LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068894.D
Acq On : 13 Oct 2021 13:42
Operator : JC/MD
Sample : M4142-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

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: VN068894.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.590	214	224	242	rVB	48252	83370	1.42%	0.362%
2	3.690	607	634	713	rBV	2109815	5862961	100.00%	25.429%
3	4.285	834	856	917	rBV	542741	1655993	28.24%	7.182%
4	4.572	939	963	996	rBV2	188350	600106	10.24%	2.603%
5	5.621	1324	1354	1386	rBV3	61384	224522	3.83%	0.974%
6	6.498	1659	1681	1698	rBV3	39987	123601	2.11%	0.536%
7	7.335	1966	1993	2013	rBV	95068	272763	4.65%	1.183%
8	7.651	2091	2111	2144	rBV	42286	124986	2.13%	0.542%
9	8.024	2228	2250	2261	rBV	278608	669814	11.42%	2.905%
10	8.088	2262	2274	2305	rVB	550092	1243368	21.21%	5.393%
11	8.440	2375	2405	2431	rBV2	325456	888991	15.16%	3.856%
12	8.641	2456	2480	2498	rBV5	32879	95043	1.62%	0.412%
13	8.968	2583	2602	2631	rBV	762010	1590000	27.12%	6.896%
14	9.156	2652	2672	2702	rBV	262872	617206	10.53%	2.677%
15	9.411	2751	2767	2783	rBV2	50102	104029	1.77%	0.451%
16	10.333	3095	3111	3125	rBV2	75893	141977	2.42%	0.616%
17	10.443	3128	3152	3167	rVV	1192939	2231915	38.07%	9.680%
18	10.508	3167	3176	3203	rVB	128331	257141	4.39%	1.115%
19	11.747	3620	3638	3660	rBV	1036208	1894647	32.32%	8.218%
20	12.278	3823	3836	3853	rVB5	36816	69418	1.18%	0.301%
21	12.734	3990	4006	4030	rVB	792560	1389009	23.69%	6.024%
22	13.678	4341	4358	4380	rBV	901564	1559687	26.60%	6.765%
23	13.772	4383	4393	4409	rVB2	97046	159616	2.72%	0.692%
24	14.997	4837	4850	4864	rVB	129399	222452	3.79%	0.965%
25	15.198	4910	4925	4939	rBV	76860	136846	2.33%	0.594%
26	15.949	5194	5205	5220	rVB3	73436	152938	2.61%	0.663%
27	16.059	5233	5246	5258	rBV	135658	265586	4.53%	1.152%
28	16.113	5259	5266	5279	rVB	45186	76516	1.31%	0.332%
29	16.217	5292	5305	5321	rVB	120608	251457	4.29%	1.091%
30	16.330	5333	5347	5371	rBV6	35687	90126	1.54%	0.391%

