LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP-1

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\82X022421W.M
Title : SW846 8260

Signal : TIC: VX021110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.164	9	13	19	rBV2	42451	44603	1.43%	0.235%
2	1.476	62	66	76	rBV	194686	216260	6.96%	1.140%
3	2.087	164	170	177	rBV	21597	36252	1.17%	0.191%
4	2.329	206	211	219	rVV	31818	50513	1.62%	0.266%
5	2.417	220	226	237	rVB	27541	45848	1.47%	0.242%
6	2.576	245	253	261	rBV	17844	35592	1.14%	0.188%
7	3.005	317	326	338	rBV	25081	59493	1.91%	0.313%
8	3.382	382	390	400	rVB	23561	54504	1.75%	0.287%
9	4.299	532	546	567	rBV	1144765	3108658	100.00%	16.381%
10	5.464	732	744	757	rBV2	131492	376118	12.10%	1.982%
11	5.629	761	772	789	rBV	200001	565337	18.19%	2.979%
12	6.035	831	841	850	rBV	143380	372039	11.97%	1.960%
13	6.829	963	976	998	rBV	347746	834299	26.84%	4.396%
14	7.265	1043	1050	1072	rBV	91760	217449	6.99%	1.146%
15	7.635	1105	1113	1123	rBV	100773	194427	6.25%	1.025%
16	8.694	1285	1293	1301	rBV	742530	1192496	38.36%	6.284%
17	8.765	1301	1305	1309	rVV	44093	72383	2.33%	0.381%
18	8.812	1309	1313	1323	rVB	16718	31808	1.02%	0.168%
19	9.277	1386	1392	1411	rBV	147764	246019	7.91%	1.296%
20	10.094	1525	1531	1542	rBV	783502	1092281	35.14%	5.756%
21	10.194	1542	1548	1561	rBV	289659	448324	14.42%	2.362%
22	10.341	1568	1573	1582	rVB2	40031	60911	1.96%	0.321%
23	10.483	1592	1597	1603	rBV	57371	76062	2.45%	0.401%
24	10.683	1623	1631	1636	rBV4	21538	48932	1.57%	0.258%
25	10.788	1644	1649	1664	rBV	102507	161436	5.19%	0.851%
26	11.118	1699	1705	1711	rBV	627635	822736	26.47%	4.335%
27	11.171	1711	1714	1720	rVB	32794	42892	1.38%	0.226%
28	11.612	1783	1789	1791	rBV	60200	78271	2.52%	0.412%
29	11.642	1791	1794	1803	rVV3	51030	88311	2.84%	0.465%
30	11.724	1803	1808	1815	rVV	365483	434465	13.98%	2.289%
31	11.789	1815	1819	1823	rVB	29689	37191	1.20%	0.196%
32	11.906	1834	1839	1847	rBV	213128	293066	9.43%	1.544%
33	11.989	1849	1853	1856	rVV	80654	113456	3.65%	0.598%
34	12.024	1856	1859	1862	rVV	163072	232460	7.48%	1.225%
35	12.059	1862	1865	1873	rVB	847978	1094316	35.20%	5.766%
36	12.253	1893	1898	1909	rBV	1260735	1714139	55.14%	9.033%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP-1

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\82X022421W.M
Title : SW846 8260

37	12.342	1909	1913	1927	rVV4	64302	151094	4.86%	0.796%
38	12.453	1927	1932	1936	rVB	33573	45035	1.45%	0.237%
39	12.630	1954	1962	1969	rVB5	22204	41862	1.35%	0.221%
40	12.830	1991	1996	2002	rBV4	21456	40835	1.31%	0.215%
41	13.648	2127	2135	2143	rBV	34997	61025	1.96%	0.322%
42	13.883	2170	2175	2182	rVV	77610	121651	3.91%	0.641%
43	13.954	2182	2187	2204	rVB	77697	143558	4.62%	0.756%
44	14.607	2293	2298	2307	rBV	470274	574311	18.47%	3.026%
45	16.024	2531	2539	2556	rBV2	1767060	3093066	99.50%	16.299%
46	16.148	2556	2560	2571	rVB2	57091	111660	3.59%	0.588%

