LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072423\
Data File : VX036635.D
Acq On : 24 Jul 2023 17:21
Operator : JC/MD
Sample : 03718-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
34585

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_X\Method\82X072123W.M
Title : SW846 8260

Signal : TIC: VX036635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	21	rVB	85013	93853	1.04%	0.418%
2	2.386	206	213	235	rBV	4474903	9020246	100.00%	40.177%
3	2.575	235	244	275	rVB	491191	1977547	21.92%	8.808%
4	4.562	559	570	589	rBV	137084	396865	4.40%	1.768%
5	5.032	635	647	664	rBV3	20881	93115	1.03%	0.415%
6	5.385	696	705	718	rBV2	100543	296398	3.29%	1.320%
7	5.550	722	732	749	rVB2	170329	488656	5.42%	2.177%
8	5.958	786	799	805	rBV	115212	299033	3.32%	1.332%
9	6.037	805	812	827	rVB	240660	641171	7.11%	2.856%
10	6.763	920	931	948	rBV	277756	664881	7.37%	2.961%
11	7.458	1037	1045	1060	rBV	706017	1393224	15.45%	6.206%
12	7.909	1112	1119	1134	rBV	153917	308010	3.41%	1.372%
13	8.647	1234	1240	1246	rBV	575544	909671	10.08%	4.052%
14	8.720	1246	1252	1267	rVB	619123	942742	10.45%	4.199%
15	9.488	1373	1378	1383	rBV	64339	93858	1.04%	0.418%
16	10.055	1463	1471	1483	rBV	598380	814942	9.03%	3.630%
17	10.299	1504	1511	1518	rVB	277240	370851	4.11%	1.652%
18	10.646	1562	1568	1581	rVB3	156436	289210	3.21%	1.288%
19	11.079	1634	1639	1645	rBV	488682	623652	6.91%	2.778%
20	12.024	1788	1794	1800	rVB	572785	757854	8.40%	3.376%
21	12.213	1821	1825	1838	rBV	291691	415839	4.61%	1.852%
22	12.414	1852	1858	1863	rBV	138230	178999	1.98%	0.797%
23	13.774	2073	2081	2088	rBV	1060562	1288631	14.29%	5.740%
24	14.634	2213	2222	2233	rVB	65429	91968	1.02%	0.410%

Sum of corrected areas: 22451216

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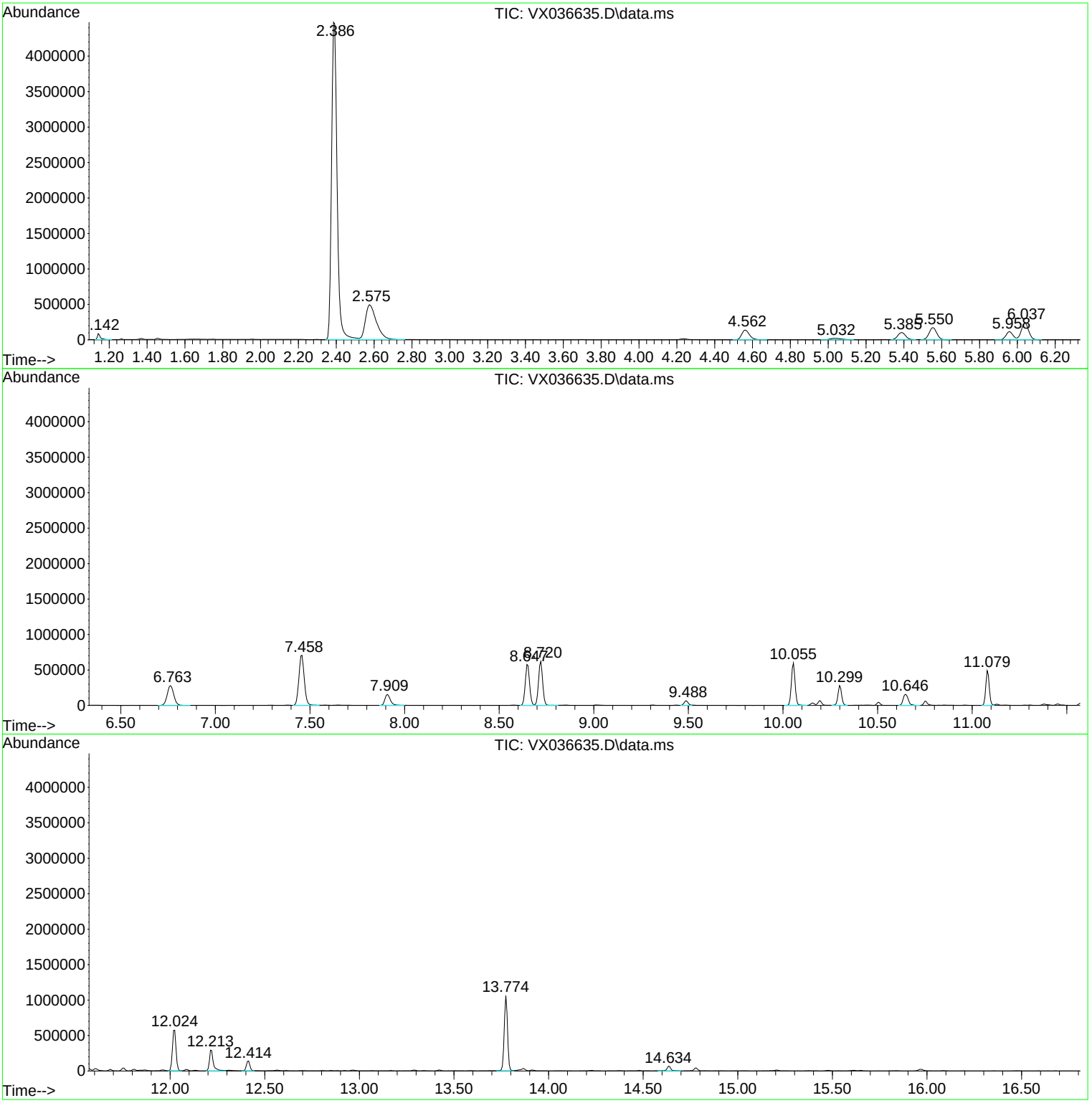
ClientSampleId :
34585