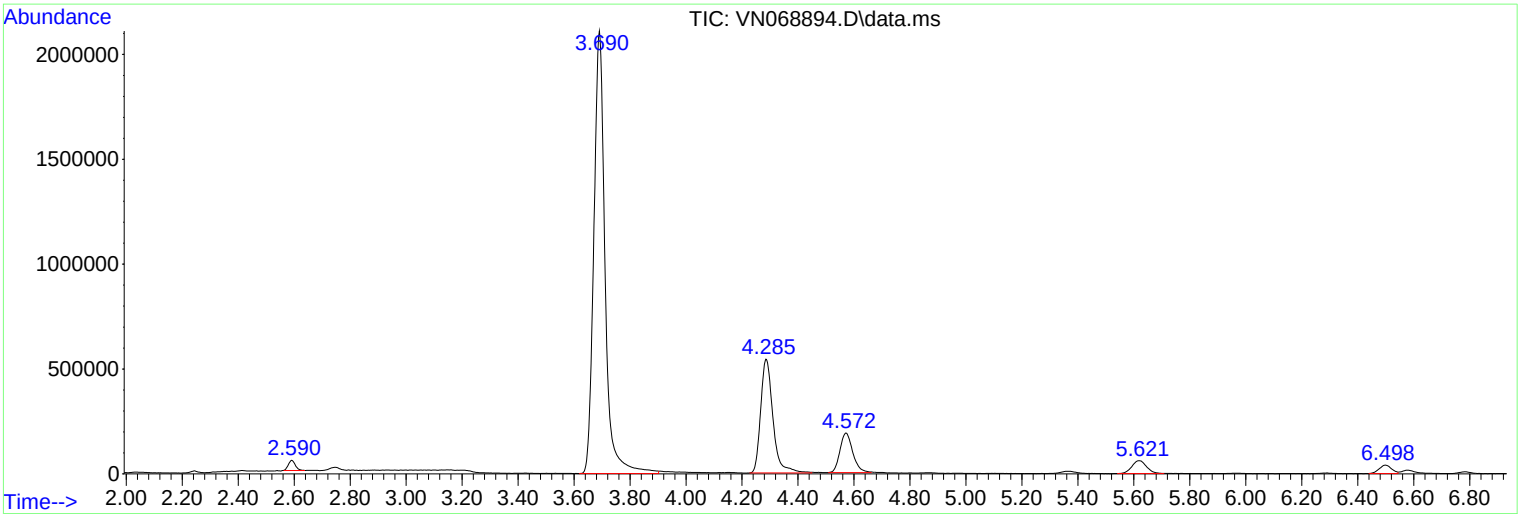
Sum of corrected areas: 23056084

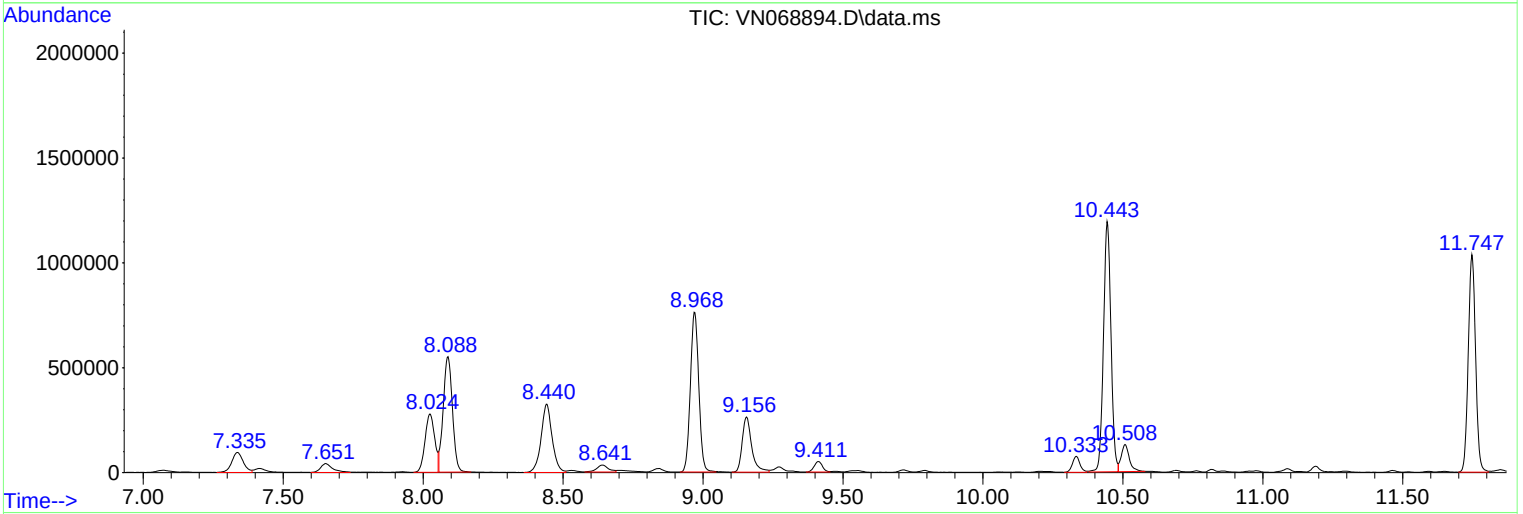
Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068894.D
Acq On : 13 Oct 2021 13:42
Operator : JC/MD
Sample : M4142-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

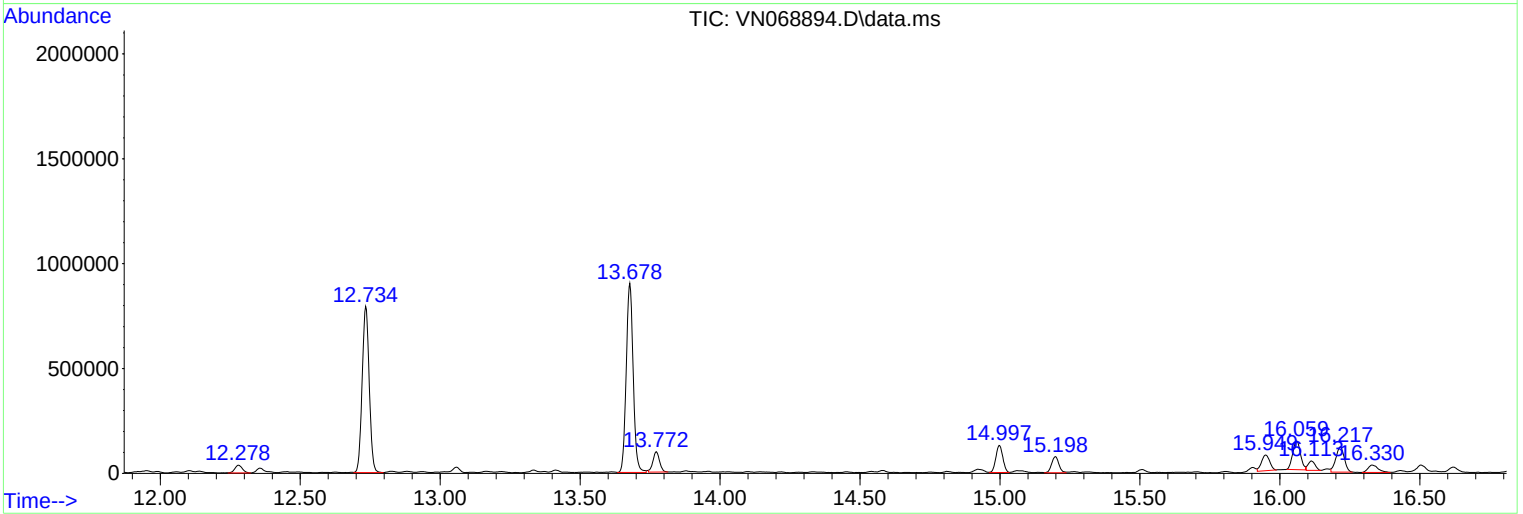
Instrument :
MSVOA_N
ClientSampleId :
2087

