LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100319\
Data File : VN058523.D
Acq On : 3 Oct 2019 20:08
Operator : JC/SP
Sample : K5176-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30464-67

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\82N092719W.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	4.037	684	704	732	rBV	153631	451729	1.34%	0.811%
2	7.355	1716	1736	1758	rBV2	132473	349978	1.04%	0.628%
3	7.574	1787	1804	1815	rBV	247699	620225	1.84%	1.113%
4	7.651	1815	1828	1849	rVB	470034	1133994	3.36%	2.035%
5	8.011	1921	1940	1961	rBV	320453	769396	2.28%	1.381%
6	8.574	2099	2115	2135	rBV	726300	1531589	4.53%	2.749%
7	10.085	2569	2585	2597	rBV	1098783	2037273	6.03%	3.656%
8	10.796	2789	2806	2852	rBV	1839604	5246487	15.53%	9.416%
9	11.410	2983	2997	3016	rBV	971565	1743194	5.16%	3.129%
10	11.847	3123	3133	3145	rBV	316652	524093	1.55%	0.941%
11	12.406	3296	3307	3328	rVB	751013	1310348	3.88%	2.352%
12	13.265	3566	3574	3589	rVB2	268176	463142	1.37%	0.831%
13	13.348	3590	3600	3613	rVB	913696	1487335	4.40%	2.669%
14	13.458	3622	3634	3671	rBV	19934240	33774319	100.00%	60.616%
15	14.213	3861	3869	3885	rBV2	418393	658641	1.95%	1.182%
16	14.319	3893	3902	3906	rBV2	472971	701817	2.08%	1.260%
17	14.352	3906	3912	3932	rVB	818511	1365780	4.04%	2.451%
18	15.008	4110	4116	4123	rVB2	375136	451718	1.34%	0.811%
19	15.159	4157	4163	4181	rVB	627292	1097048	3.25%	1.969%

Sum of corrected areas: 55718106

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN100319\
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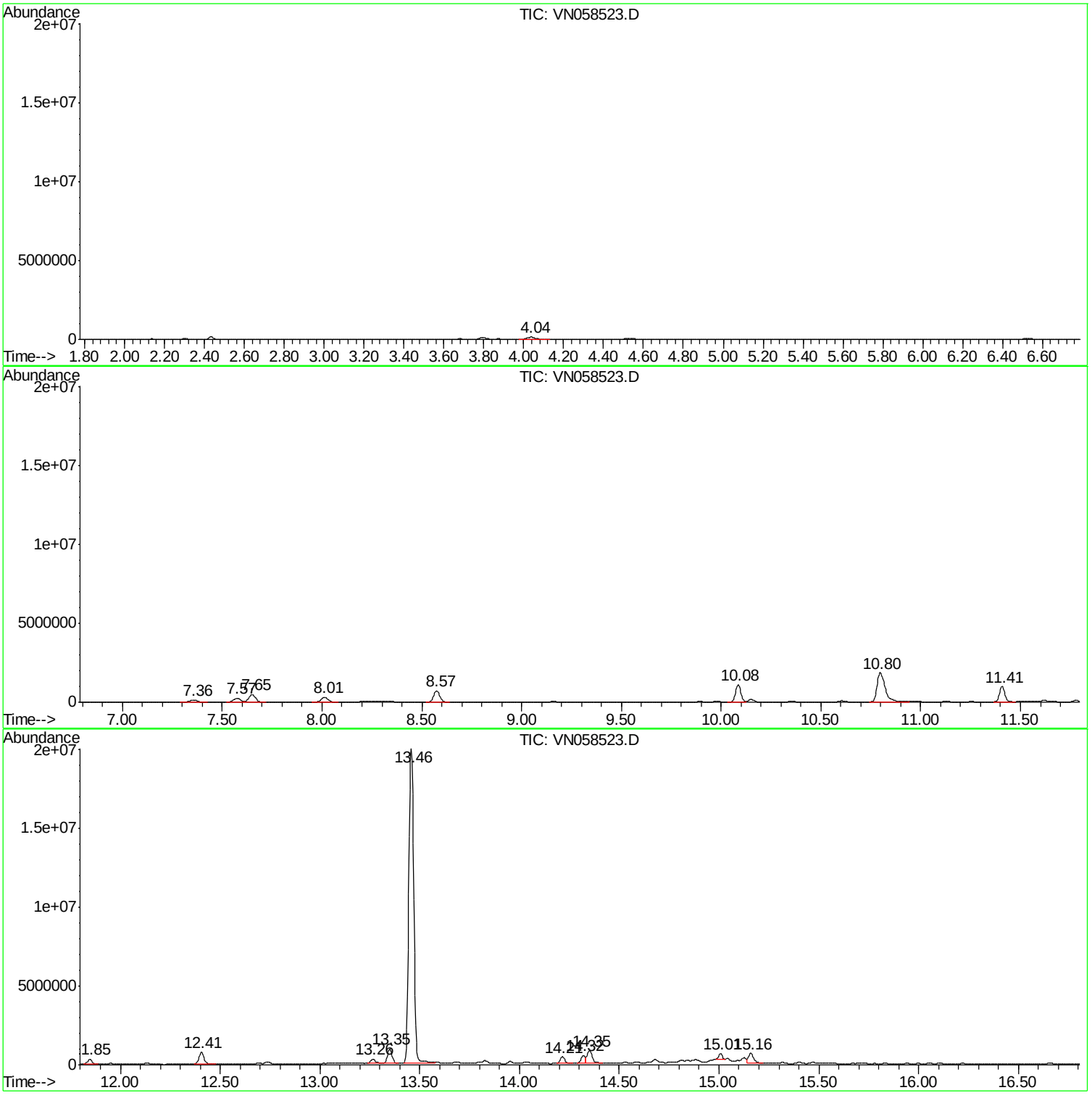
Operator : JC/SP
Sample : K5176-10
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30464-67