Sum of corrected areas: 18977444

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
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Operator : JC/MD
Sample : M1578-01
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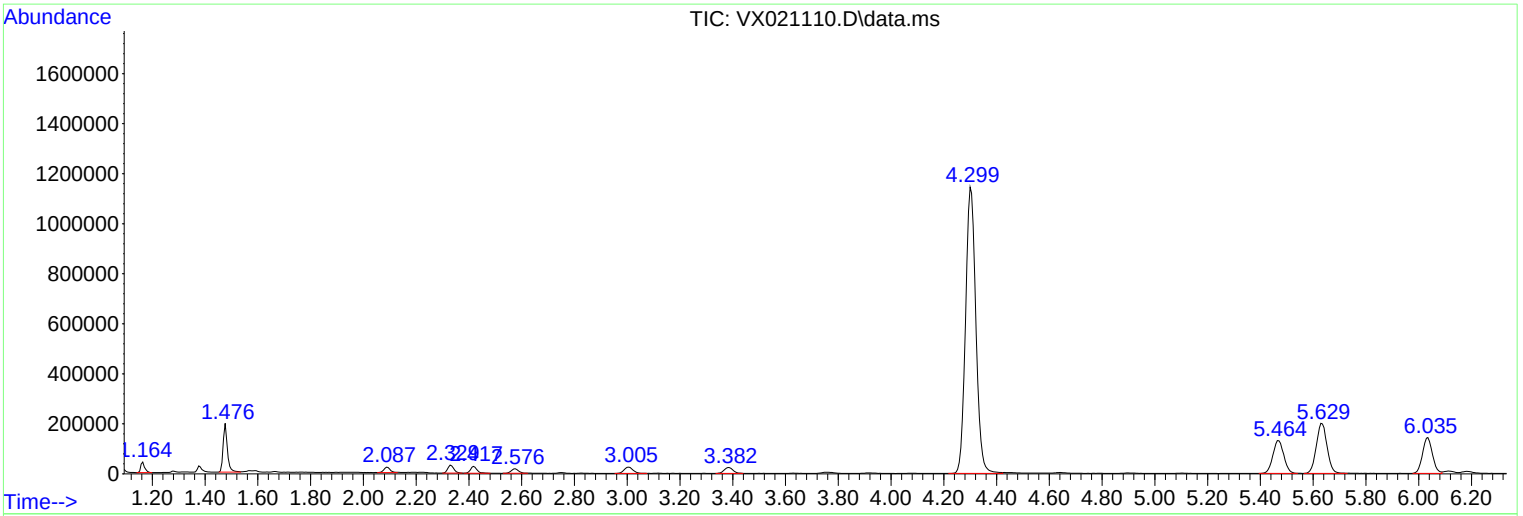
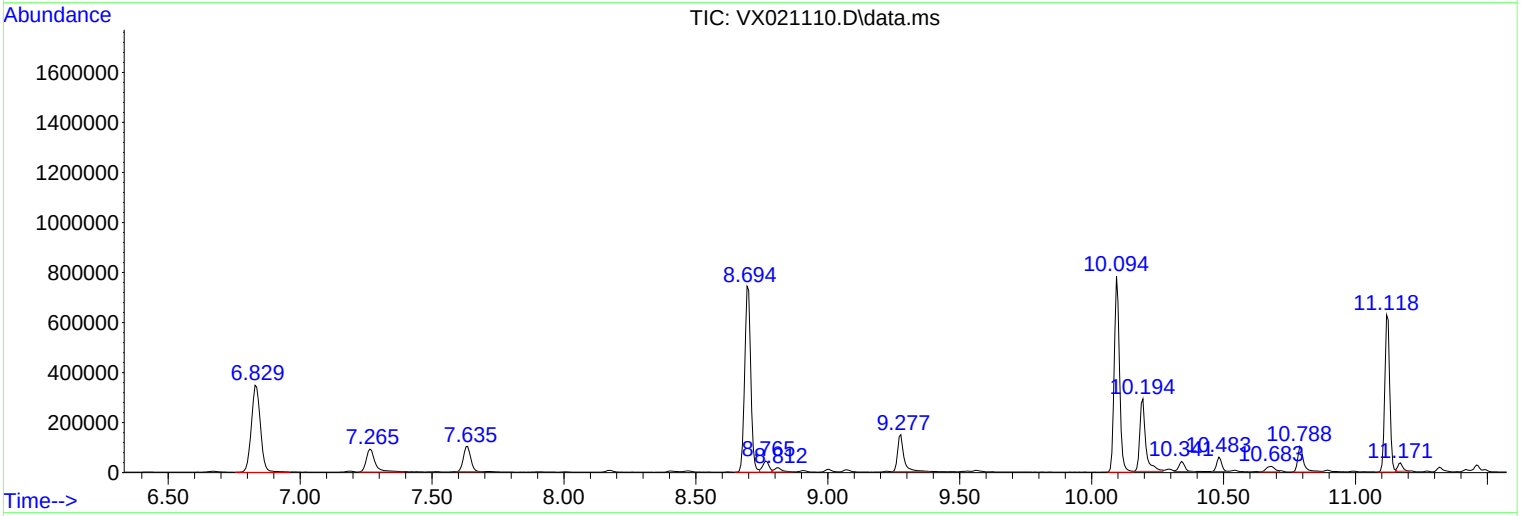
ALS Vial : 15 Sample Multiplier: 1

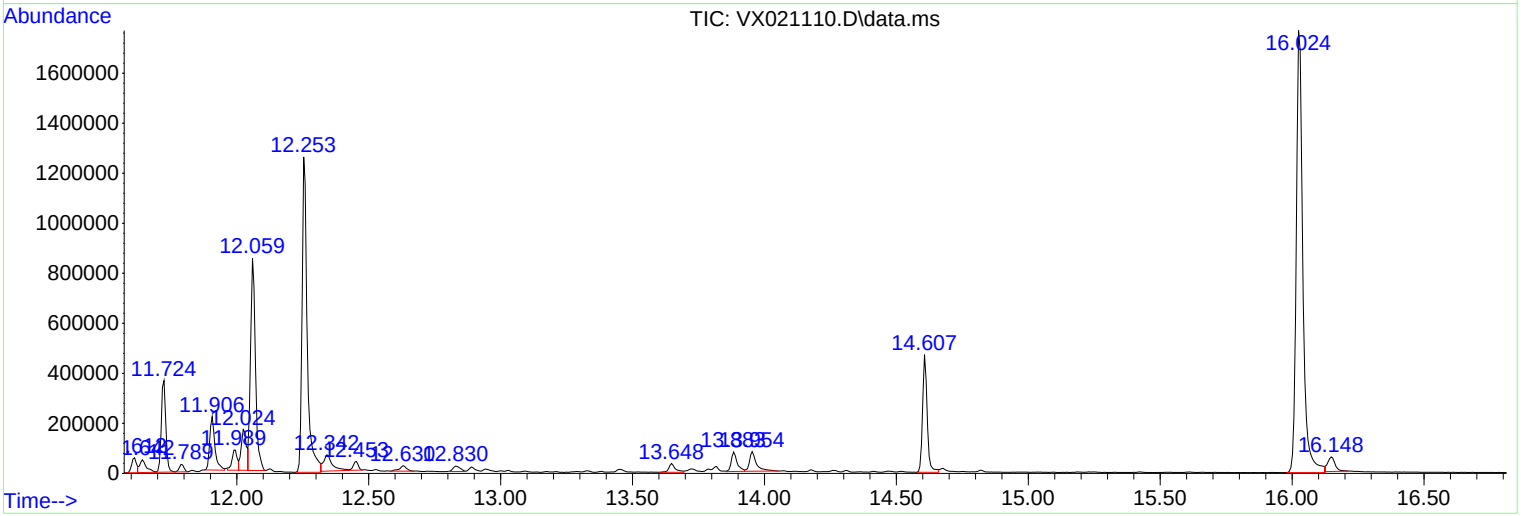
Instrument :
MSVOA_X
ClientSampleId :
COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