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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Data File : VX036635.D
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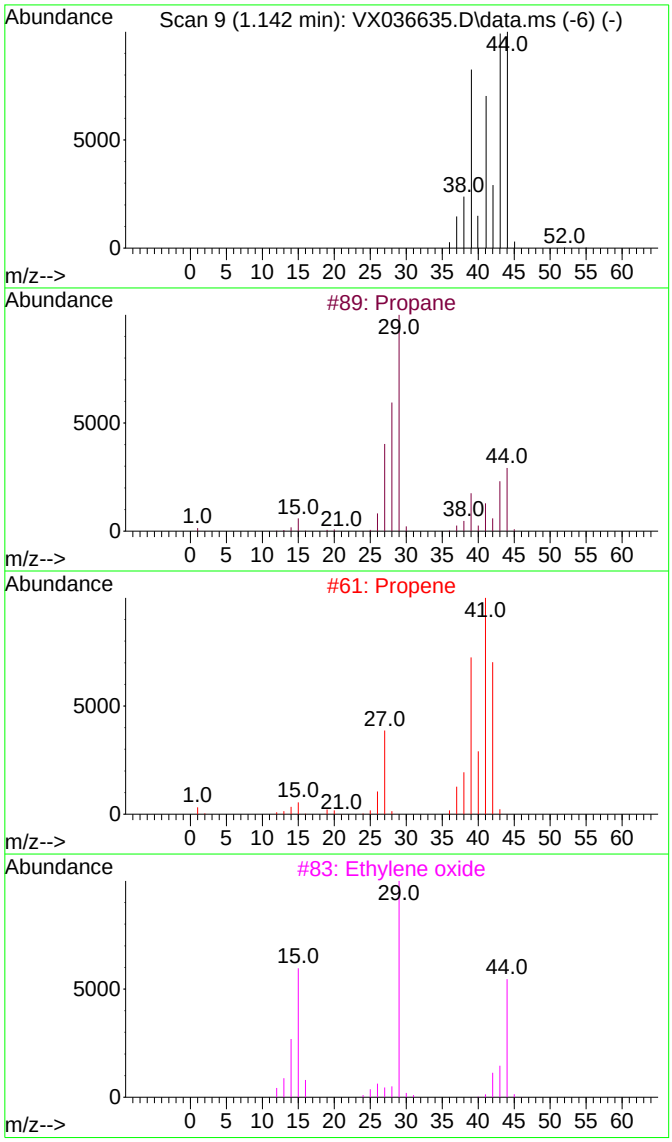
Quant Title : SW846 8260