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.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\VN100319\
Data File : VN058523.D
Acq On : 3 Oct 2019 20:08
Operator : JC/SP
Sample : K5176-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30464-67

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.M
Quant Title : SW846 8260

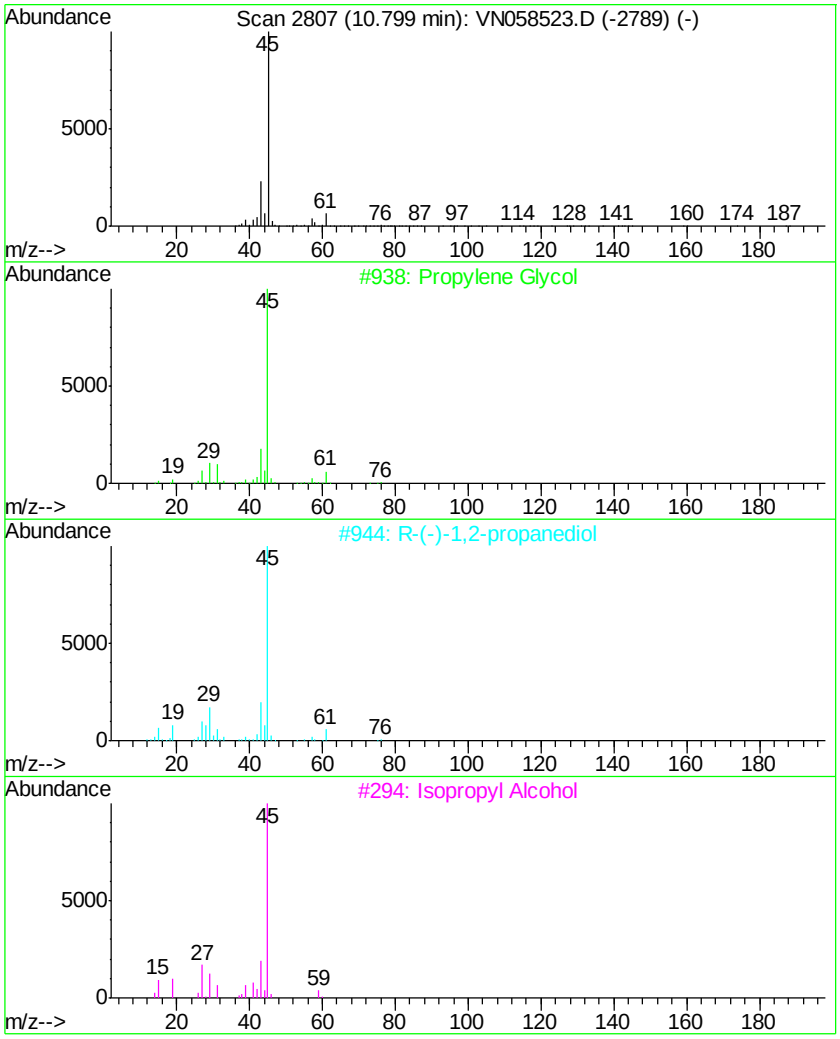
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