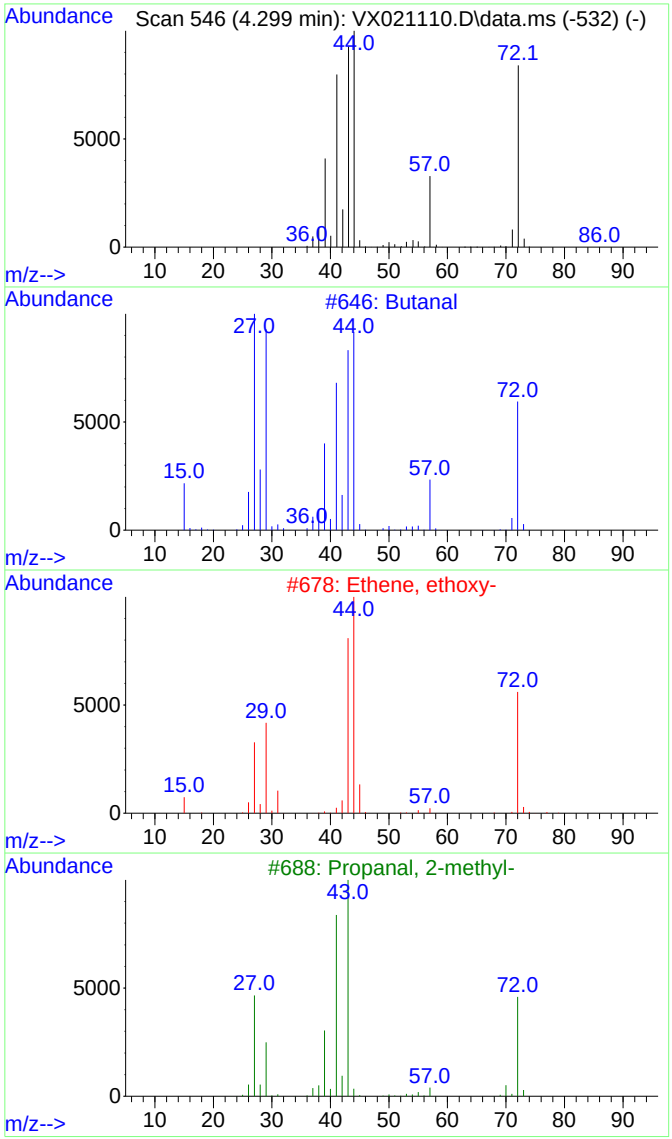
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

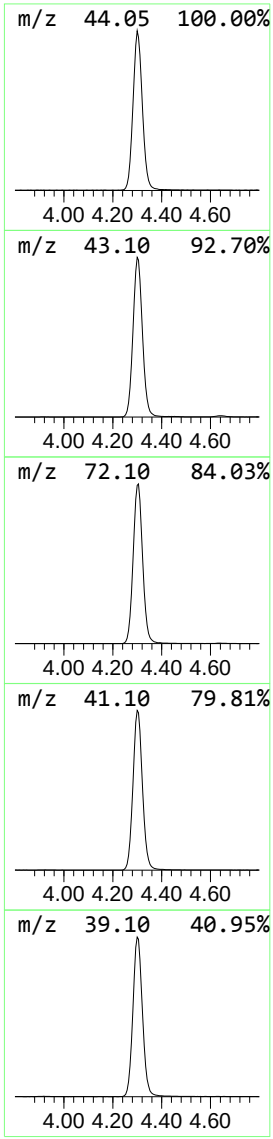
****

Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	274.94 ug/l	3108660	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	58
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5	Isobutylene epoxide	72	C4H8O	000558-30-5	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

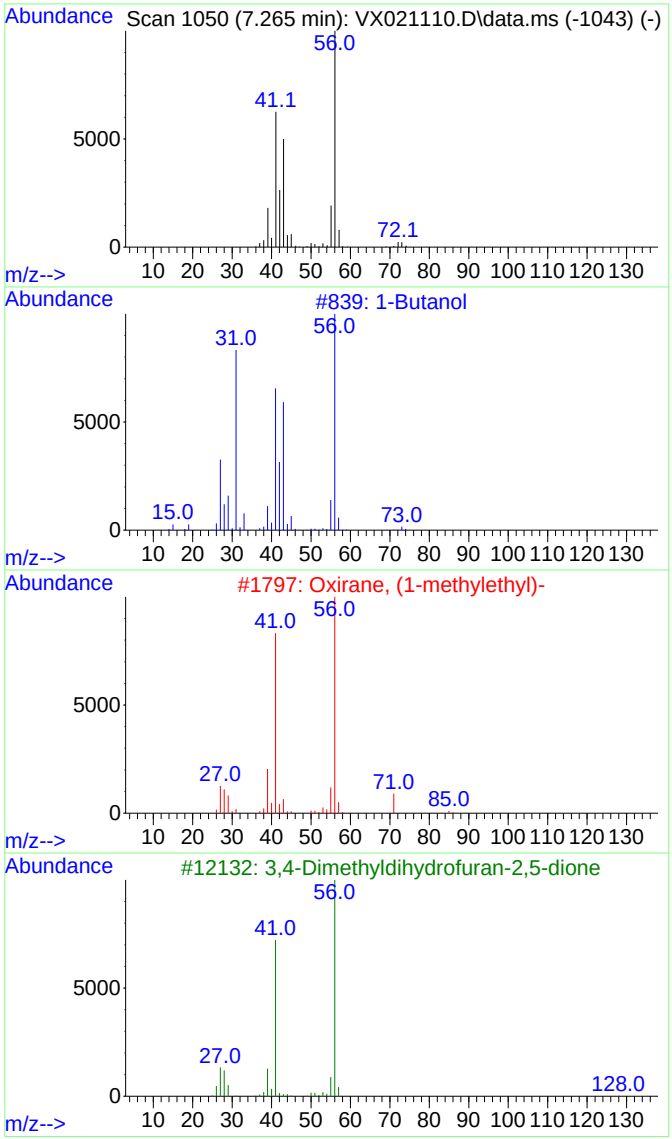
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

