LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068902.D
Acq On : 13 Oct 2021 17:13
Operator : JC/MD
Sample : M4175-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30784

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: VN068902.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.021	2226	2249	2253	rBV	273549	561943	2.38%	1.202%
2	8.166	2289	2303	2326	rVB2	120952	301956	1.28%	0.646%
3	8.289	2326	2349	2383	rBV	573823	1351781	5.73%	2.892%
4	8.434	2384	2403	2427	rVB	276162	627966	2.66%	1.344%
5	8.550	2427	2446	2464	rBV4	91190	241547	1.02%	0.517%
6	8.820	2528	2547	2574	rBV	887300	1781774	7.56%	3.812%
7	8.965	2581	2601	2636	rVB	716984	1506835	6.39%	3.224%
8	9.453	2748	2783	2796	rBV3	162831	411847	1.75%	0.881%
9	10.443	3133	3152	3161	rBV	1083758	2039539	8.65%	4.364%
10	10.507	3161	3176	3208	rVB	12645353	23570733	100.00%	50.432%
11	11.746	3622	3638	3660	rBV	980165	1793719	7.61%	3.838%
12	11.956	3695	3716	3738	rBV3	246079	524711	2.23%	1.123%
13	12.280	3811	3837	3853	rBV3	85001	265635	1.13%	0.568%
14	12.733	3994	4006	4029	rVB	799071	1404356	5.96%	3.005%
15	12.985	4088	4100	4108	rBV	207971	369058	1.57%	0.790%
16	13.053	4116	4125	4140	rVB4	405027	785279	3.33%	1.680%
17	13.372	4230	4244	4272	rBV	562098	1039367	4.41%	2.224%
18	13.559	4302	4314	4327	rBV7	182986	384577	1.63%	0.823%
19	13.677	4345	4358	4391	rVB2	1004421	2118075	8.99%	4.532%
20	13.841	4407	4419	4424	rBV2	158688	256208	1.09%	0.548%
21	13.913	4438	4446	4466	rVB5	204761	462945	1.96%	0.991%
22	13.997	4467	4477	4491	rBV5	179112	289310	1.23%	0.619%
23	14.123	4513	4524	4534	rBV4	232541	407513	1.73%	0.872%
24	14.219	4549	4560	4573	rVB	170685	272377	1.16%	0.583%
25	14.651	4704	4721	4742	rVB	708461	1277862	5.42%	2.734%
26	14.911	4807	4818	4837	rBV7	153800	359798	1.53%	0.770%
27	16.325	5327	5345	5369	rVB2	1167895	2330758	9.89%	4.987%

Sum of corrected areas: 46737469

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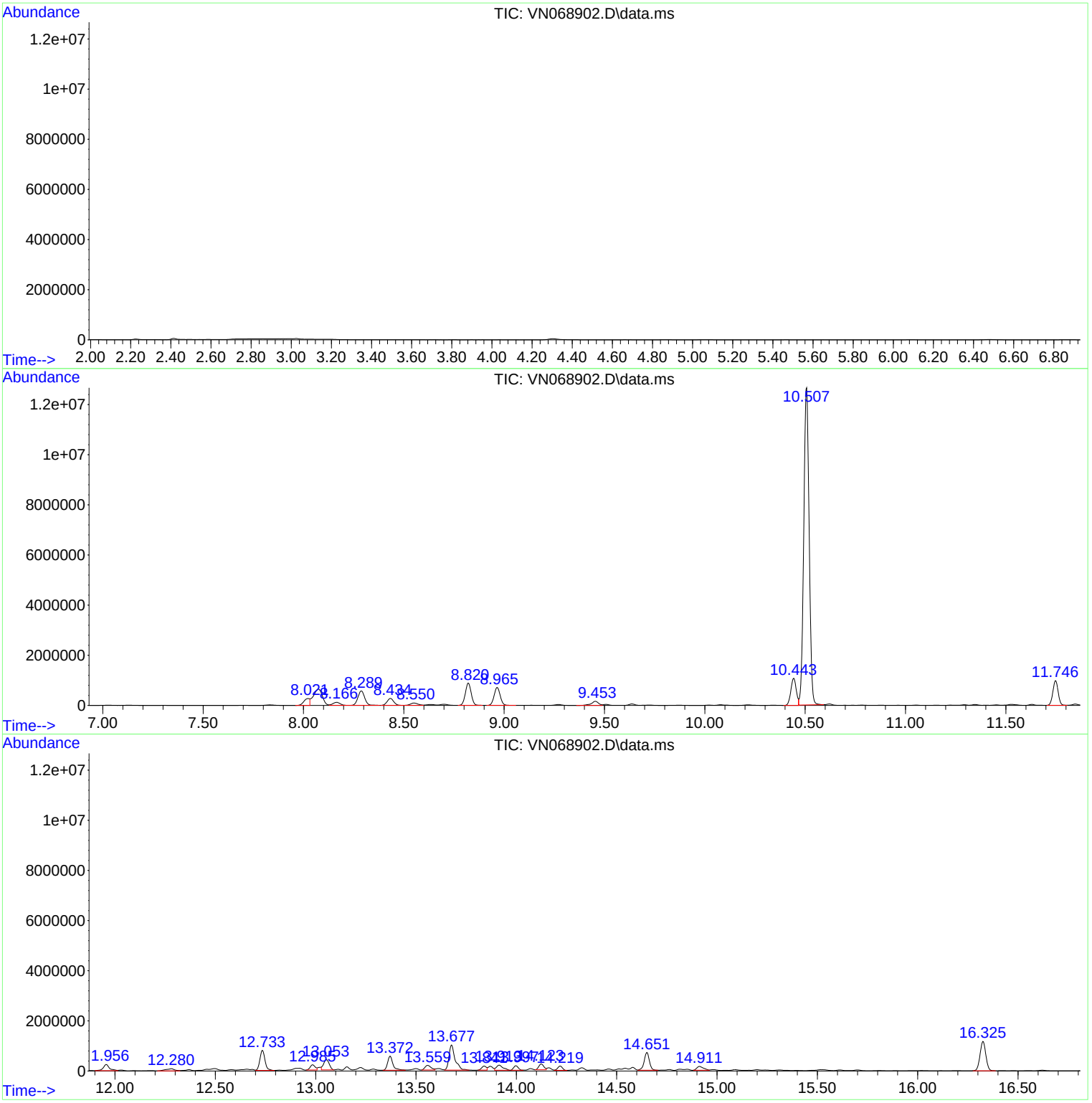
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30784