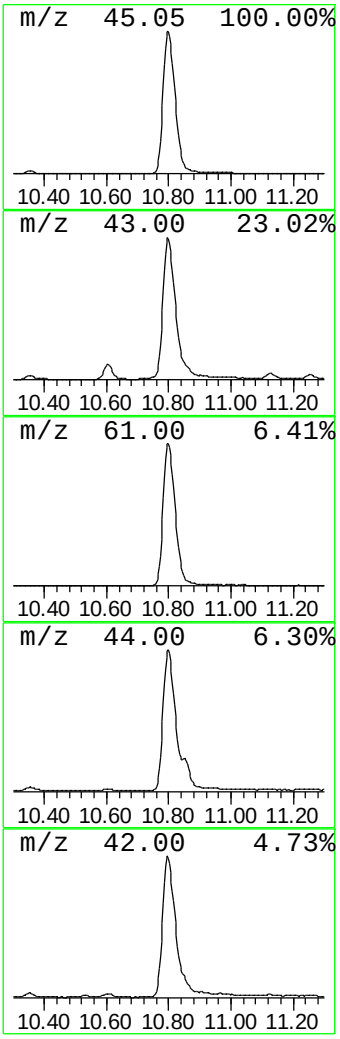
****

Peak Number 1 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	150.49 ug/l	5246490	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9





Library Search Compound Report

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Data File : VN058523.D
Acq On : 3 Oct 2019 20:08
Operator : JC/SP
Sample : K5176-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30464-67

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.M
Quant Title : SW846 8260

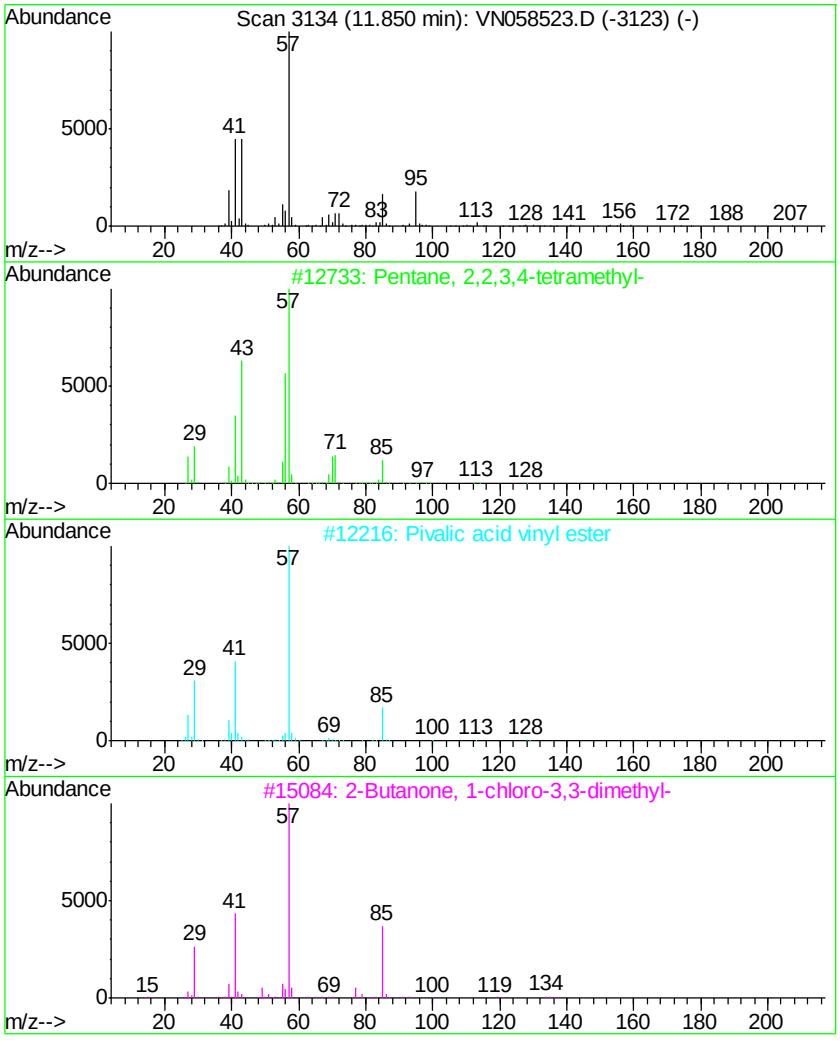
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

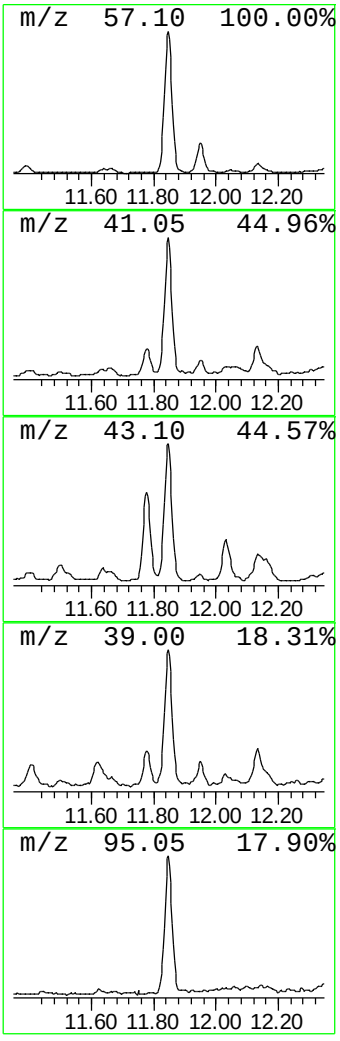
****

Peak Number 2 unknown11.85 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	15.03 ug/l	524093	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	43
2	Pivalic acid vinyl ester	128	C7H12O2	003377-92-2	43
3	2-Butanone, 1-chloro-3,3-dimethyl-	134	C6H11ClO	013547-70-1	43
4	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	37
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	37





