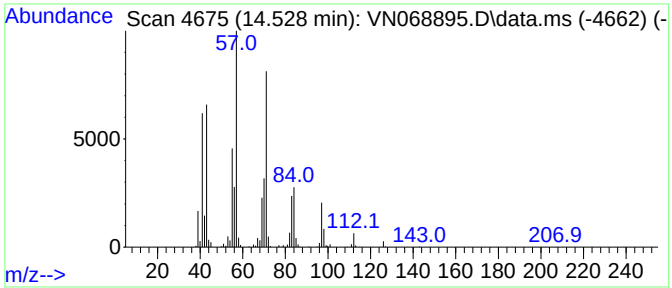
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

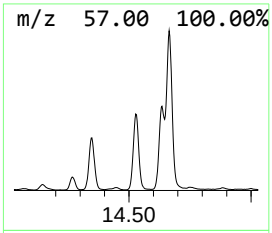
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

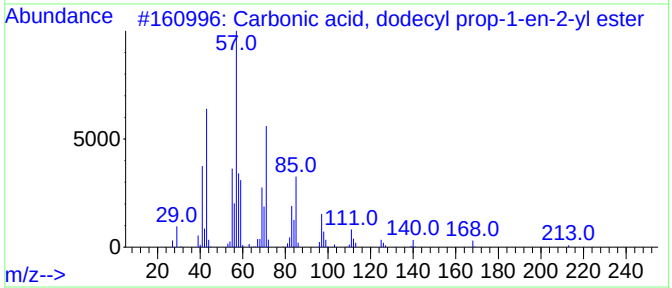
****
Peak Number 6 Carbonic acid, dodecyl prop... Concentration Rank 7

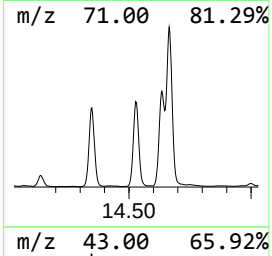
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.528	32.39 ug/l	1074640	1,4-Dichlorobenzene-d4	13.675

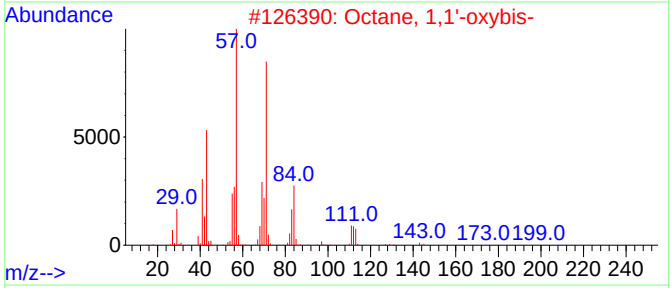
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	72
2	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
3	Hexadecyl octyl ether	354	C24H50O	1000406-38-6	64
4	Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	64
5	Tetradecane	198	C14H30	000629-59-4	50