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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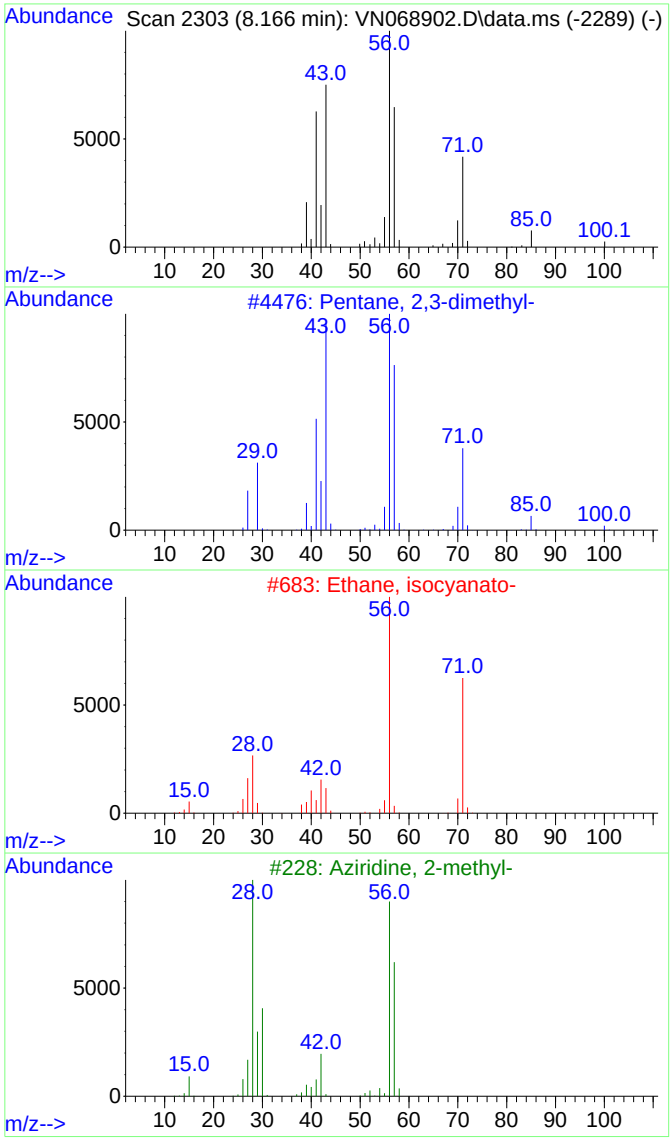
Quant Title : SW846 8260

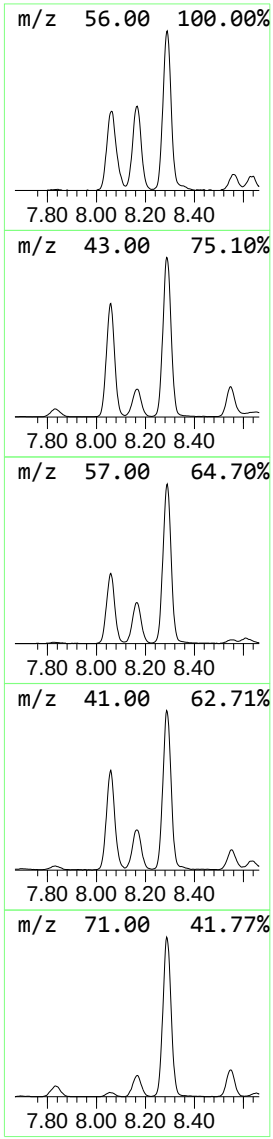
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.166	26.87 ug/l	301956	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Ethane, isocyanato-	71	C3H5NO	000109-90-0	53
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
5	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	40





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Data File : VN068902.D
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Operator : JC/MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30784