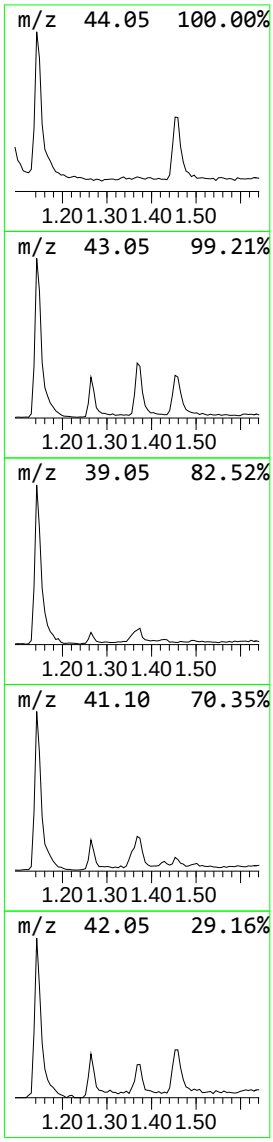
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	9.60 ug/l	93853	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Propene	42	C3H6	000115-07-1	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Cyclopropene	40	C3H4	002781-85-3	4
5	Alanine	89	C3H7NO2	000056-41-7	2





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
34585

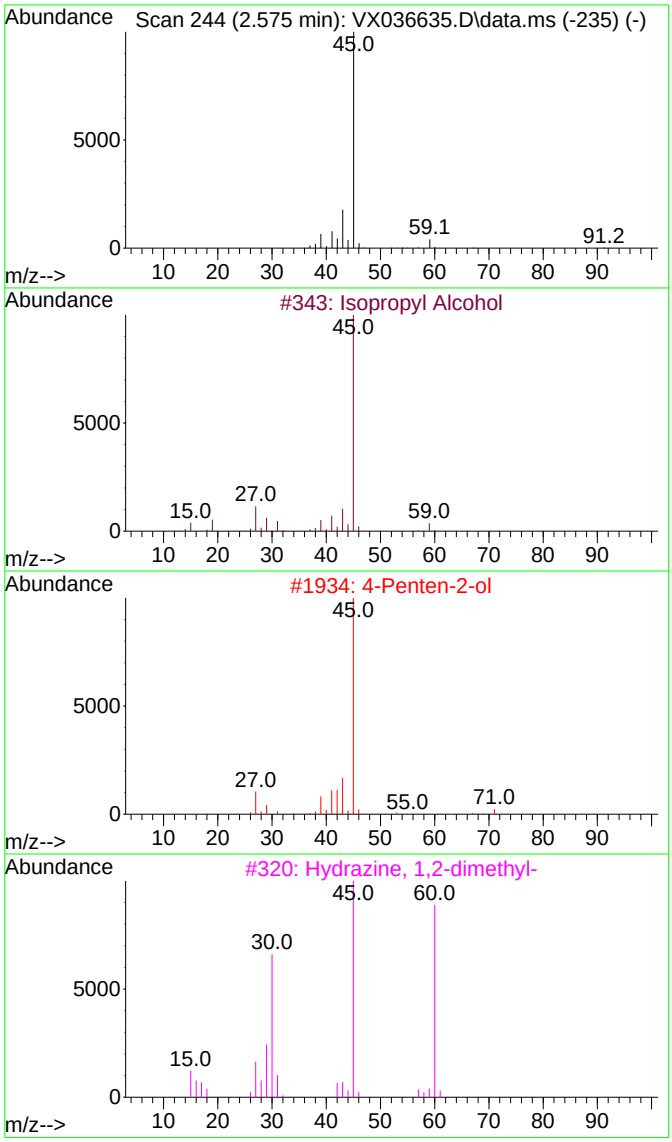
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

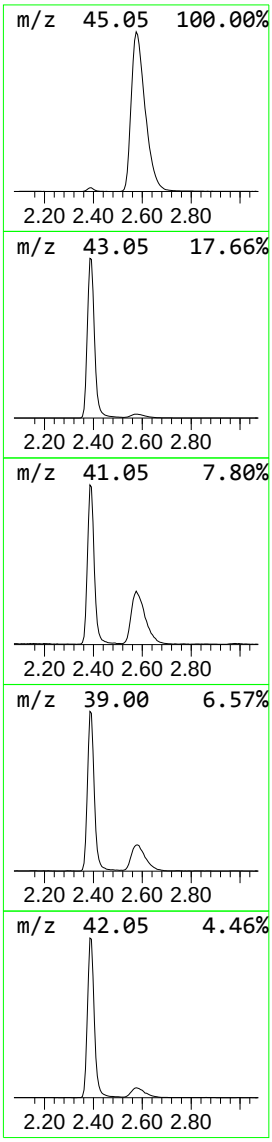
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.575	202.35 ug/l	1977550	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	4-Penten-2-ol	86	C5H10O	000625-31-0	9
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
34585