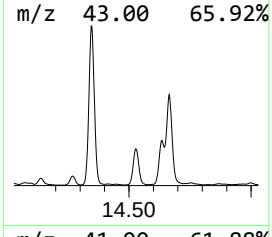


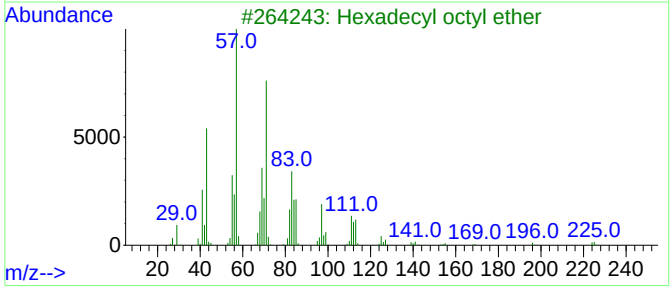


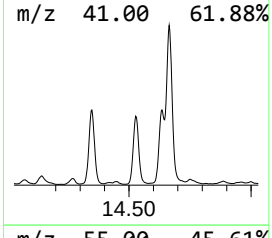


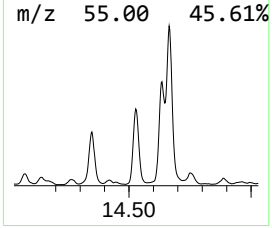












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Instrument : MSVOA_N
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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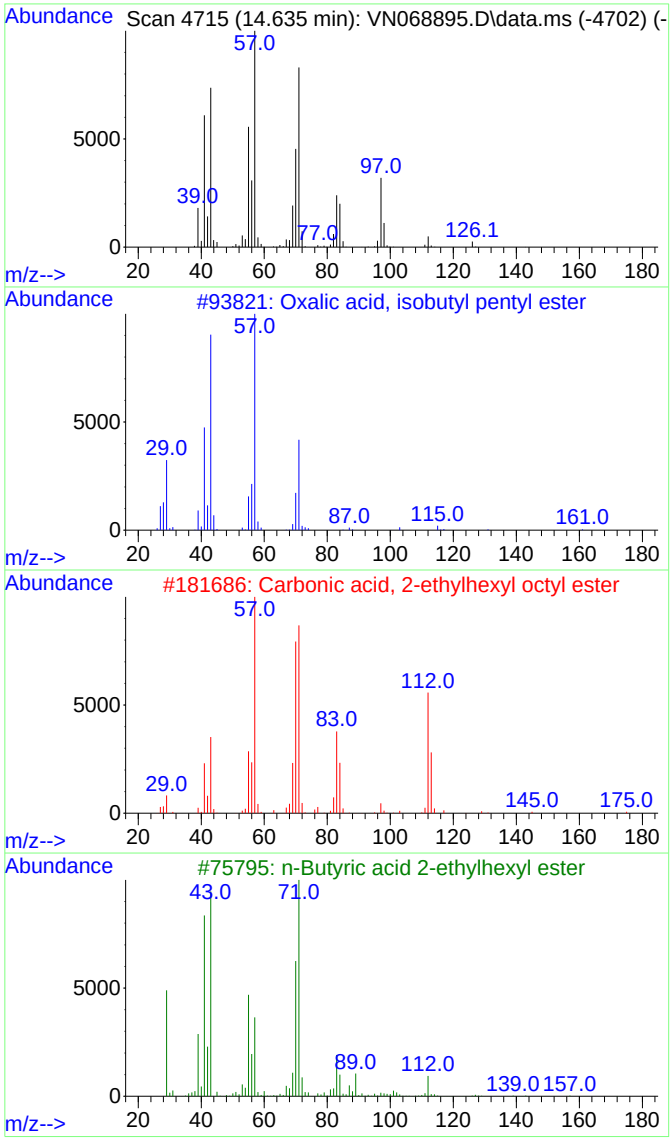
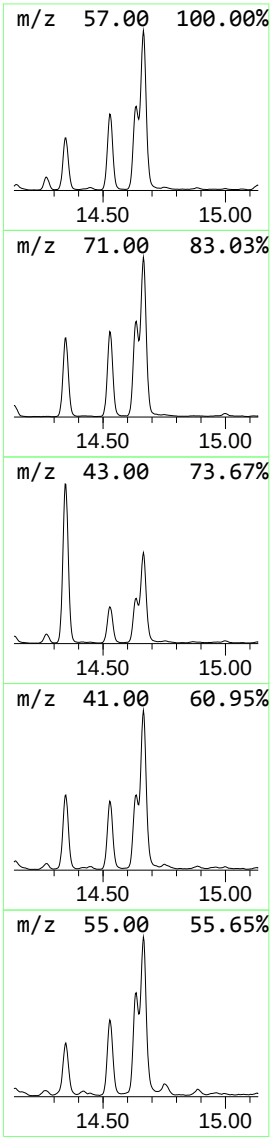
Peak Number 7 unknown14.635 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.635	34.33 ug/l	1138950	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	47