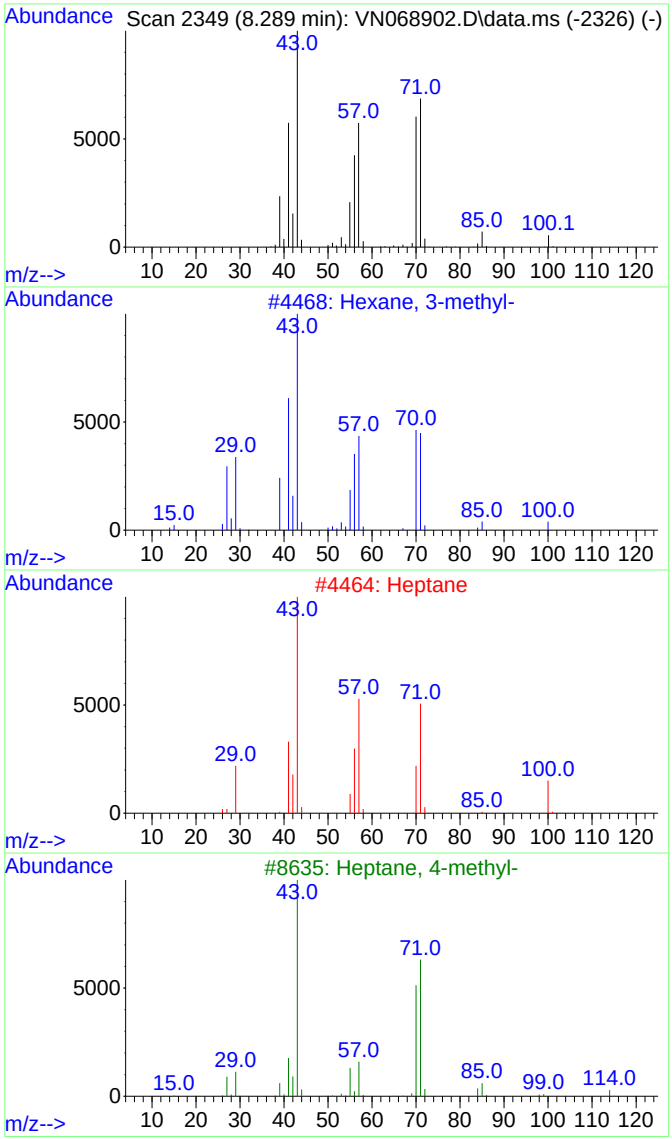
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

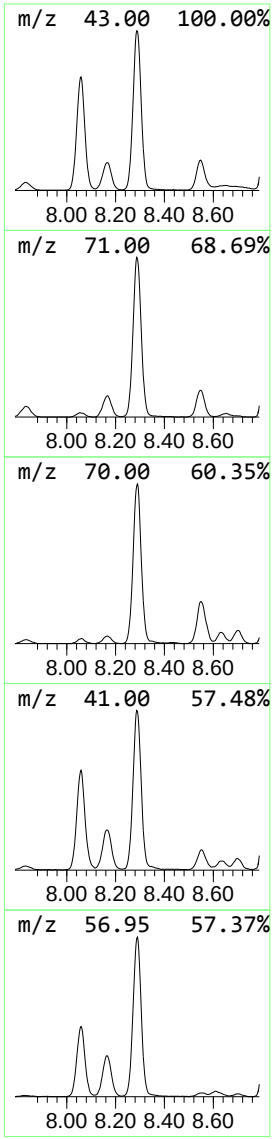
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.289	120.28 ug/l	1351780	Pentafluorobenzene	8.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53





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Operator : JC/MD
Sample : M4175-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

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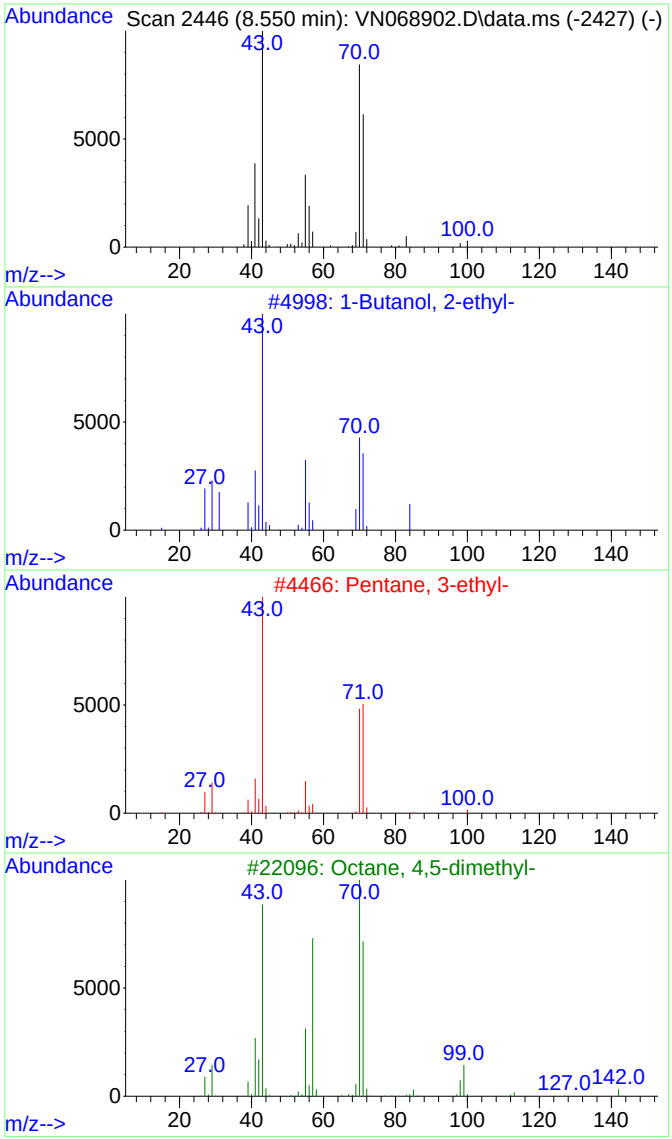
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