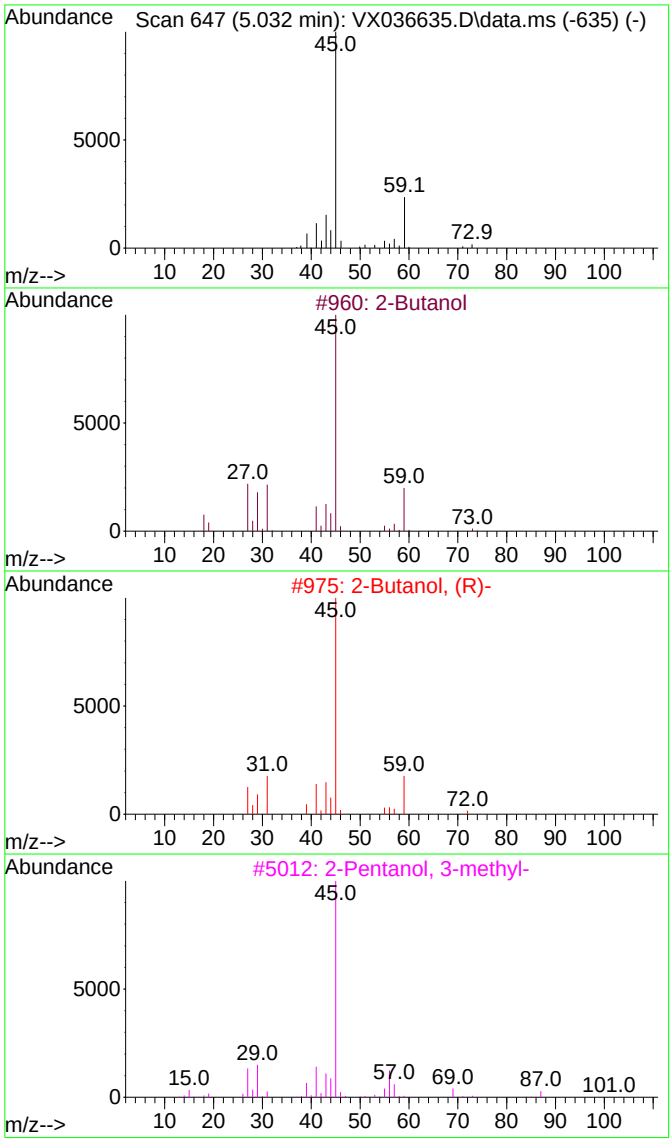
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

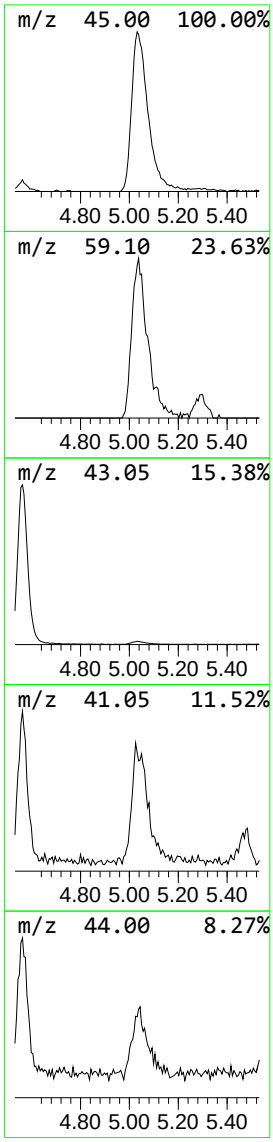
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.032	9.53 ug/l	93115	Pentafluorobenzene	5.556

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	45
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	45
5	2-Hexanol, (S)-	102	C6H14O	052019-78-0	38





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Data File : VX036635.D
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Operator : JC/MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
34585