2	Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	47
3	n-Butyric acid 2-ethylhexyl ester	200	C12H24O2	025415-84-3	47
4	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	43
5	Carbonic acid, butyl octyl ester	230	C13H26O3	1010314-63-5	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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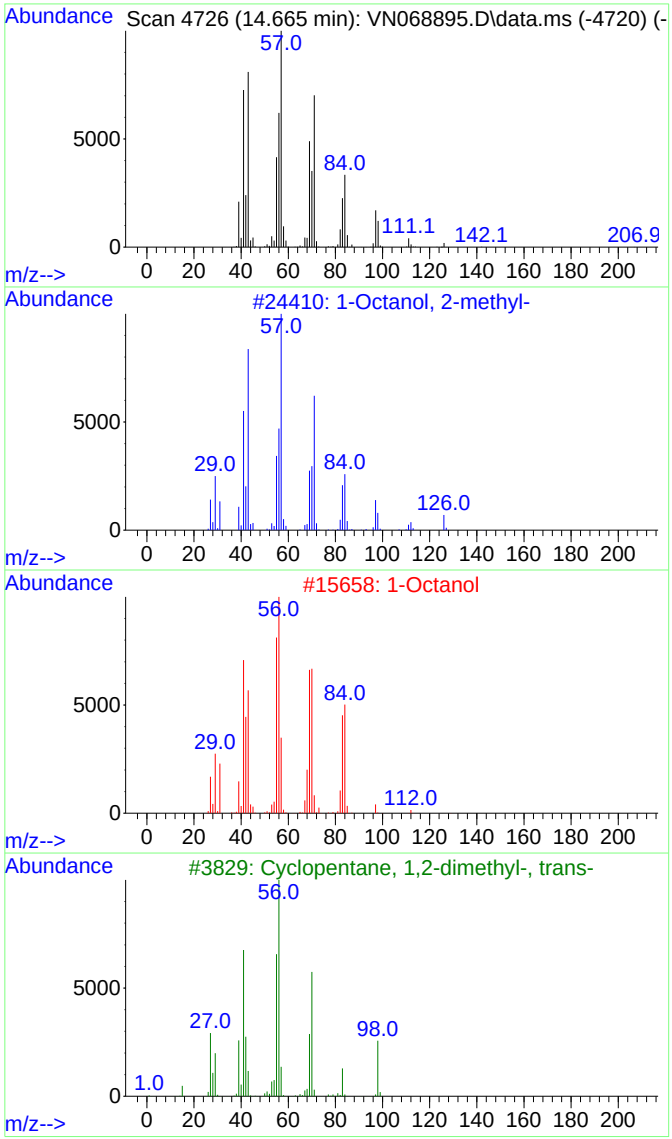
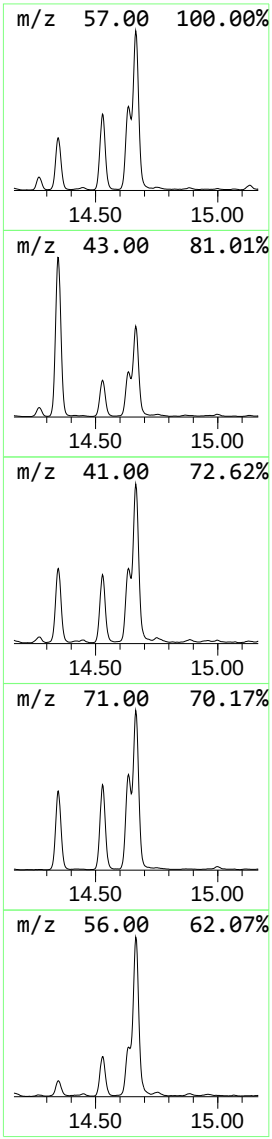
Peak Number 8 1-Octanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.665	72.94 ug/l	2420040	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	90
2	1-Octanol	130	C8H18O	000111-87-5	47