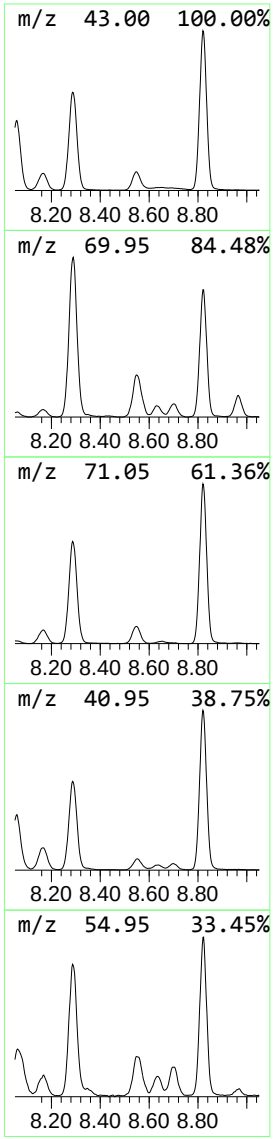
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Butanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.550	8.02 ug/l	241547	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	78
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	59
3	Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	56
4	Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	56
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	50





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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30784

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

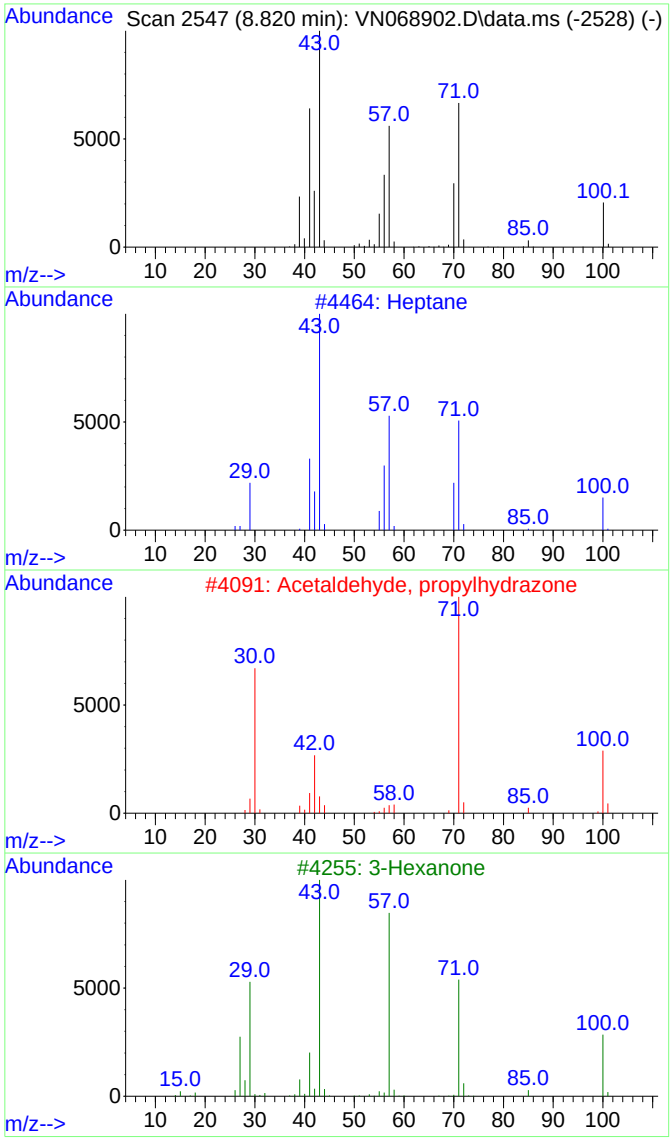
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

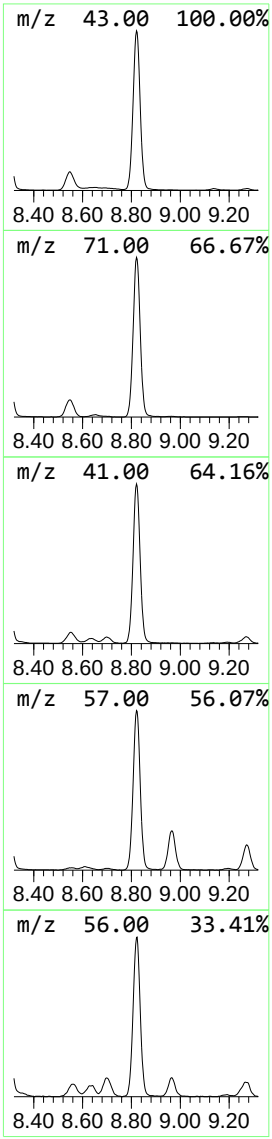
****

Peak Number 4 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.820	59.12 ug/l	1781770	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	49
3	3-Hexanone	100	C6H12O	000589-38-8	46
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	40
5	Hexane, 3-methyl-	100	C7H16	000589-34-4	40





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Operator : JC/MD
Sample : M4175-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30784