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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Data File : VN068894.D
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Instrument : MSVOA_N
ClientSampleId : 2087

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

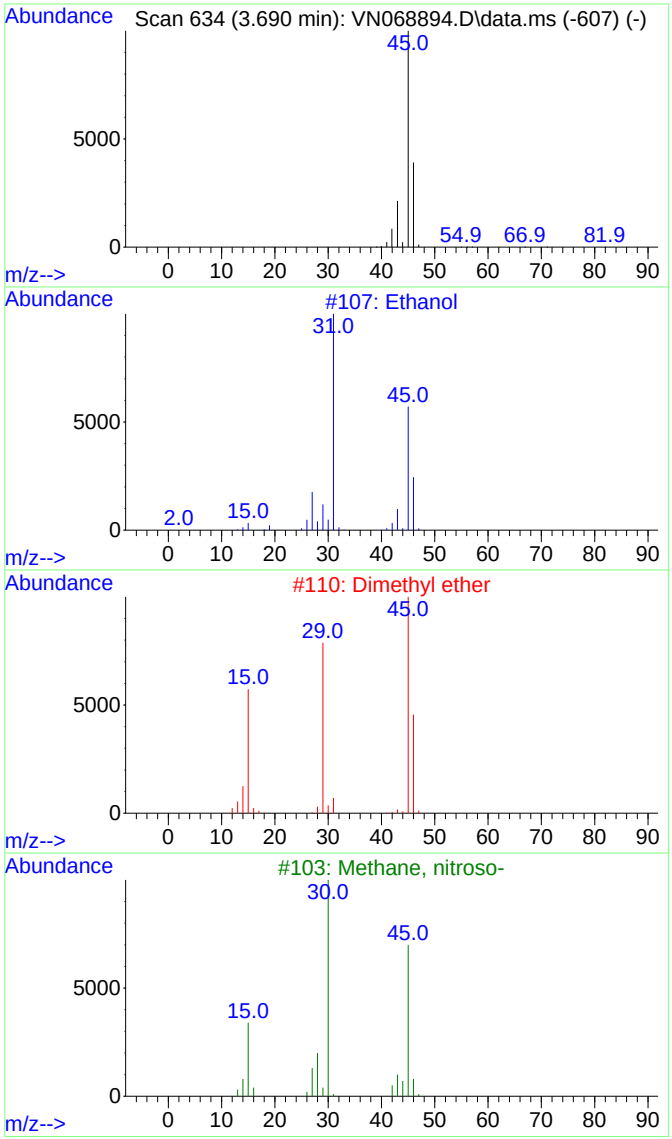
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

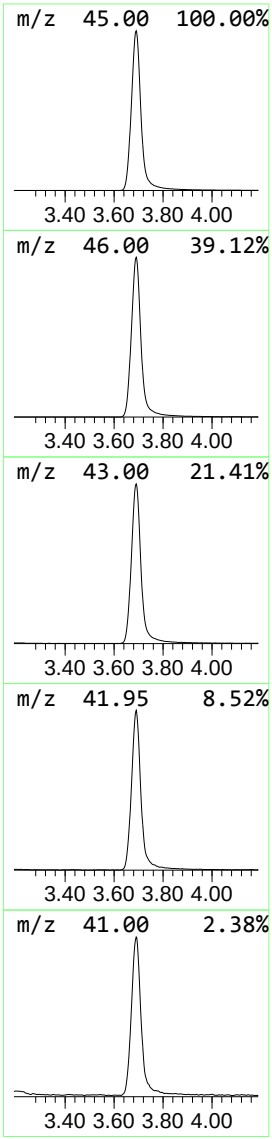
****

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.690	235.77 ug/l	5862960	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068894.D
Acq On : 13 Oct 2021 13:42
Operator : JC/MD
Sample : M4142-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