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN100319\
Data File : VN058523.D
Acq On : 3 Oct 2019 20:08
Operator : JC/SP
Sample : K5176-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30464-67

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.M
Quant Title : SW846 8260

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

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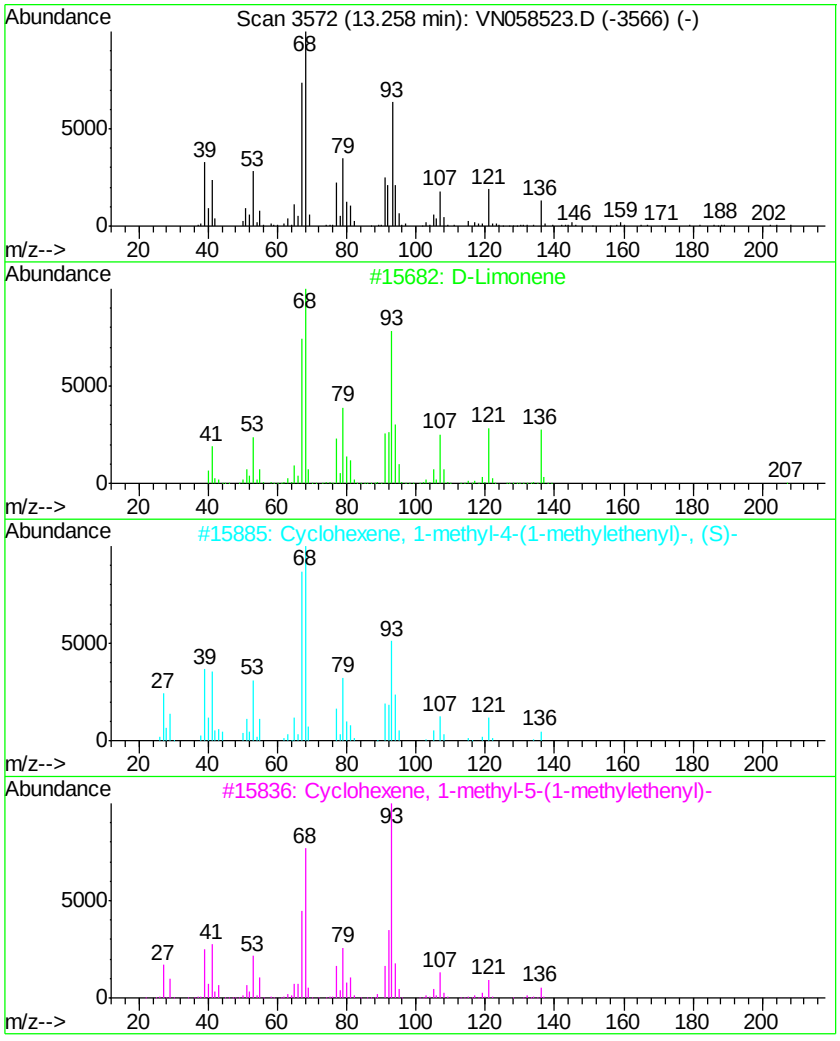
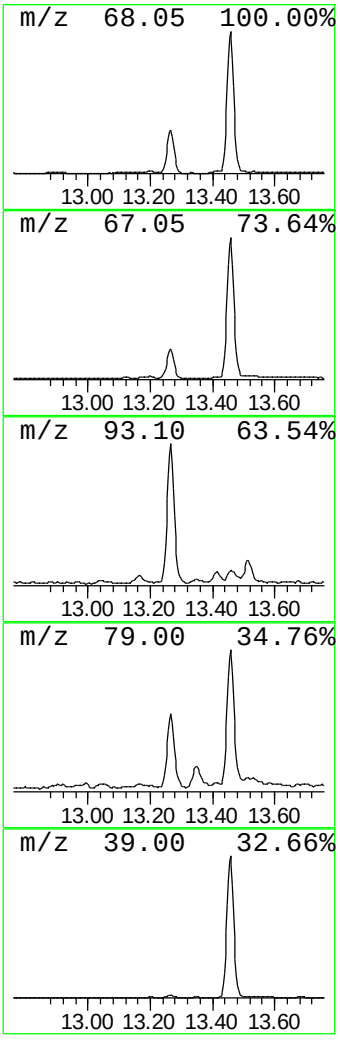
Peak Number 3 D-Limonene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	15.57 ug/l	463142	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	98
2	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	93
3	Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	90
4	Limonene	136	C10H16	000138-86-3	87
5	Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	76