3	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	38
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	38
5	Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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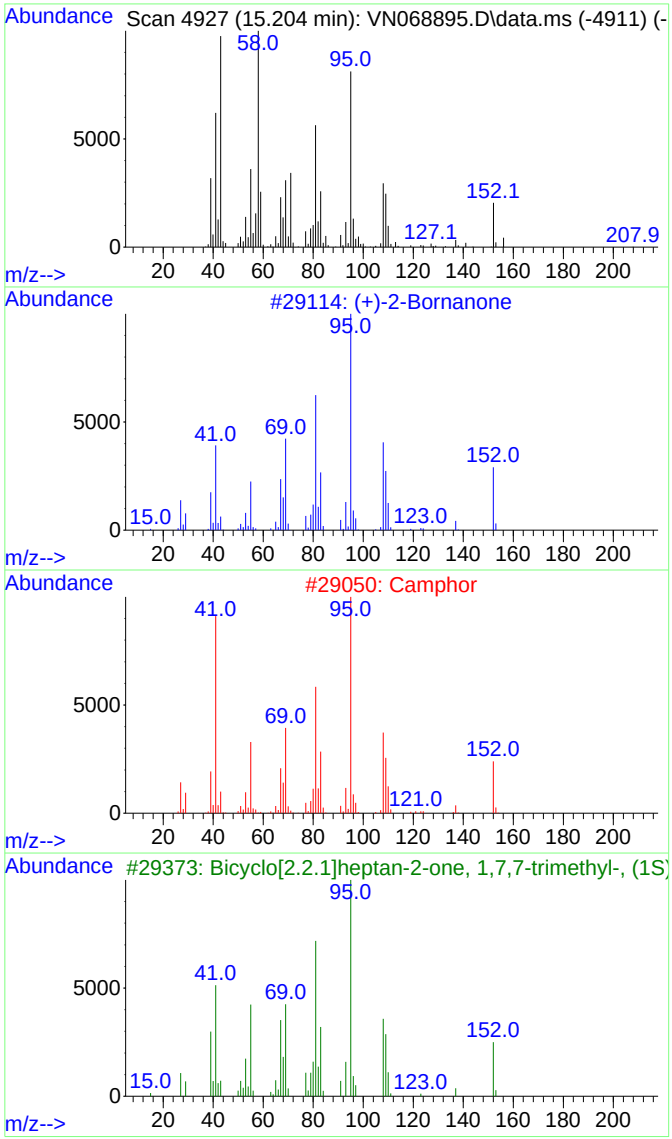
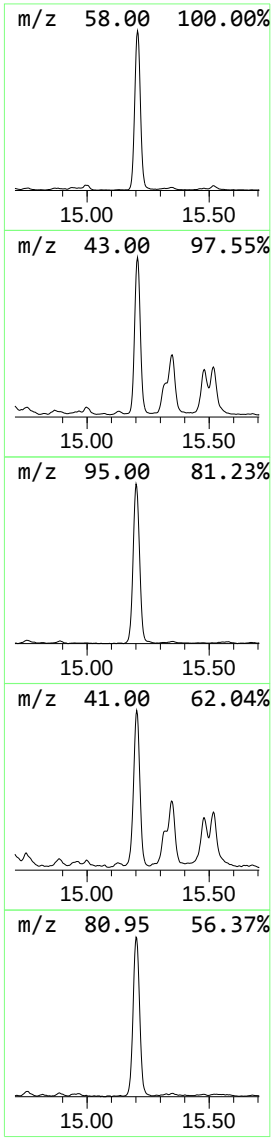
Peak Number 9 (+)-2-Bornanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	41.90 ug/l	1389990	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	96
2	Camphor	152	C10H16O	000076-22-2	96
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	95
4	2-Decanone	156	C10H20O	000693-54-9	70
5	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