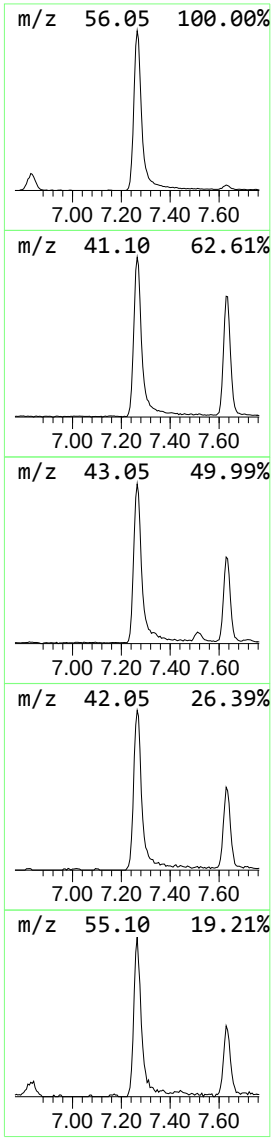
****

Peak Number 3 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.265	13.03 ug/l	217449	1,4-Difluorobenzene	6.829

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	86
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	36
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	36
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

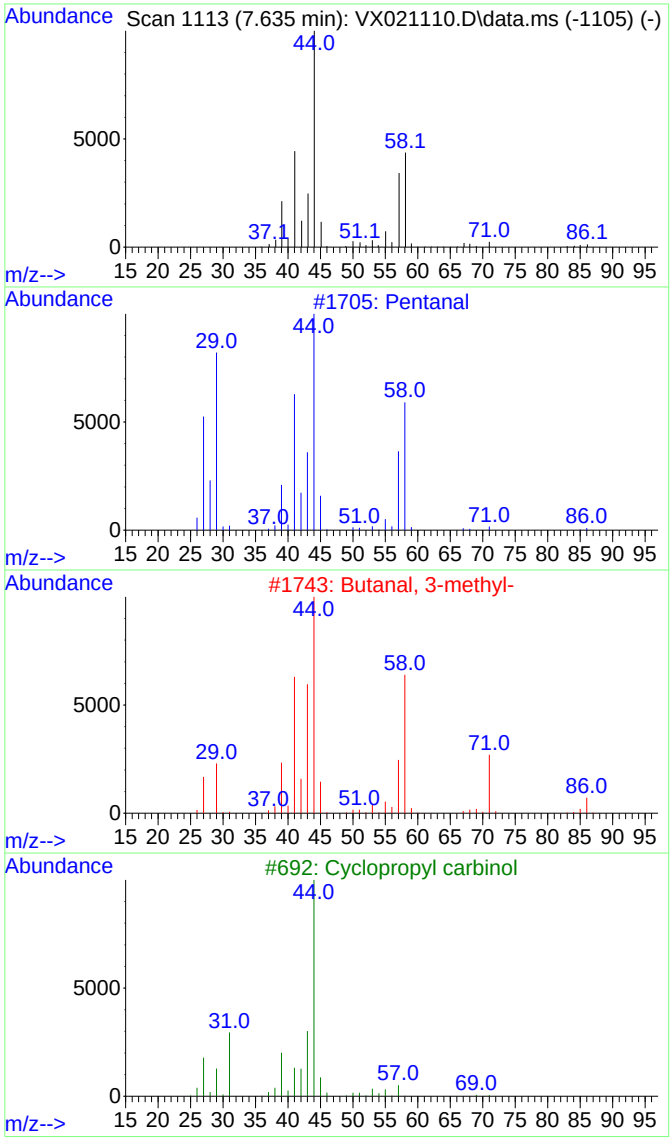
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

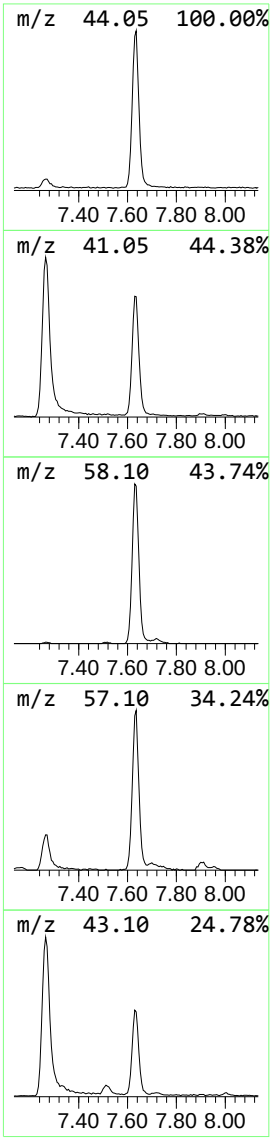
****

Peak Number 4 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.635	11.65 ug/l	194427	1,4-Difluorobenzene	6.829