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Data File : VN058523.D
Acq On : 3 Oct 2019 20:08
Operator : JC/SP
Sample : K5176-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30464-67

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.M
Quant Title : SW846 8260

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

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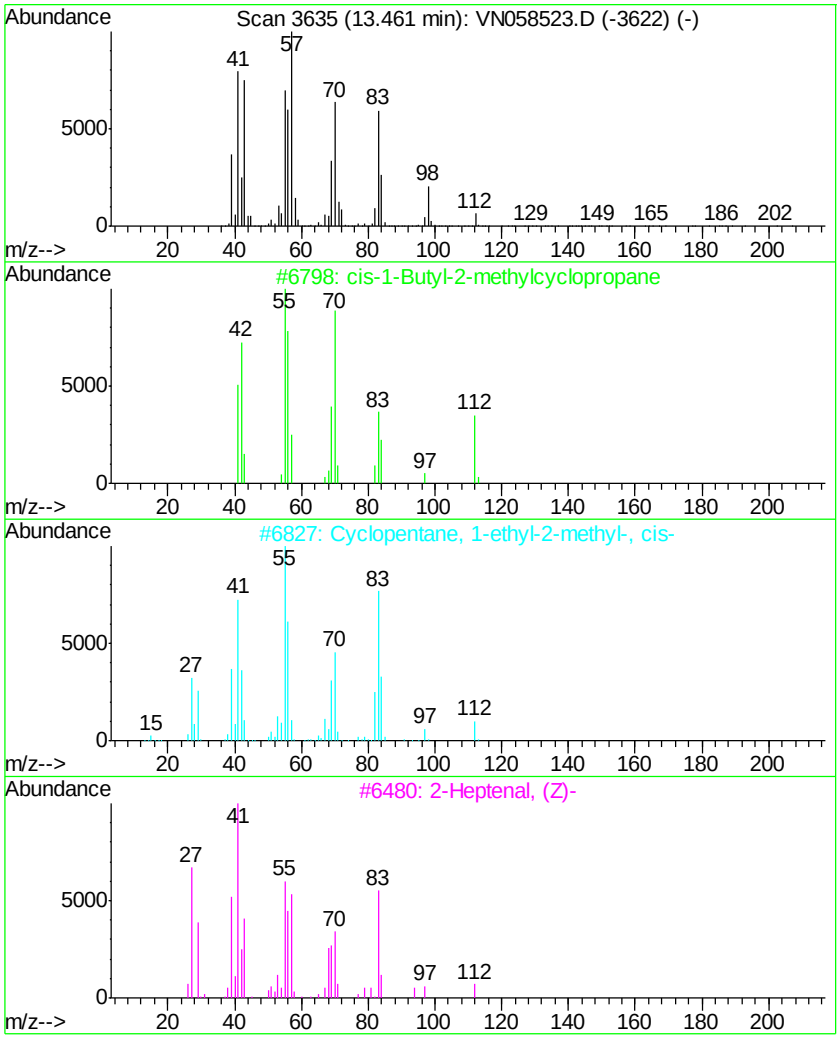
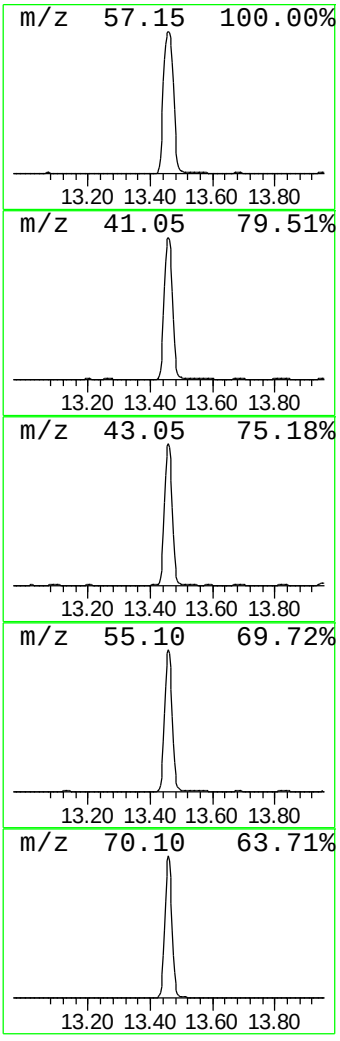
Peak Number 4 cis-1-Butyl-2-methylcyclopr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	1135.40 ug/l	33774300	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	70
2	Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	53
3	2-Heptenal, (Z)-	112	C7H12O	057266-86-1	52
4	Cyclopentane, 1-ethyl-3-methyl-,...	112	C8H16	002613-65-2	46
5	Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	46