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

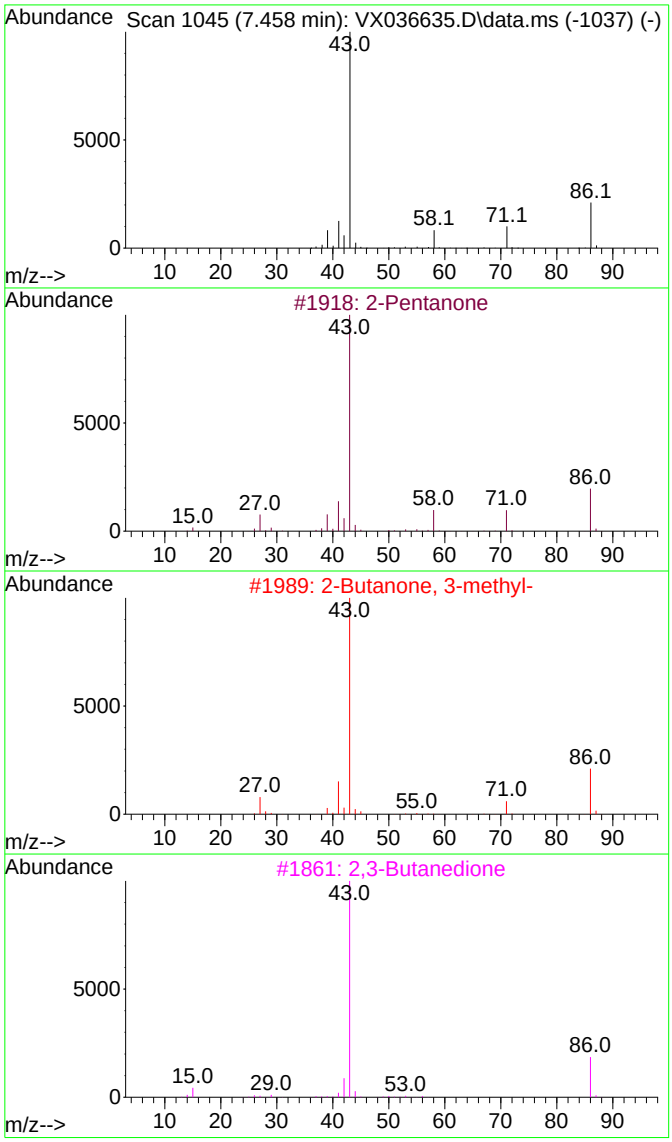
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

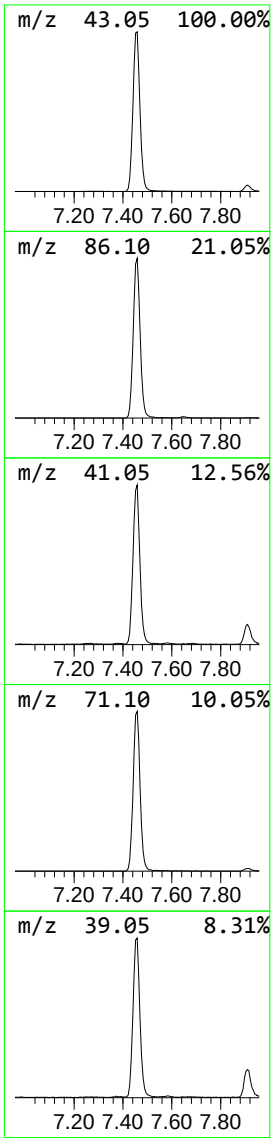
****

Peak Number 4 2-Pentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	104.77 ug/l	1393220	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	2,3-Butanedione	86	C4H6O2	000431-03-8	9
4	Butane	58	C4H10	000106-97-8	9
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





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Operator : JC/MD
Sample : 03718-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
34585

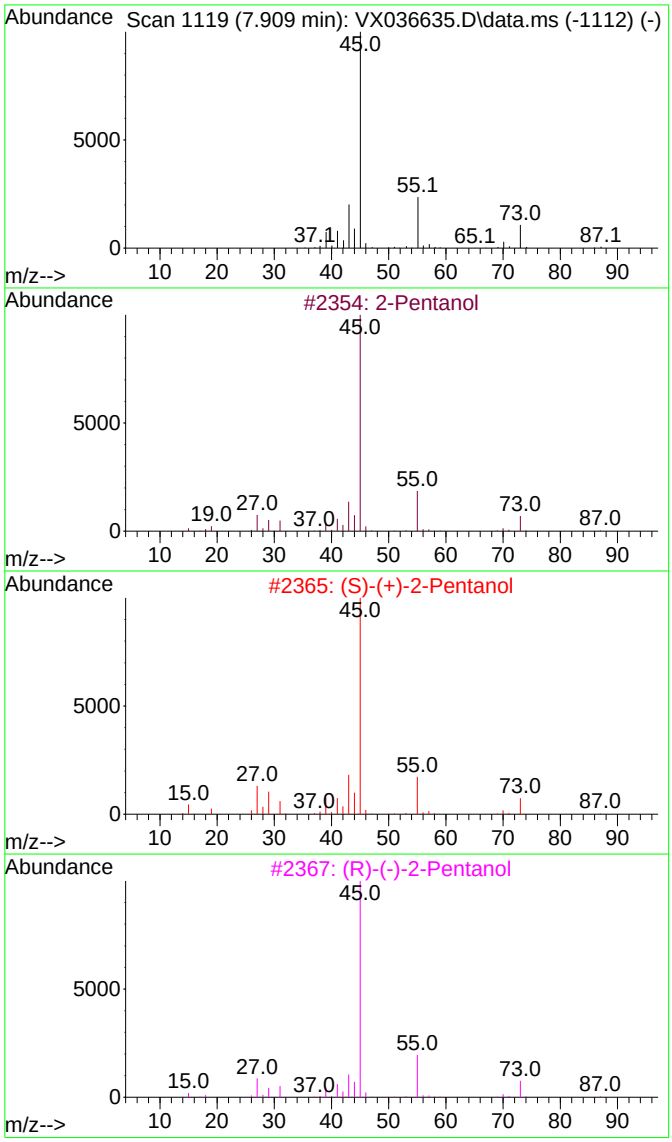
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