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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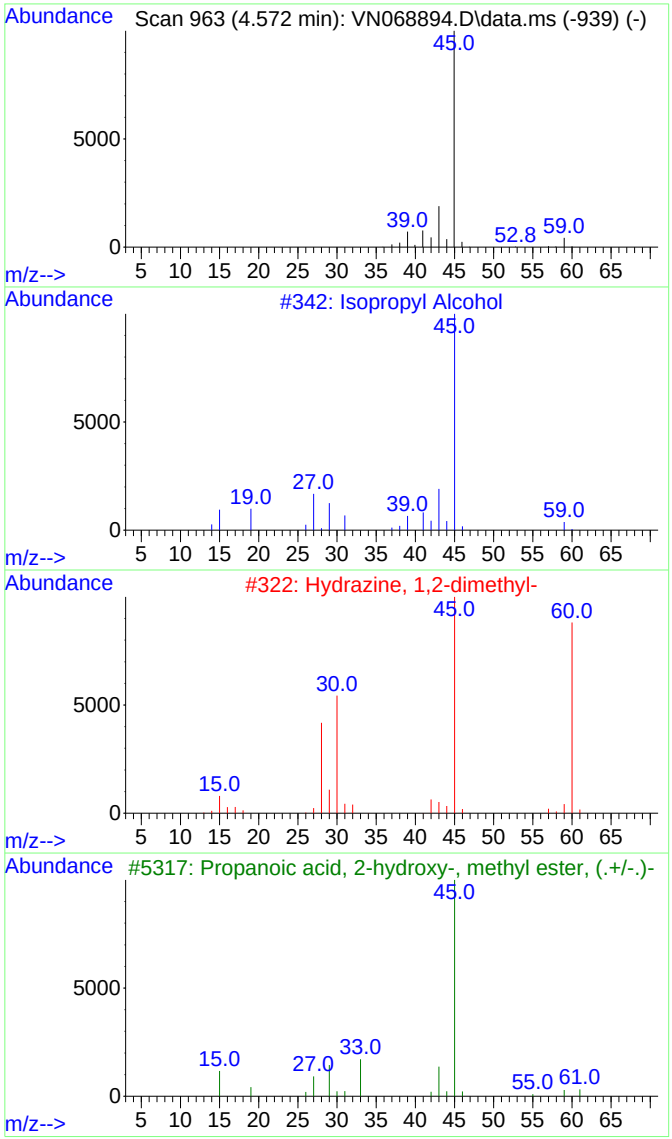
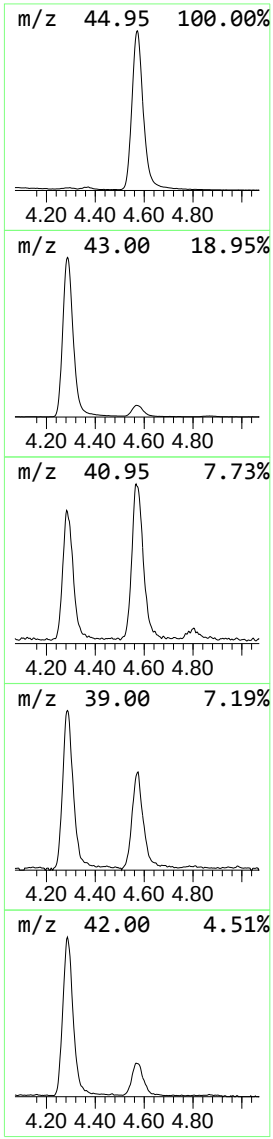
Peak Number 2 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.572	24.13 ug/l	600106	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4	Formamide	45	CH3NO	000075-12-7	7
5	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068894.D
Acq On : 13 Oct 2021 13:42
Operator : JC/MD
Sample : M4142-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

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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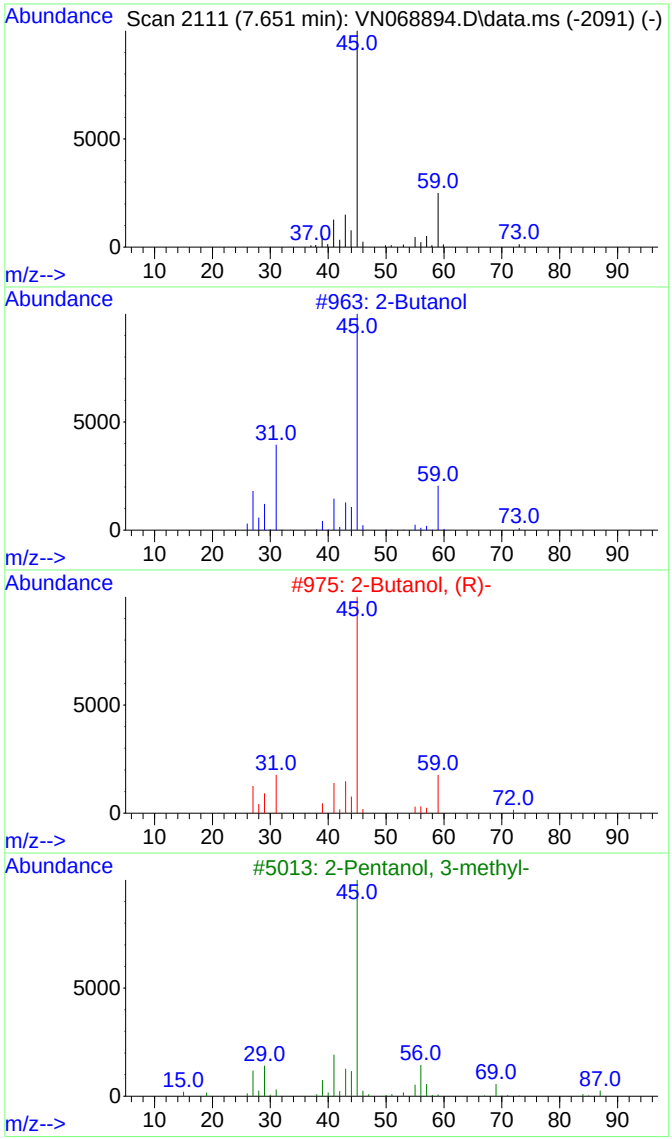
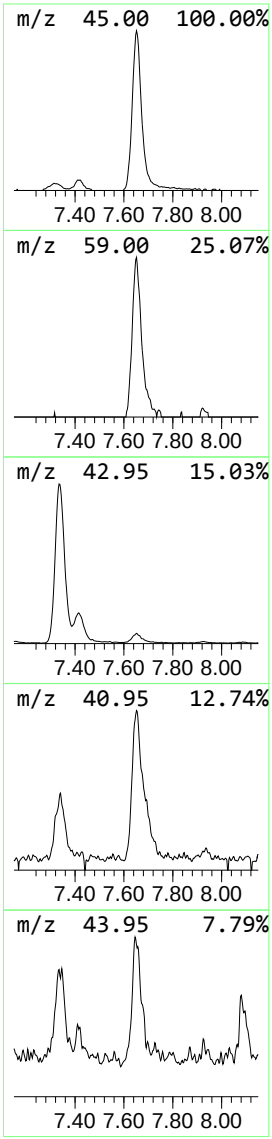
Peak Number 3 2-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.651	5.03 ug/l	124986	Pentafluorobenzene	8.088