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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30464-67

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.M
Quant Title : SW846 8260

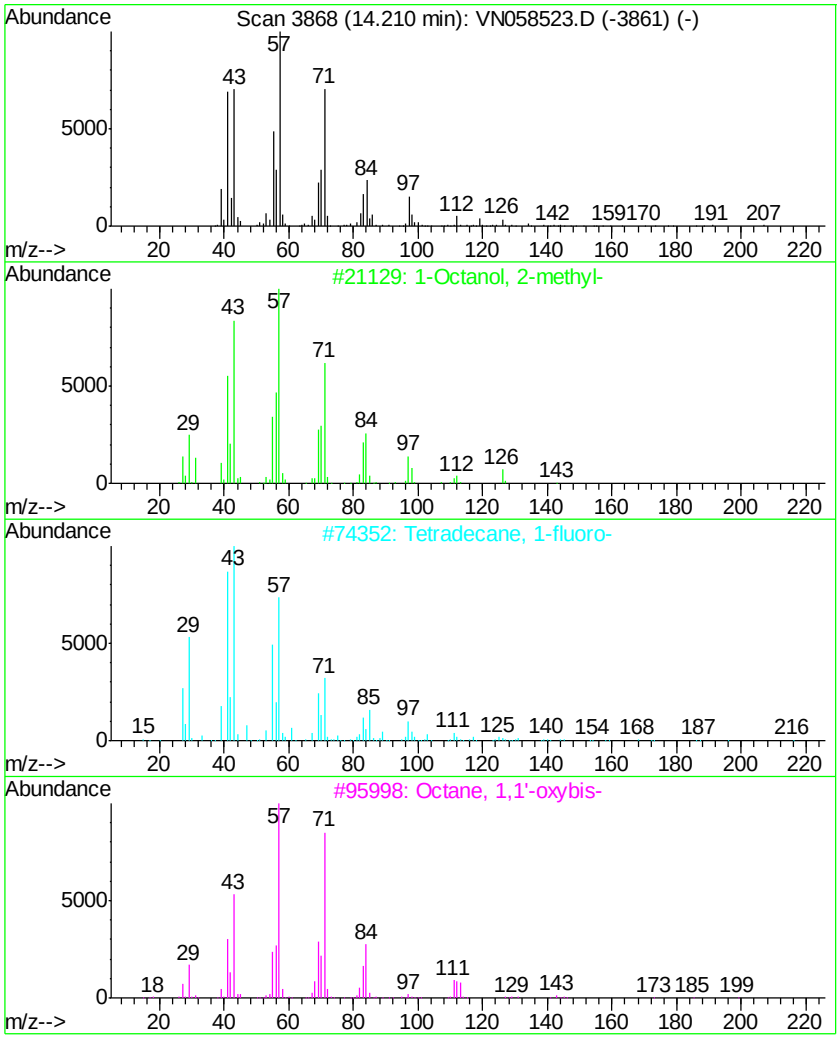
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

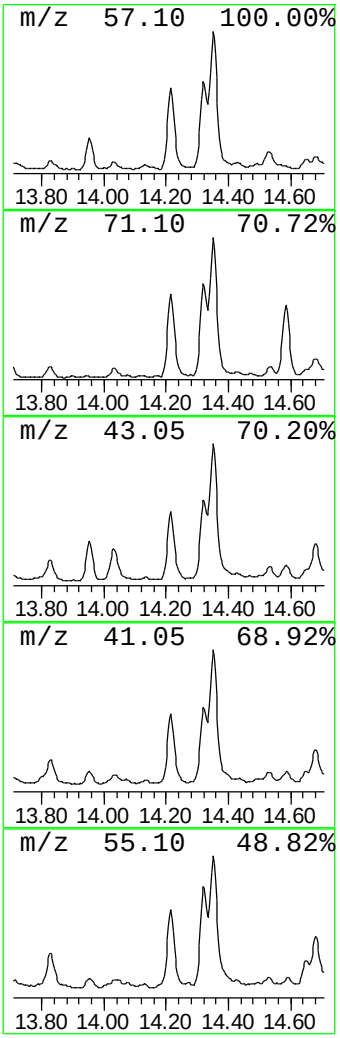
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	22.14 ug/l	658641	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	72
2	Tetradecane, 1-fluoro-	216	C14H29F	000593-33-9	72
3	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	59
4	Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	50
5	Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	47





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Instrument : MSVOA_N
ClientSampleId : 30464-67