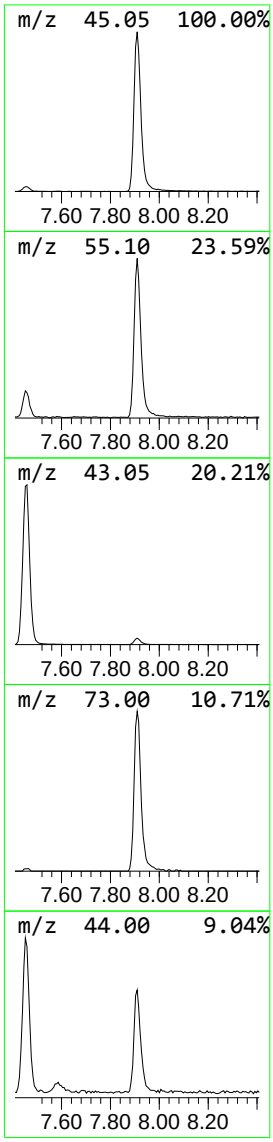
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.909	23.16 ug/l	308010	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol	88	C5H12O	006032-29-7	83
2	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	78
3	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	74
4	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	64
5	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	64





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
34585

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

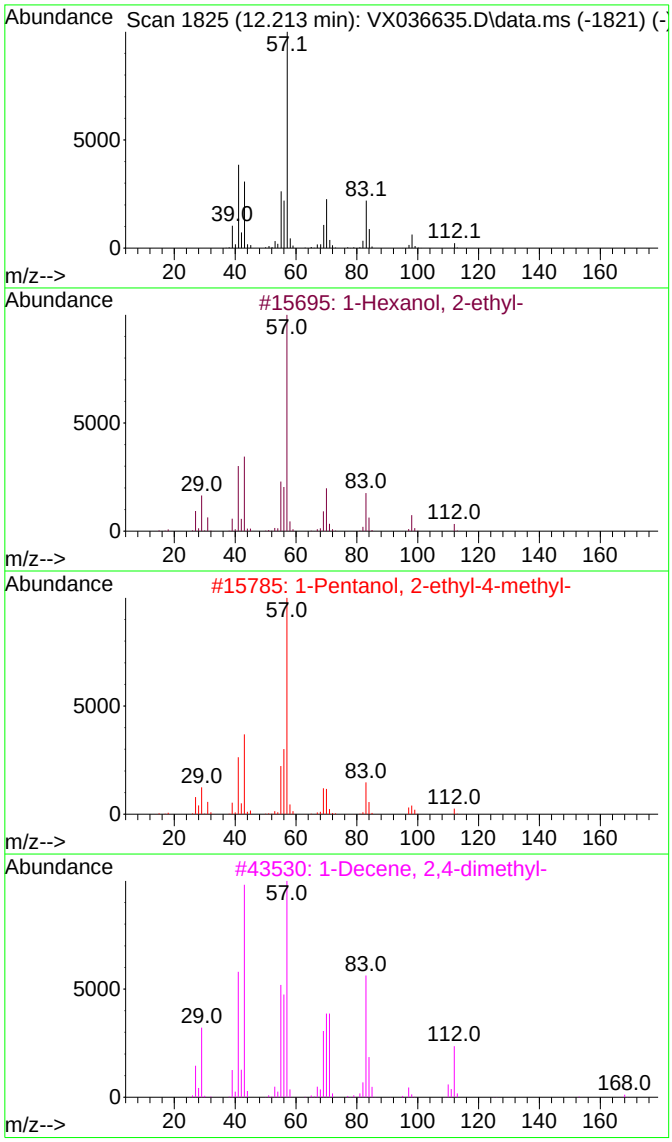
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