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	91
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	33
4	Oxiranemethanol, (S)-	74	C3H6O2	060456-23-7	9
5	Ala-gly, trimethylsilyl ester	218	C8H18N2O3Si	1000333-70-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

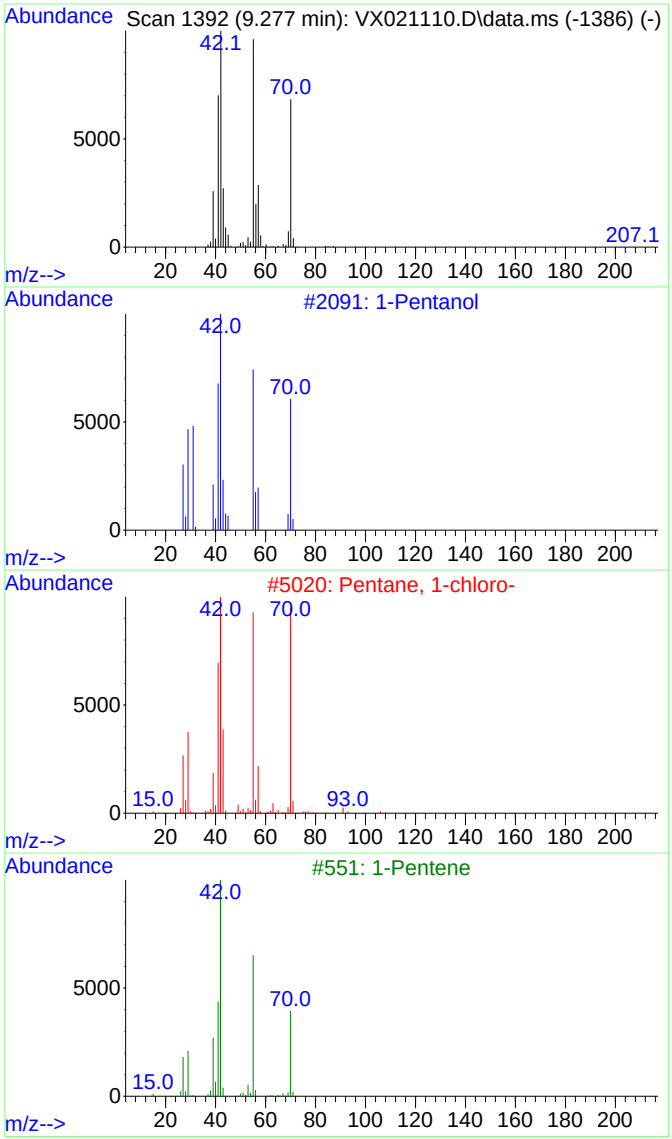
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

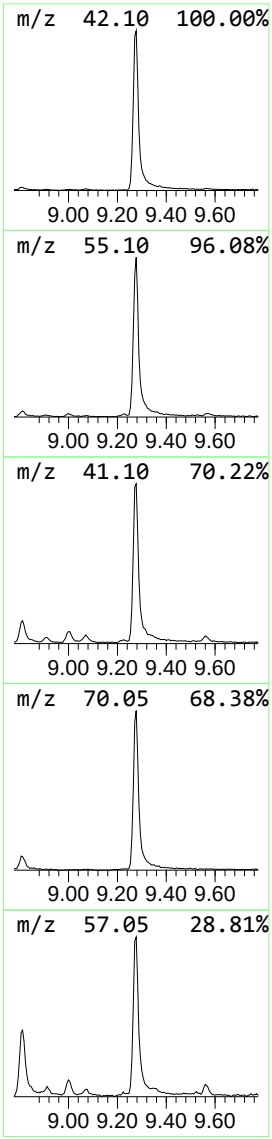
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Pentanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.277	11.26 ug/l	246019	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	83
2	Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	64
3	1-Pentene	70	C5H10	000109-67-1	64
4	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	64
5	Formic acid, pentyl ester	116	C6H12O2	000638-49-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

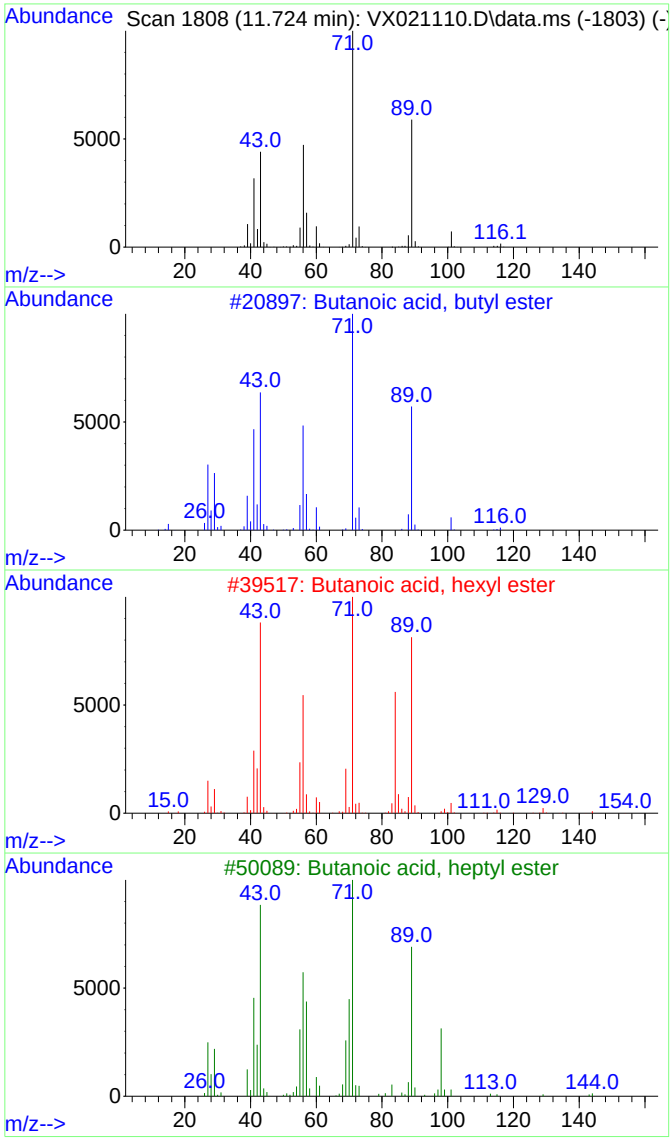
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