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.M
Quant Title : SW846 8260

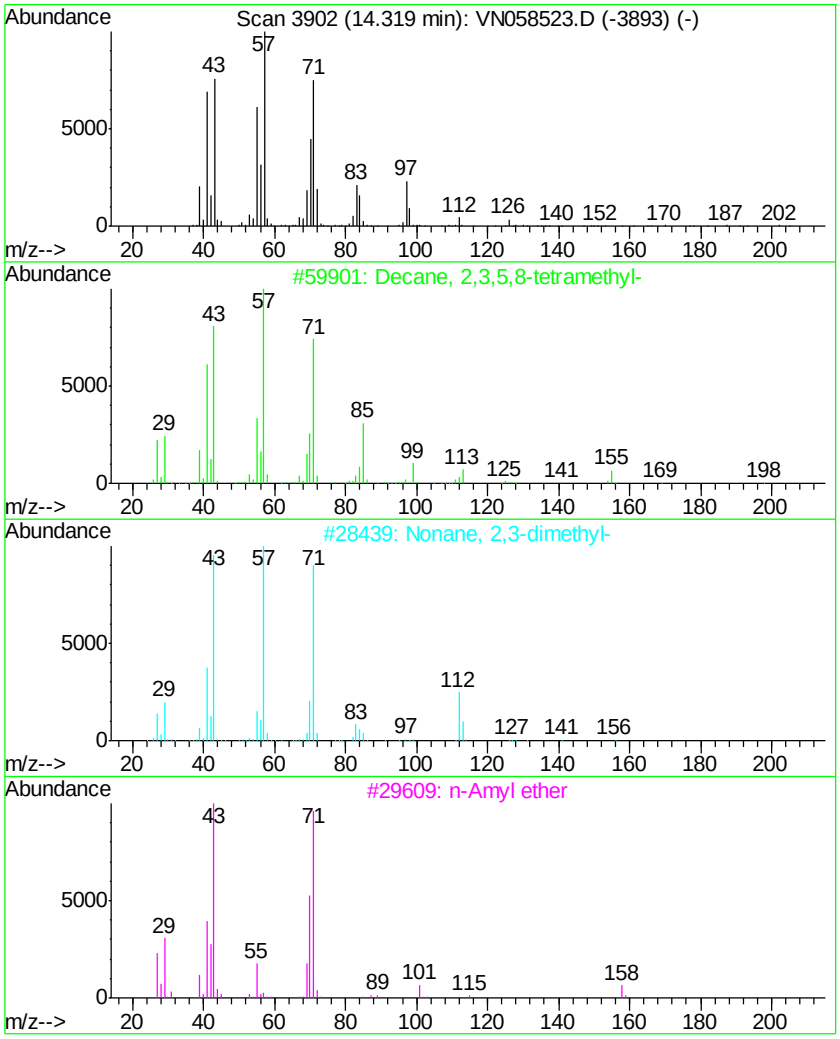
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

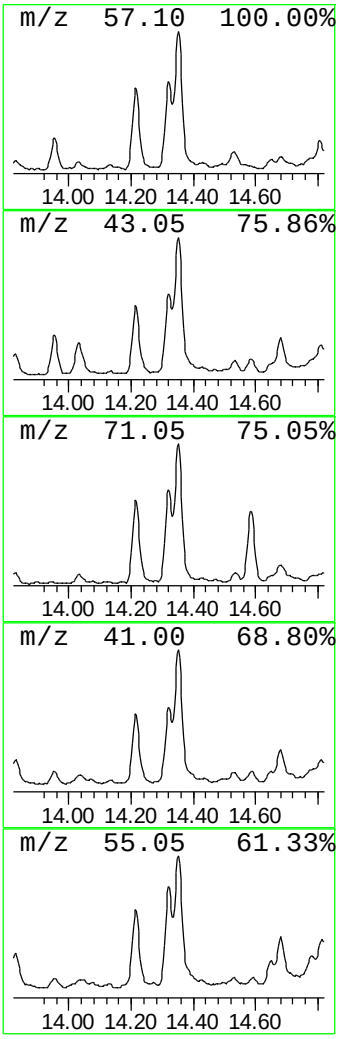
****

Peak Number 6 unknown14.32 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	23.59 ug/l	701817	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	47
2	Nonane, 2,3-dimethyl-	156	C11H24	002884-06-2	38
3	n-Amyl ether	158	C10H22O	000693-65-2	38
4	2-Ethyl-1-hexanol, heptafluorobu...	326	C12H17F7O2	1000365-16-0	35
5	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	1000365-19-6	35