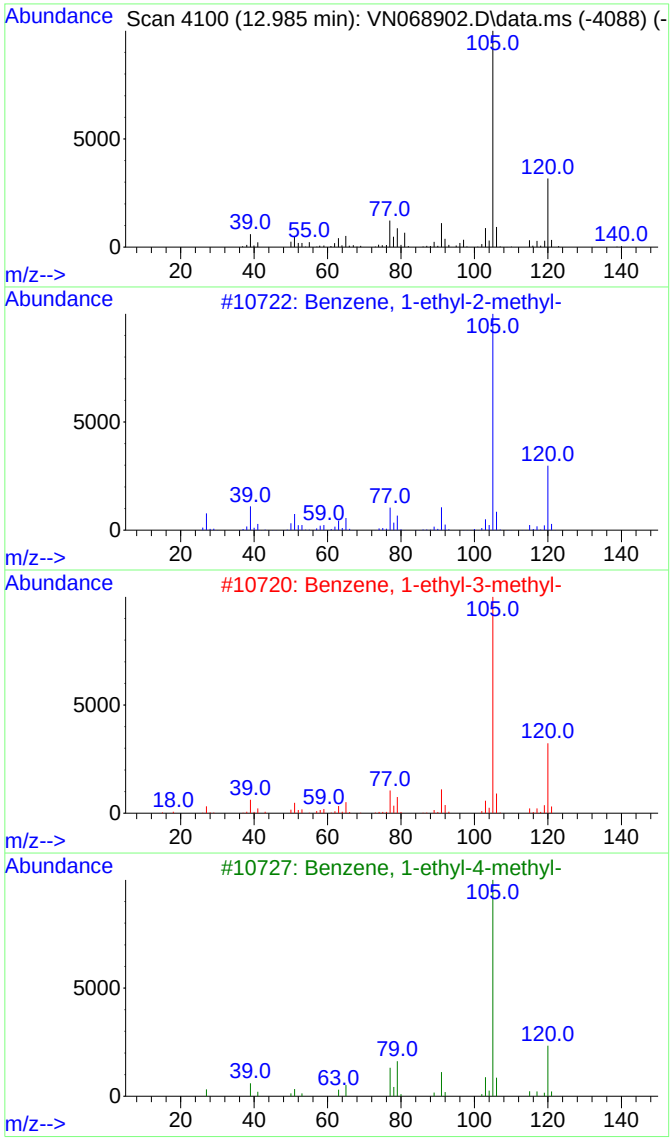
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

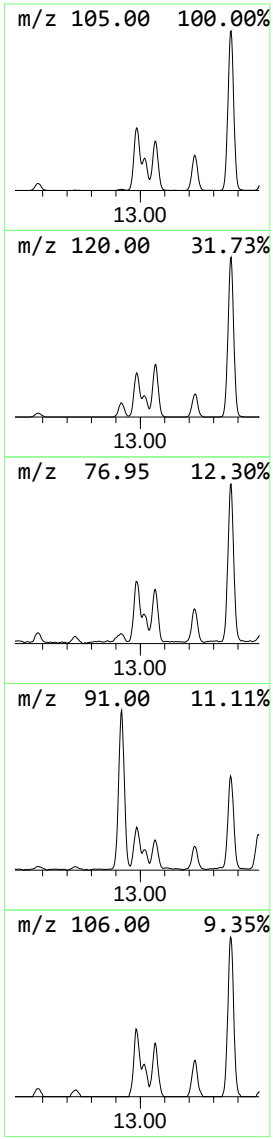
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.986	8.71 ug/l	369058	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	91





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Instrument : MSVOA_N
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TIC Library : C:\Database\NIST20.L
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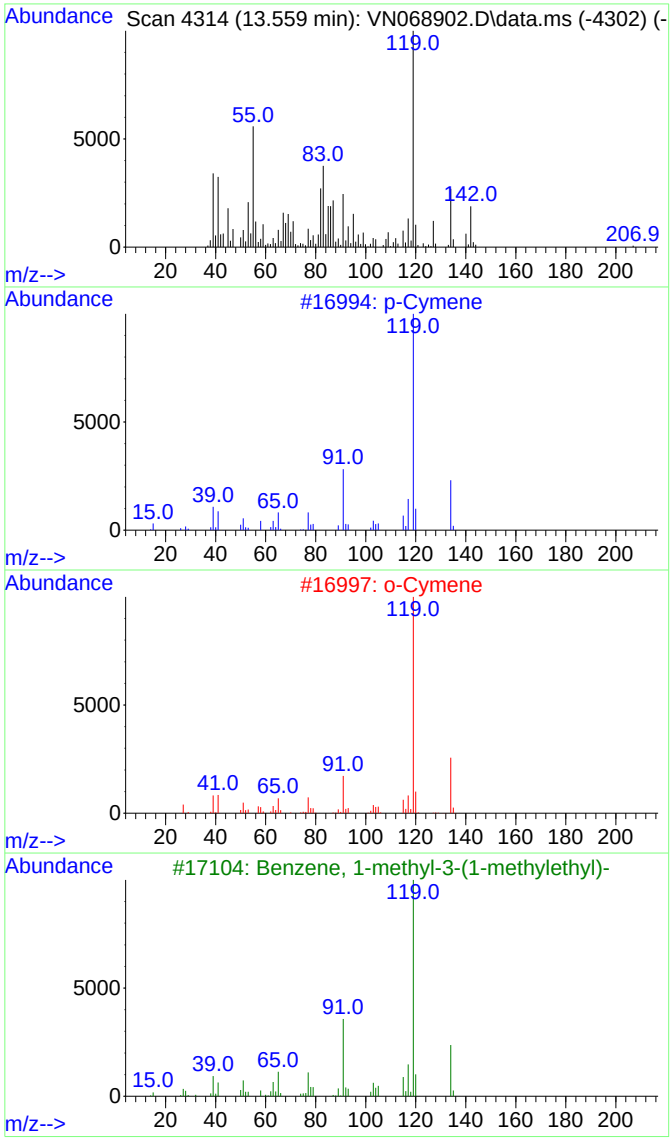
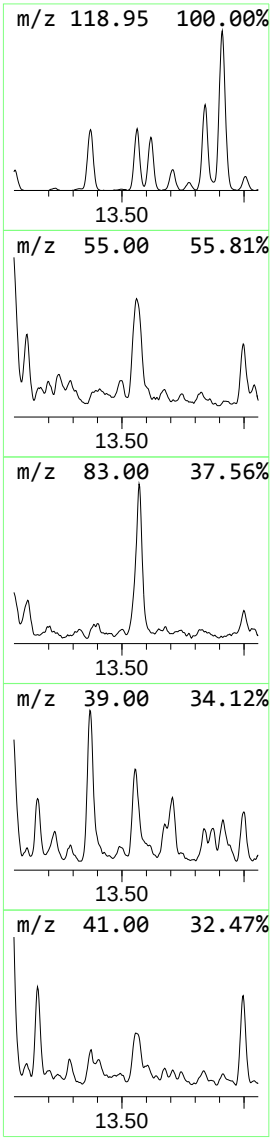
****