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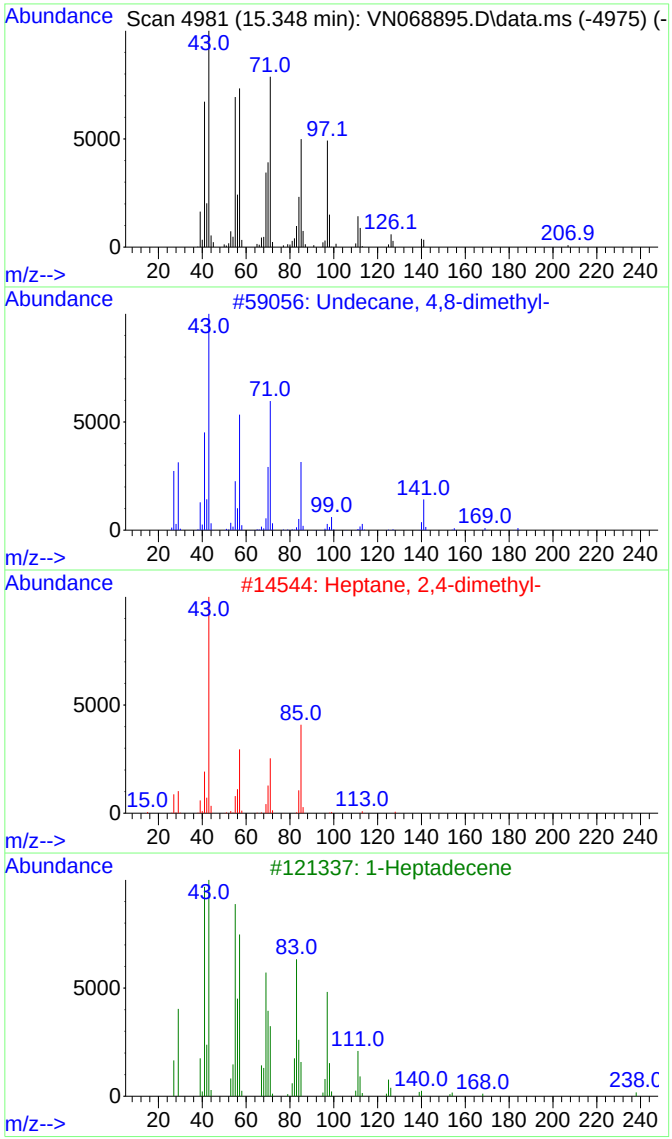
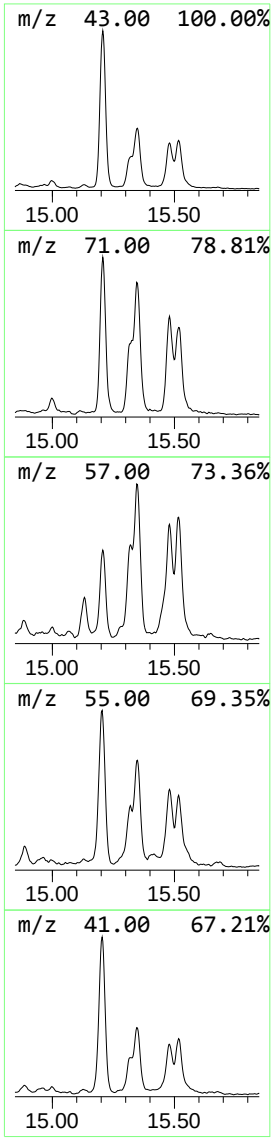
Peak Number 10 Undecane, 4,8-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.348	11.45 ug/l	379961	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	53
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53
3	1-Heptadecene	238	C17H34	006765-39-5	47
4	Oxalic acid, 6-ethyloct-3-yl iso...	286	C16H30O4	1010309-34-1	38
5	Ether, heptyl hexyl	200	C13H28O	007289-40-9	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068895.D
Acq On : 13 Oct 2021 14:07
Operator : JC/MD
Sample : M4142-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2158

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.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
Sulfur dioxide	2.314	25.8	ug/l	631284	1	8.088	1224020	50.0
2-Octanone	13.412	69.8	ug/l	2316590	4	13.675	1658860	50.0
Eucalyptol	13.739	65.3	ug/l	2164950	4	13.675	1658860	50.0
4-Nonanone	14.142	7.9	ug/l	262933	4	13.675	1658860	50.0
2-Nonanone	14.348	59.2	ug/l	1963140	4	13.675	1658860	50.0
Carbonic acid, ...	14.528	32.4	ug/l	1074640	4	13.675	1658860	50.0
unknown14.635	14.635	34.3	ug/l	1138950	4	13.675	1658860	50.0
1-Octanol, 2-me...	14.665	72.9	ug/l	2420040	4	13.675	1658860	50.0
(+)-2-Bornanone	15.204	41.9	ug/l	1389990	4	13.675	1658860	50.0
Undecane, 4,8-d...	15.348	11.4	ug/l	379961	4	13.675	1658860	50.0