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol	74	C4H10O	000078-92-2	83
2	2-Butanol, (R)-	74	C4H10O	014898-79-4	78
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	59
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	45
5	2-Hexanol	102	C6H14O	000626-93-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068894.D
Acq On : 13 Oct 2021 13:42
Operator : JC/MD
Sample : M4142-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

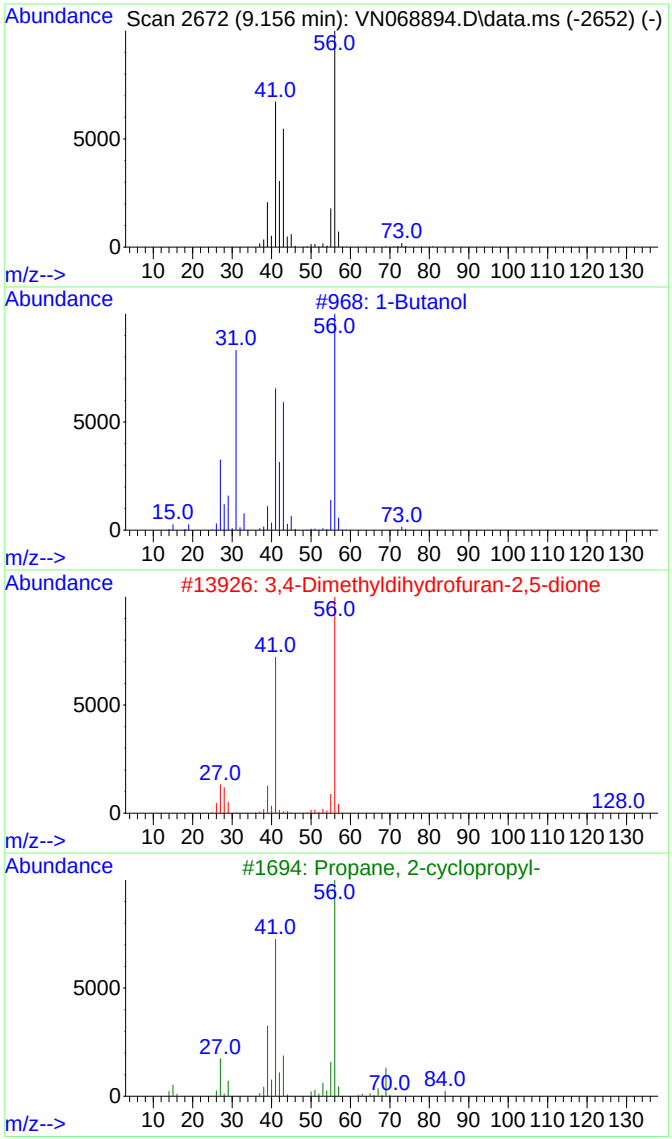
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

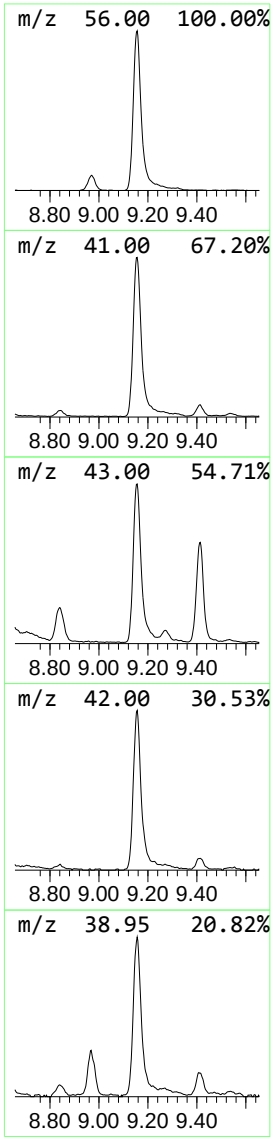
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.156	19.41 ug/l	617206	1,4-Difluorobenzene	8.971

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
4	2-Butene, (Z)-	56	C4H8	000590-18-1	9
5	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068894.D
Acq On : 13 Oct 2021 13:42
Operator : JC/MD
Sample : M4142-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