Peak Number 6 p-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.559	9.08 ug/l	384577	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	92
2	o-Cymene	134	C10H14	000527-84-4	91
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	90
4	1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	78
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	60





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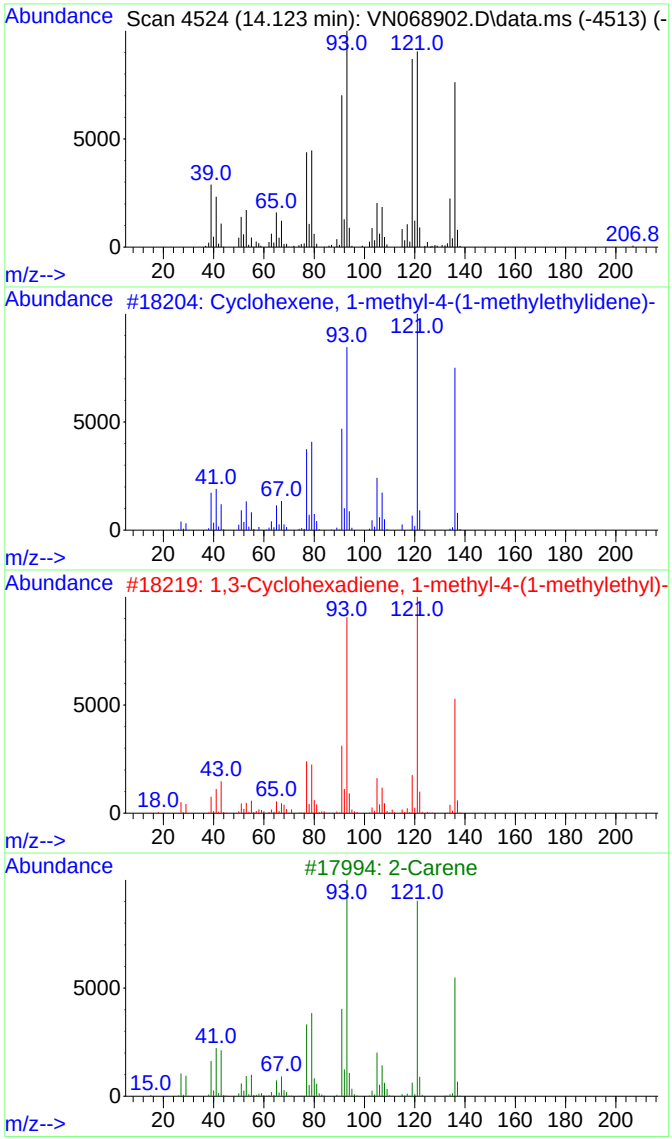
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

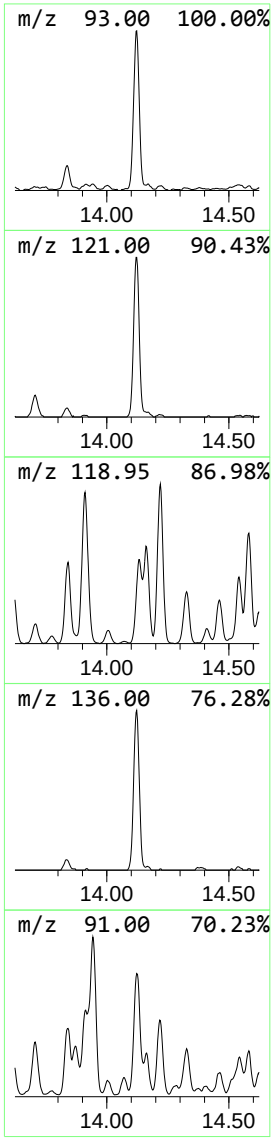
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.123	9.62 ug/l	407513	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	96
2	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	95
3	2-Carene	136	C10H16	000554-61-0	89
4	(+)-4-Carene	136	C10H16	029050-33-7	89
5	Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	76