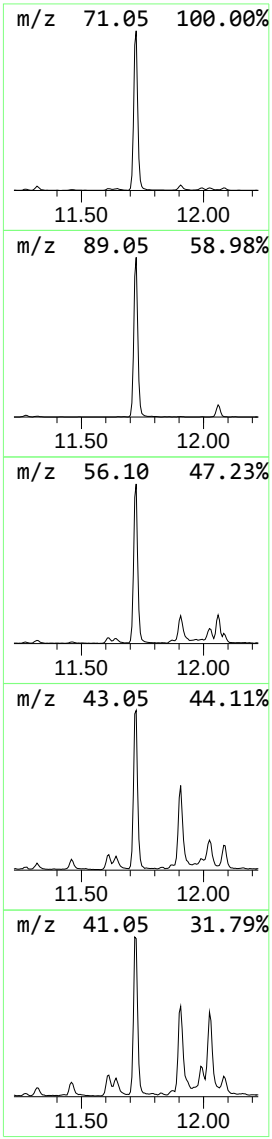
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.724	19.85 ug/l	434465	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
3	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	64
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP-1

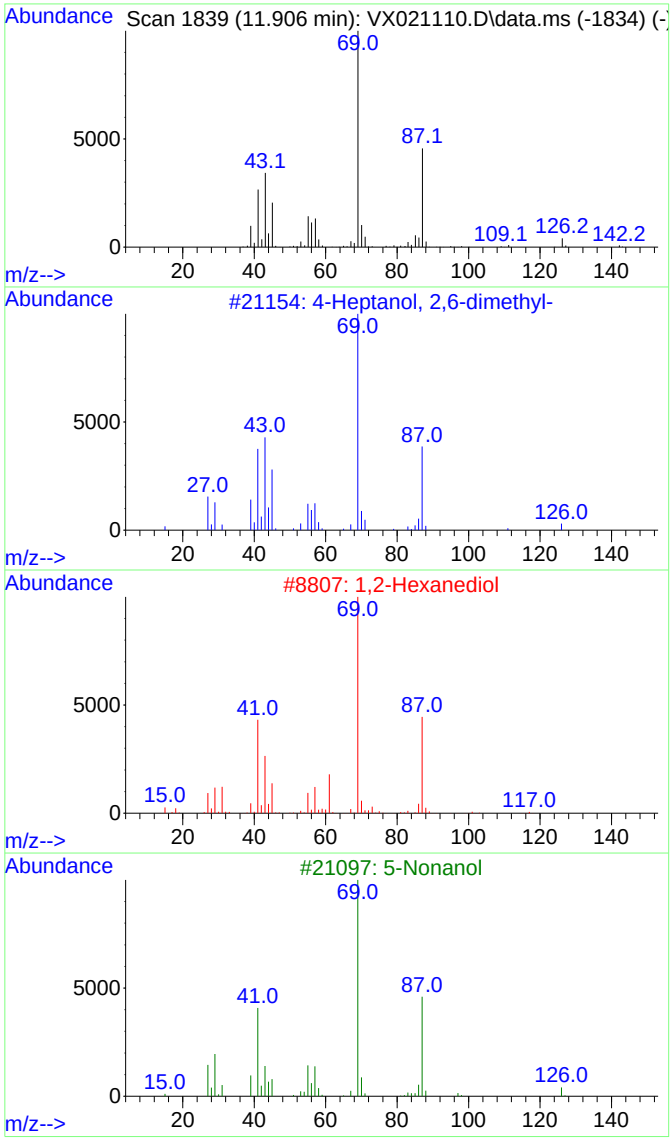
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

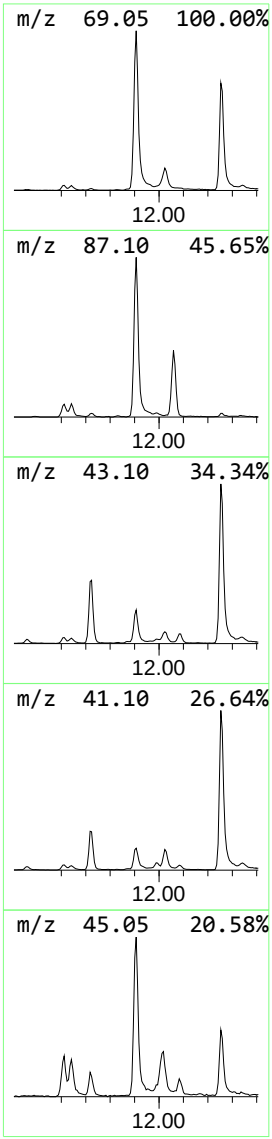
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Heptanol, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.906	13.39 ug/l	293066	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2	1,2-Hexanediol	118	C6H14O2	006920-22-5	78
3	5-Nonanol	144	C9H20O	000623-93-8	72
4	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72
5	3-Heptanol, 2,2-dimethyl-	144	C9H20O	019549-70-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