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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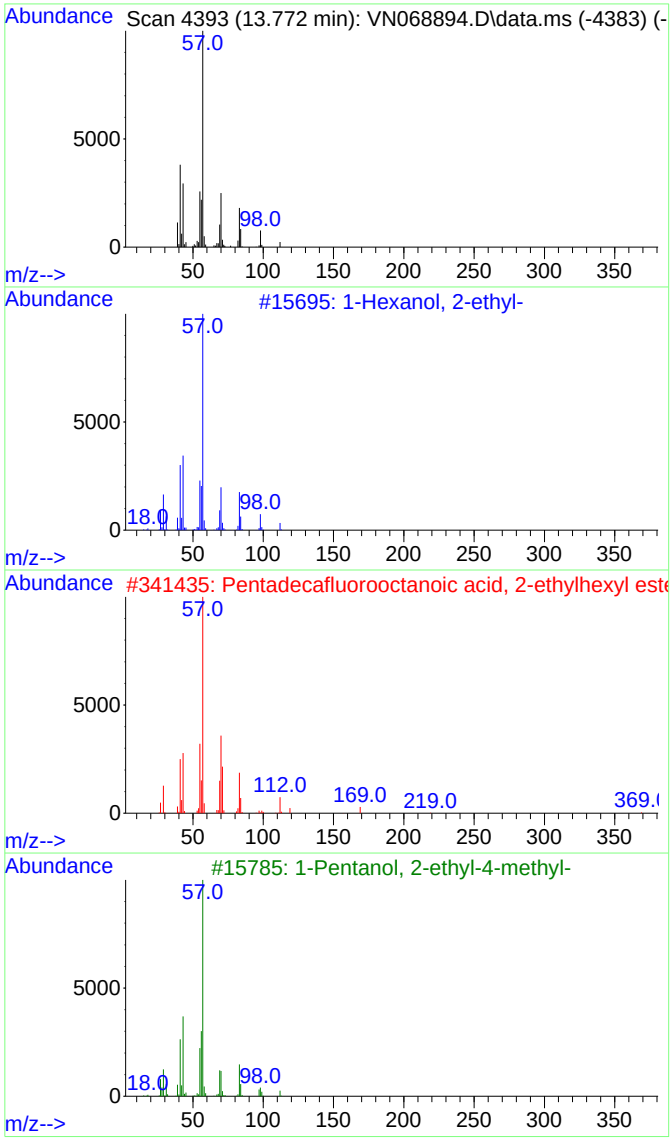
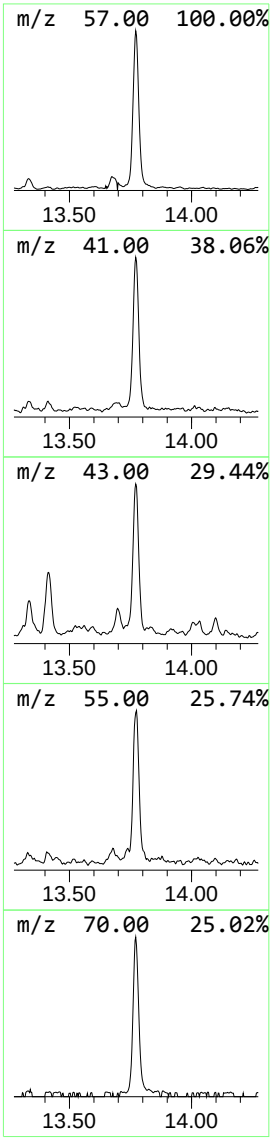
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.772	5.12 ug/l	159616	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	72
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59





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Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

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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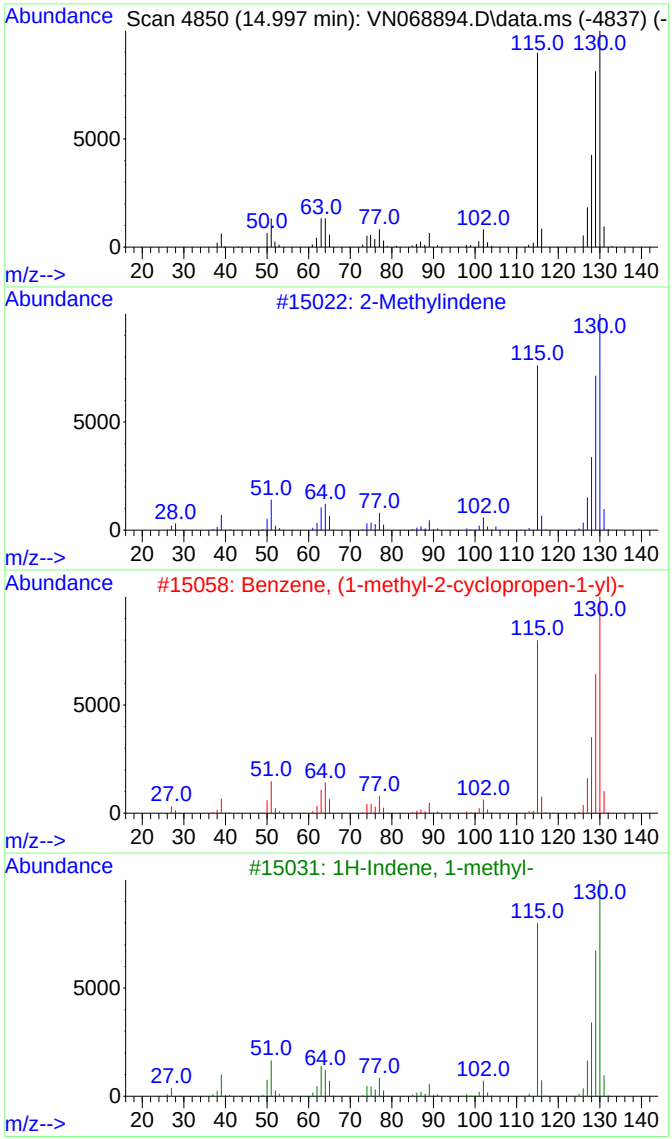
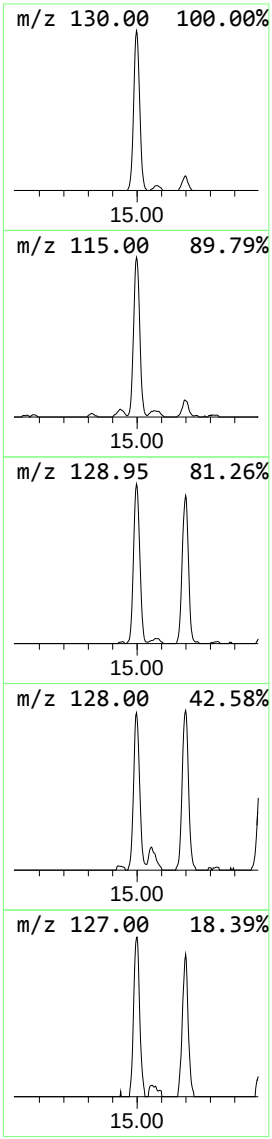
Peak Number 6 2-Methylindene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.997	7.13 ug/l	222452	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	97
2	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	97
3	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95
4	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	94