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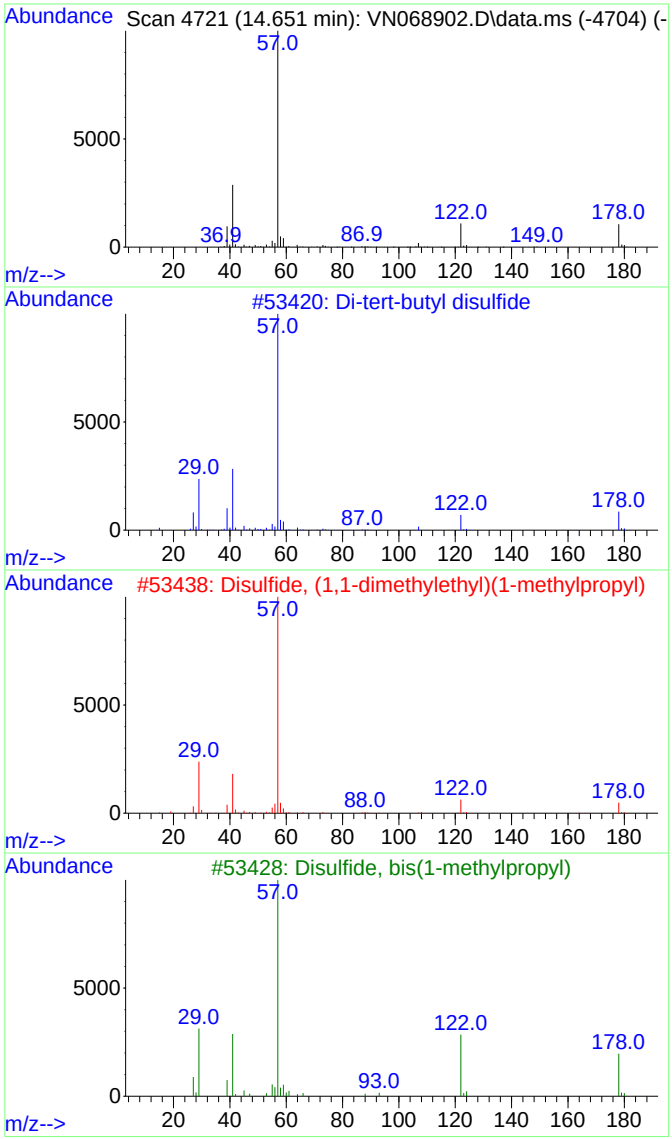
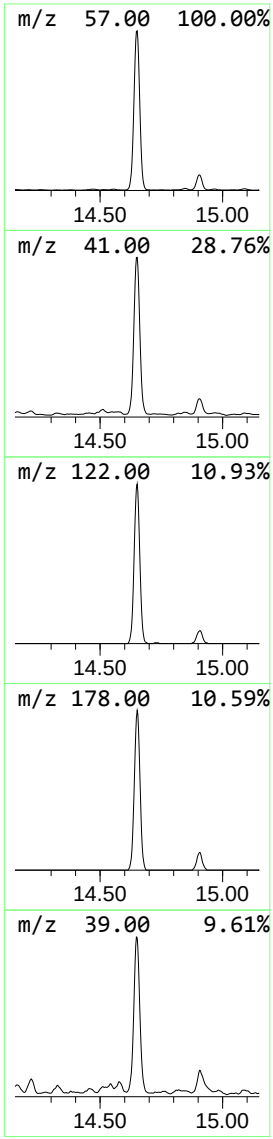
Peak Number 8 Di-tert-butyl disulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	30.17 ug/l	1277860	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	90
2	Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	64
3	Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	50
4	Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	50
5	Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	32





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ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30784

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

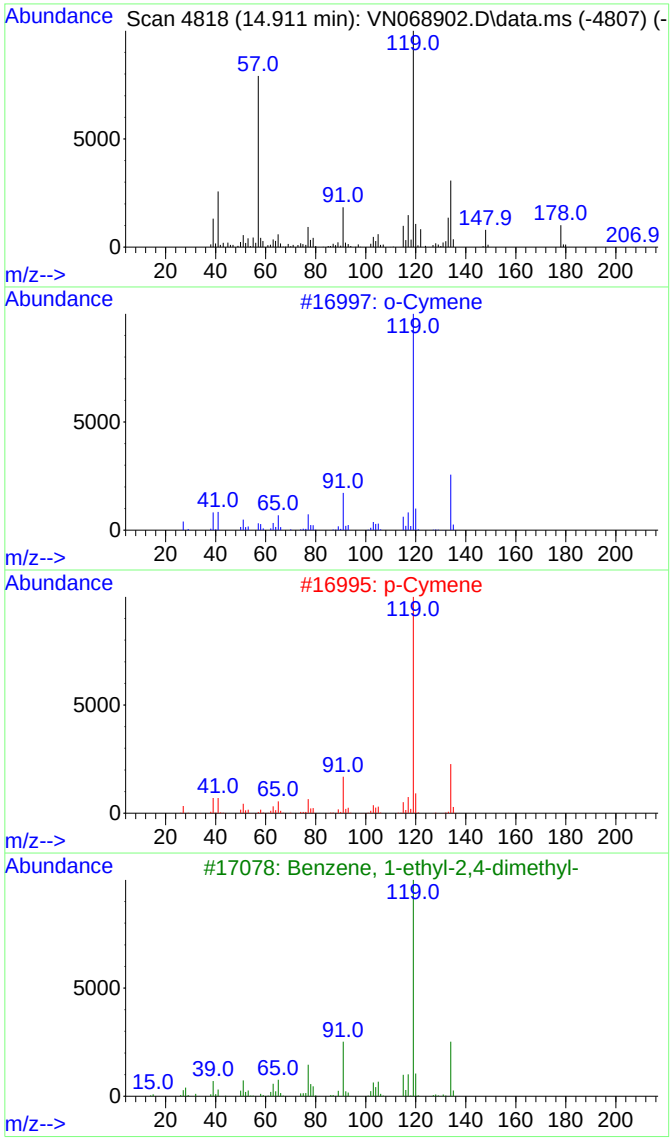
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

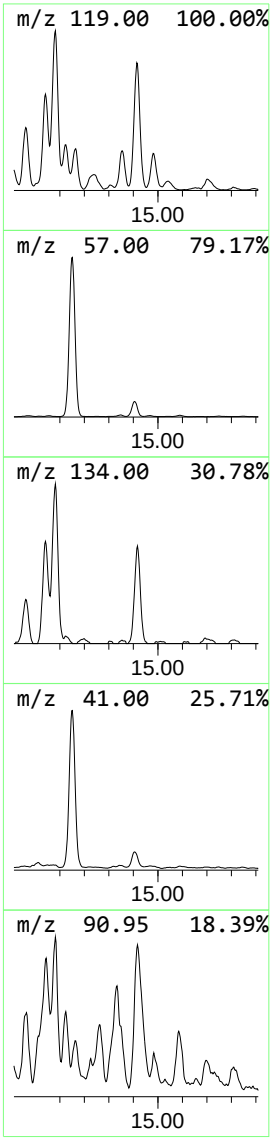
****

Peak Number 9 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.911	8.49 ug/l	359798	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	95
2	p-Cymene	134	C10H14	000099-87-6	93
3	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93
4	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	89
5	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	86