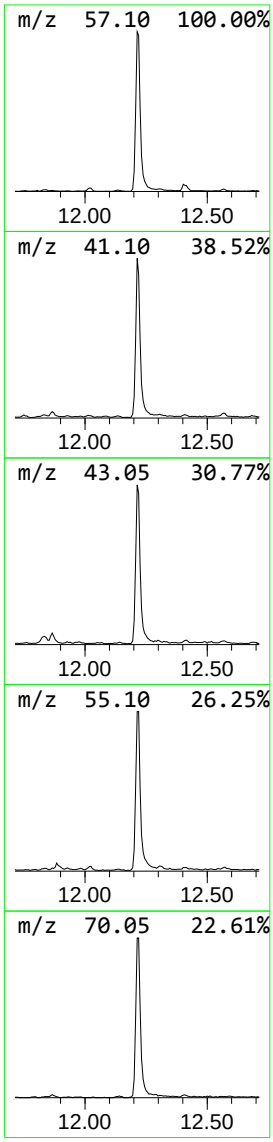
****

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	27.44 ug/l	415839	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	47





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MSVOA_X
ClientSampleId :
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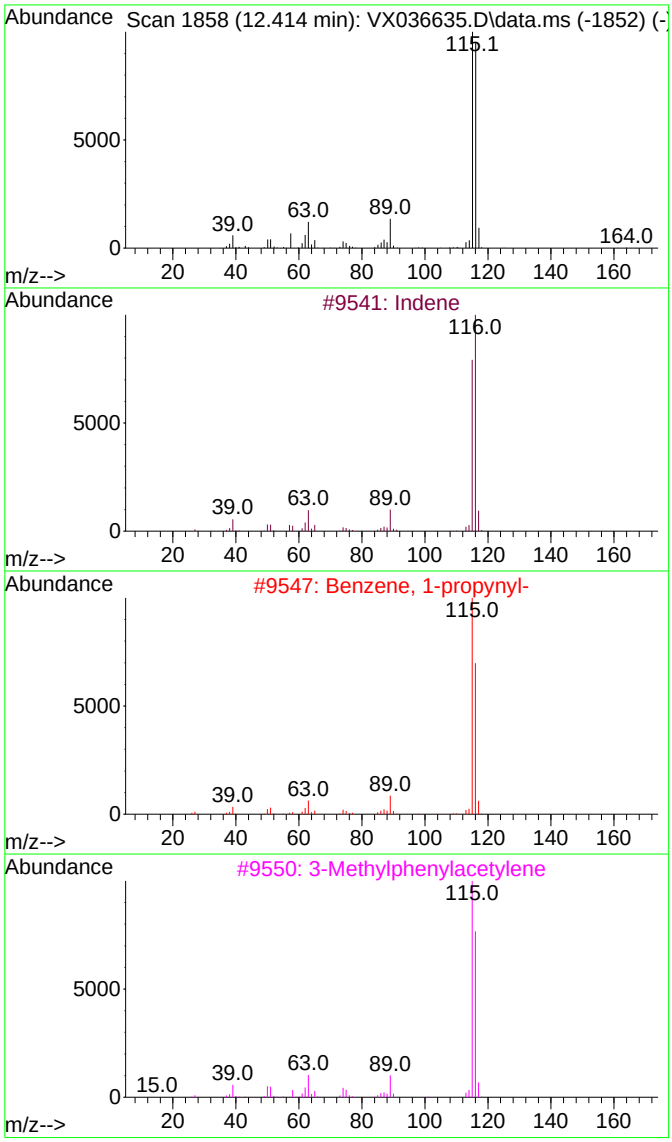
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

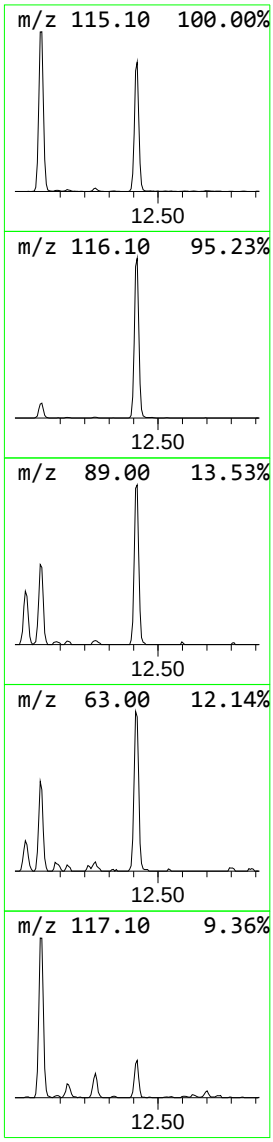
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	11.81 ug/l	178999	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	86