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Data File : VN068894.D
Acq On : 13 Oct 2021 13:42
Operator : JC/MD
Sample : M4142-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

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

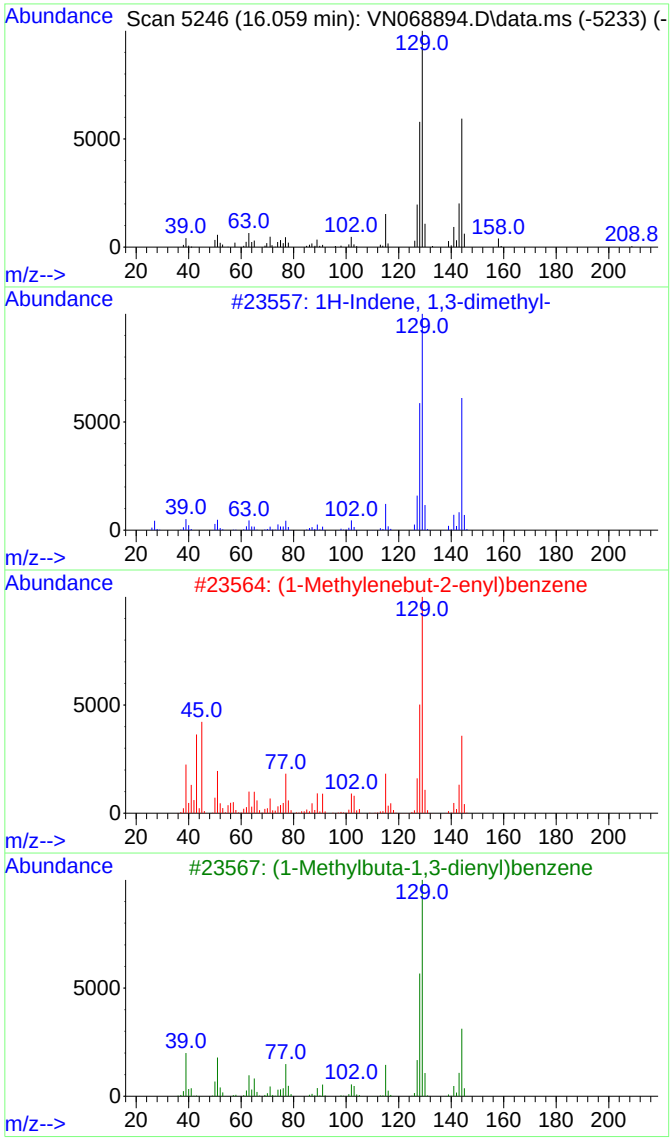
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

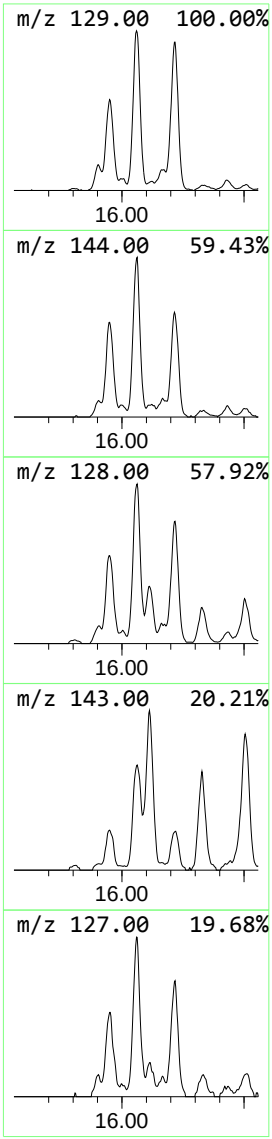
****

Peak Number 7 1H-Indene, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.059	8.51 ug/l	265586	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1,3-dimethyl-	144	C11H12	002177-48-2	96
2	(1-Methylenebut-2-enyl)benzene	144	C11H12	070588-46-4	91
3	(1-Methylbuta-1,3-dienyl)benzene	144	C11H12	054758-36-0	91
4	1H-Indene, 1-ethenyl-2,3-dihydro-	144	C11H12	051783-46-1	90
5	Benzene, (1-methyl-2-butynyl)-	144	C11H12	087712-69-4	83