Library Search Compound Report

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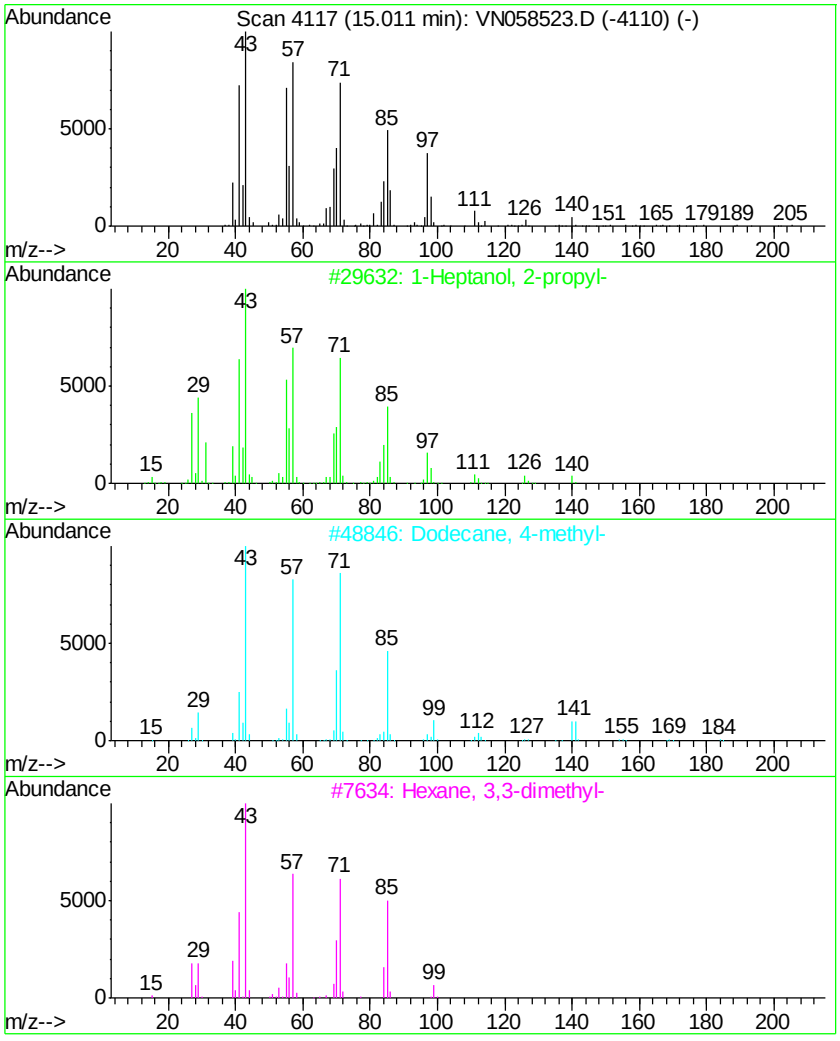
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

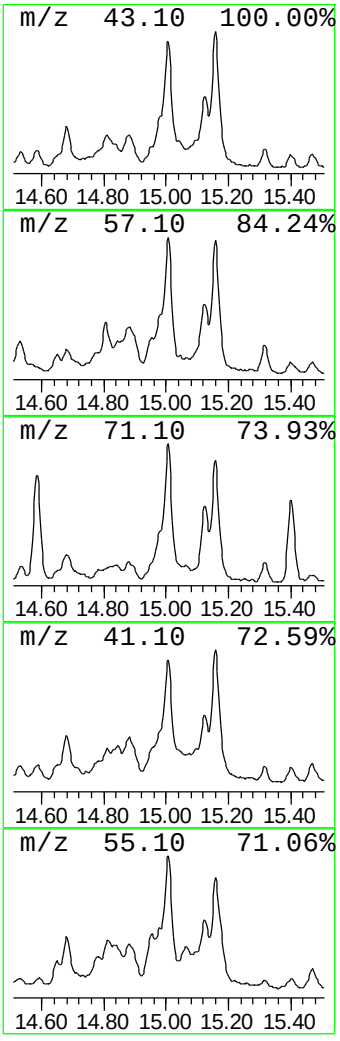
****

Peak Number 8 1-Heptanol, 2-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	15.19 ug/l	451718	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	58
2	Dodecane, 4-methyl-	184	C13H28	006117-97-1	53
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
4	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	41
5	4-Octanone	128	C8H16O	000589-63-9	38





Tentatively Identified Compound (LSC) summary

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ALS Vial : 23 Sample Multiplier: 1

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N092719W.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
Propylene Glycol	10.80	150.5	ug/l	5246490	3	11.41	1743190	50.0
unknown11.85	11.85	15.0	ug/l	524093	3	11.41	1743190	50.0
D-Limonene	13.26	15.6	ug/l	463142	4	13.35	1487340	50.0
cis-1-Butyl-2-met...	13.46	1135.4	ug/l	33774300	4	13.35	1487340	50.0
1-Octanol, 2-methyl-	14.21	22.1	ug/l	658641	4	13.35	1487340	50.0
unknown14.32	14.32	23.6	ug/l	701817	4	13.35	1487340	50.0
1-Heptanol, 2-pro...	15.01	15.2	ug/l	451718	4	13.35	1487340	50.0