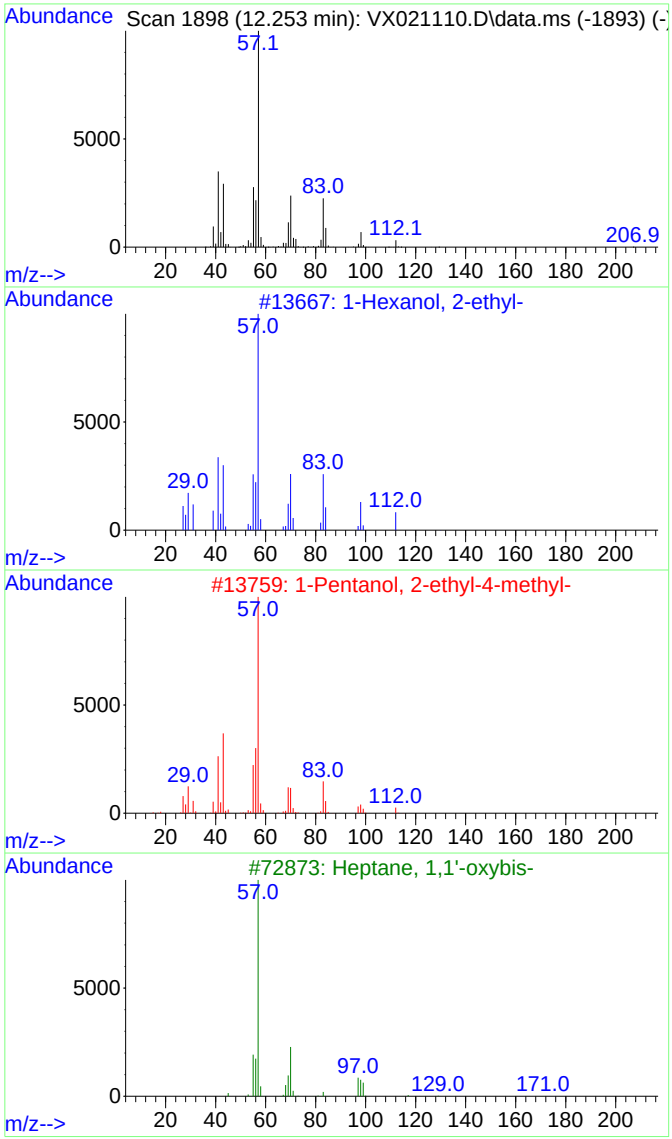
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

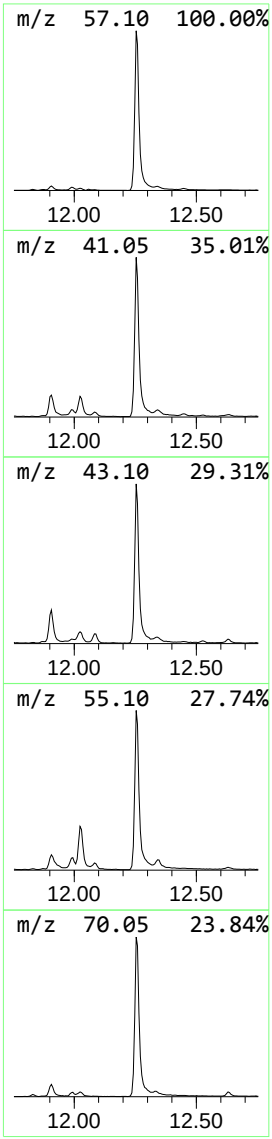
****

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	78.32 ug/l	1714140	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

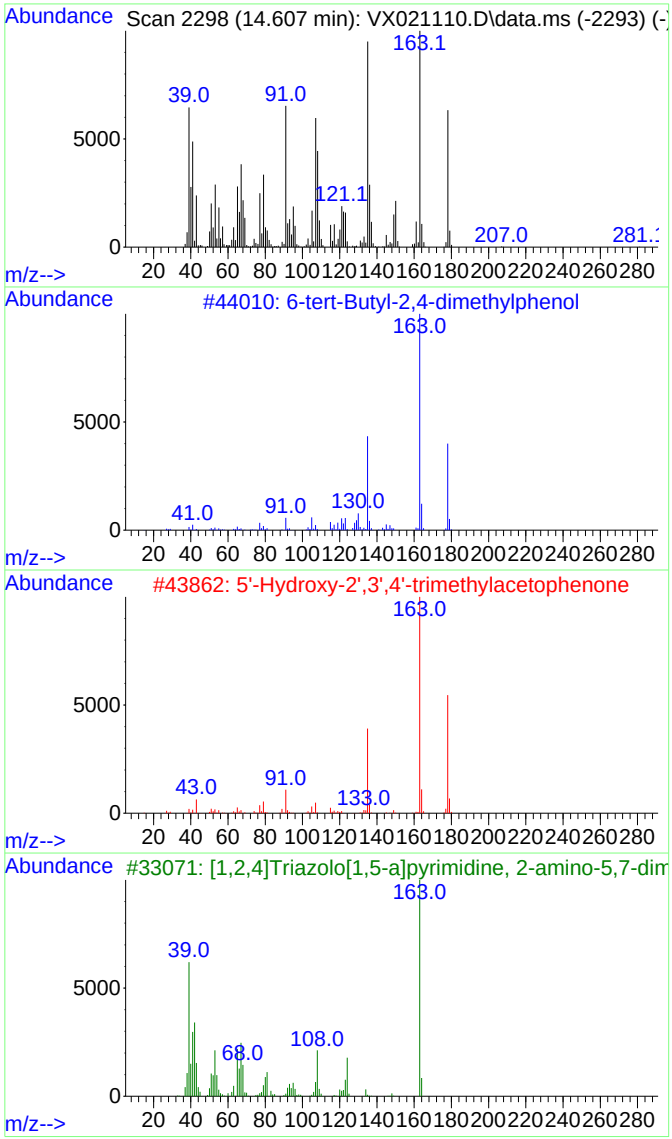
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