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MSVOA_X
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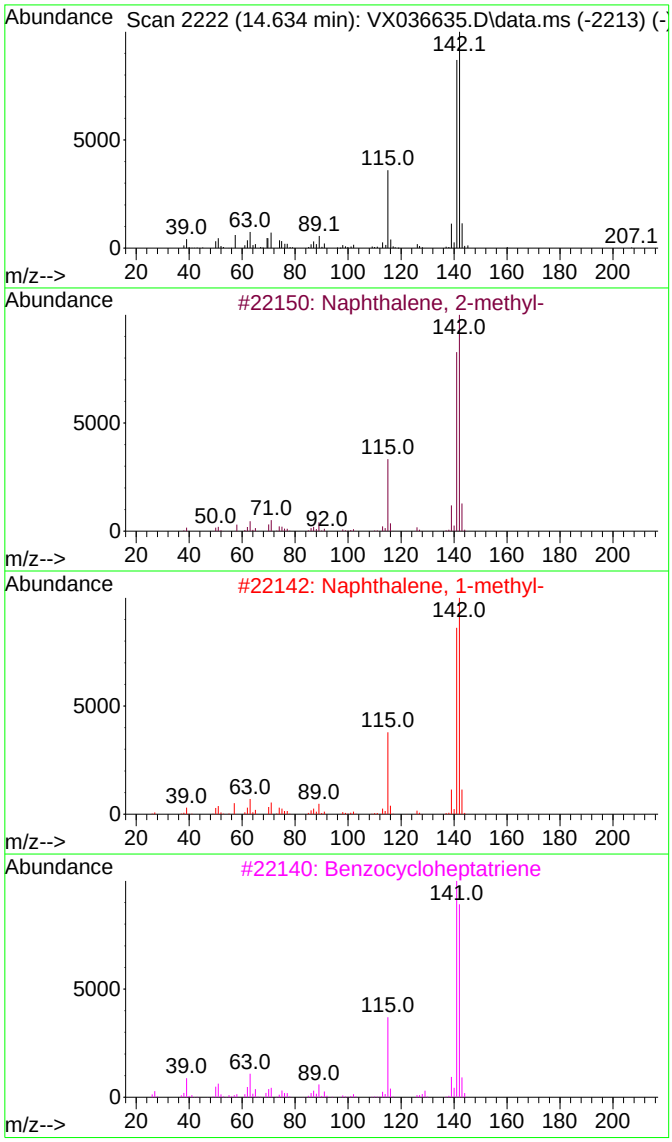
Quant Title : SW846 8260

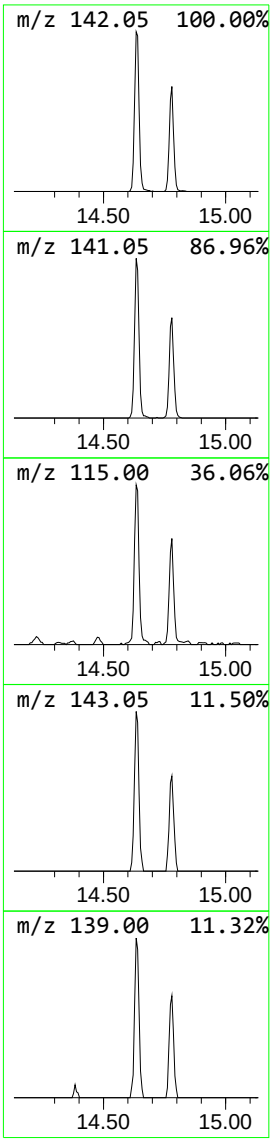
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	6.07 ug/l	91968	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Tentatively Identified Compound (LSC) summary

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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
Propane	1.142	9.6	ug/l	93853	1	5.556	488656	50.0
Isopropyl Alcohol	2.575	202.3	ug/l	1977550	1	5.556	488656	50.0
2-Butanol	5.032	9.5	ug/l	93115	1	5.556	488656	50.0
2-Pentanone	7.458	104.8	ug/l	1393220	2	6.763	664881	50.0
2-Pentanol	7.909	23.2	ug/l	308010	2	6.763	664881	50.0
1-Hexanol, 2-et...	12.213	27.4	ug/l	415839	4	12.024	757854	50.0
Indene	12.414	11.8	ug/l	178999	4	12.024	757854	50.0
Naphthalene, 2-...	14.634	6.1	ug/l	91968	4	12.024	757854	50.0