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ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

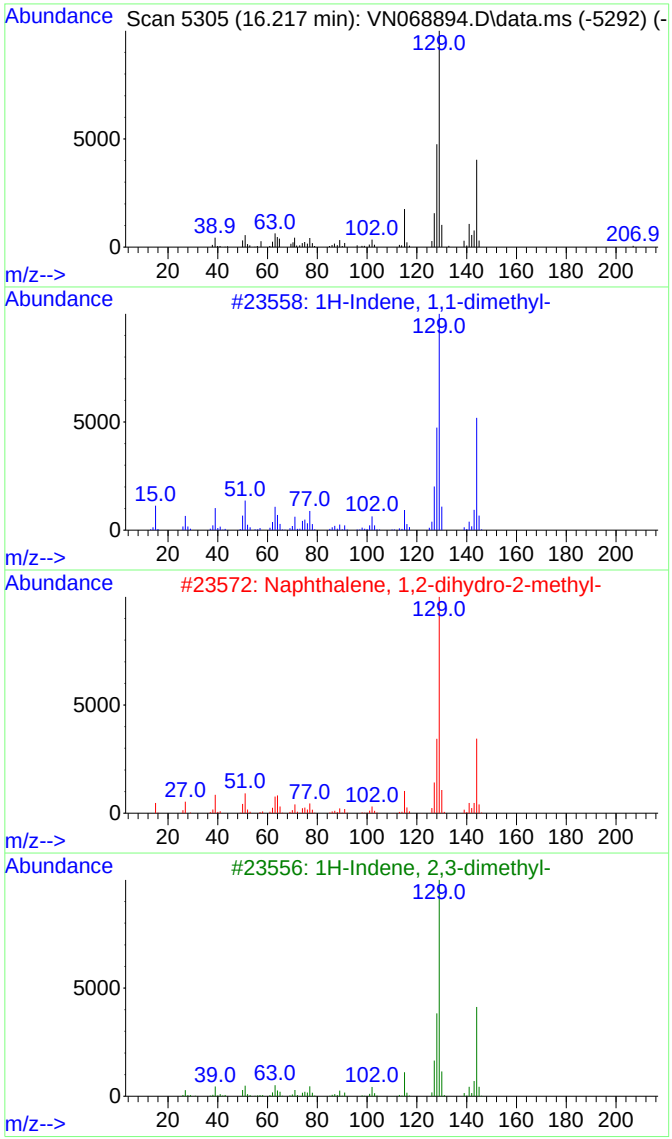
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

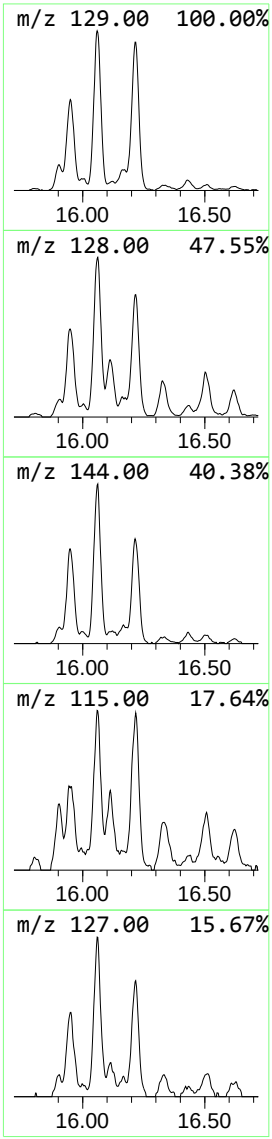
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1H-Indene, 1,1-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.218	8.06 ug/l	251457	1,4-Dichlorobenzene-d4	13.678

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1,1-dimethyl-	144	C11H12	018636-55-0	86
2	Naphthalene, 1,2-dihydro-2-methyl-	144	C11H12	021564-79-4	83
3	1H-Indene, 2,3-dimethyl-	144	C11H12	004773-82-4	81
4	(1-Methylbuta-1,3-dienyl)benzene	144	C11H12	054758-36-0	78
5	1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101321\
Data File : VN068894.D
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Operator : JC/MD
Sample : M4142-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 2087

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
Ethanol	3.690	235.8	ug/l	5862960	1	8.088	1243370	50.0
Isopropyl Alcohol	4.572	24.1	ug/l	600106	1	8.088	1243370	50.0
2-Butanol	7.651	5.0	ug/l	124986	1	8.088	1243370	50.0
1-Butanol	9.156	19.4	ug/l	617206	2	8.971	1590000	50.0
1-Hexanol, 2-et...	13.772	5.1	ug/l	159616	4	13.678	1559690	50.0
2-Methylindene	14.997	7.1	ug/l	222452	4	13.678	1559690	50.0
1H-Indene, 1,3-...	16.059	8.5	ug/l	265586	4	13.678	1559690	50.0
1H-Indene, 1,1-...	16.218	8.1	ug/l	251457	4	13.678	1559690	50.0