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Data File : VN068902.D
Acq On : 13 Oct 2021 17:13
Operator : JC/MD
Sample : M4175-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30784

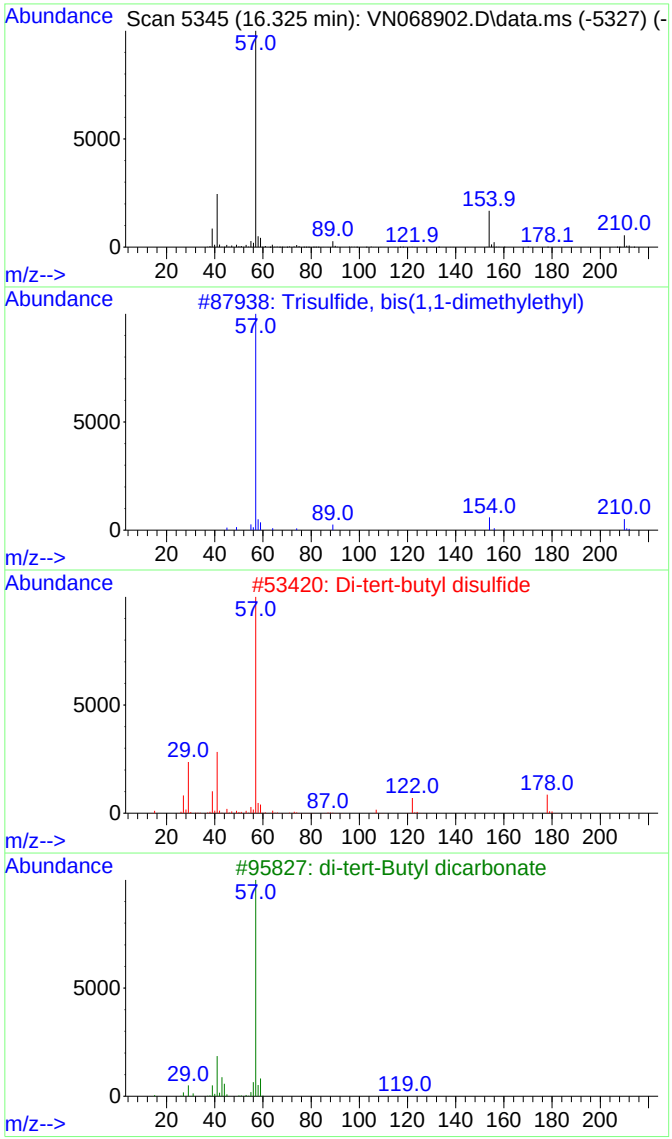
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

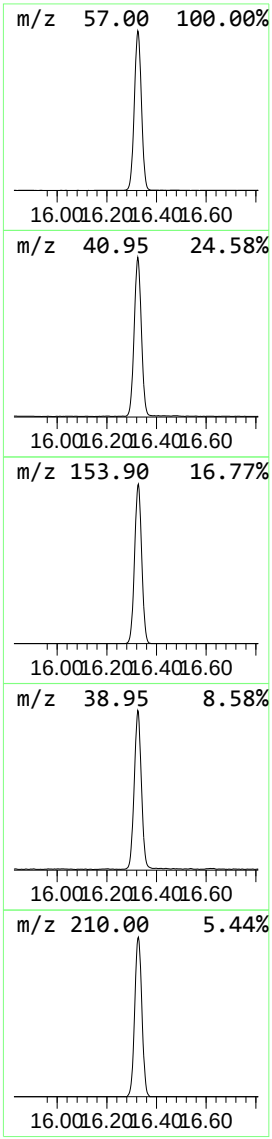
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Trisulfide, bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.325	55.02 ug/l	2330760	1,4-Dichlorobenzene-d4	13.677

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	74
2	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	43
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	22
4	Hypophosphonous dichloride, bis(...	246	C8H18Cl2P2	079898-85-4	10
5	Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068902.D
Acq On : 13 Oct 2021 17:13
Operator : JC/MD
Sample : M4175-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30784

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
Pentane, 2,3-di...	8.166	26.9	ug/l	301956	1	8.080	561943	50.0
Hexane, 3-methyl-	8.289	120.3	ug/l	1351780	1	8.080	561943	50.0
1-Butanol, 2-et...	8.550	8.0	ug/l	241547	2	8.965	1506840	50.0
Heptane	8.820	59.1	ug/l	1781770	2	8.965	1506840	50.0
Benzene, 1-ethy...	12.986	8.7	ug/l	369058	4	13.677	2118080	50.0
p-Cymene	13.559	9.1	ug/l	384577	4	13.677	2118080	50.0
Cyclohexene, 1-...	14.123	9.6	ug/l	407513	4	13.677	2118080	50.0
Di-tert-butyl d...	14.651	30.2	ug/l	1277860	4	13.677	2118080	50.0
o-Cymene	14.911	8.5	ug/l	359798	4	13.677	2118080	50.0
Trisulfide, bis...	16.325	55.0	ug/l	2330760	4	13.677	2118080	50.0