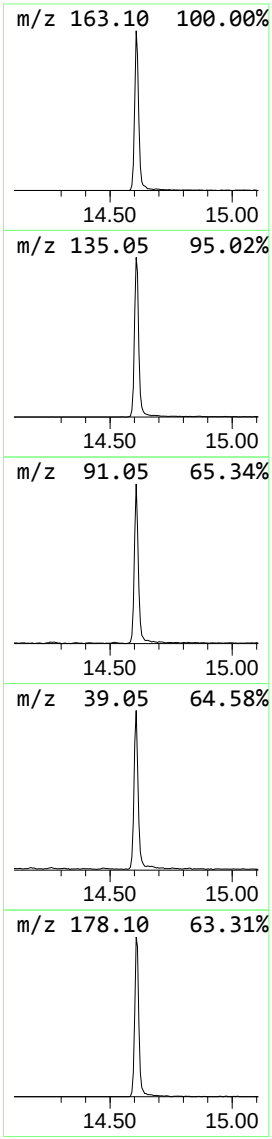
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 6-tert-Butyl-2,4-dimethylph... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.607	26.24 ug/l	574311	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	55
2	5'-Hydroxy-2',3',4'-trimethylace...	178	C11H14O2	013667-28-2	53
3	[1,2,4]Triazolo[1,5-a]pyrimidine...	163	C7H9N5	007135-02-6	46
4	1-(2,3-Dihydro-benzo[1,4]dioxin-...	178	C10H10O3	1000318-48-7	38
5	2-Benzothiazolamine, 5,6-dimethyl-	178	C9H10N2S	029927-08-0	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-1

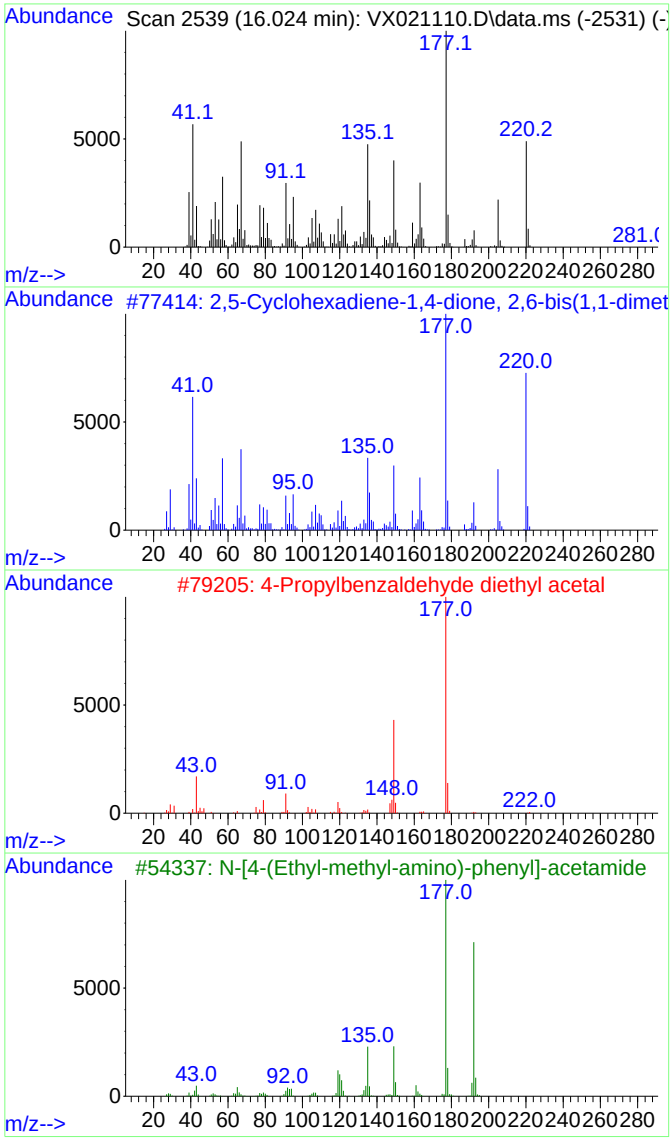
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

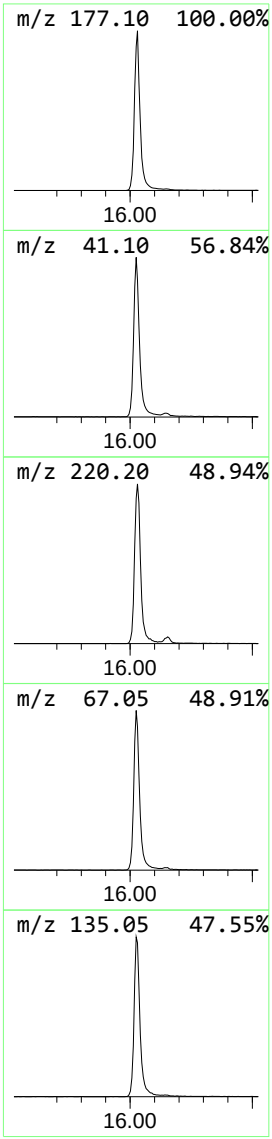
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.025	141.32 ug/l	3093070	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	4-Propylbenzaldehyde diethyl acetal	222	C14H22O2	089557-35-7	38
3	N-[4-(Ethyl-methyl-amino)-phenyl...	192	C11H16N2O	099981-45-0	38
4	1,3,5,7-Tetramethyl-adamantane	192	C14H24	001687-36-1	35
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021110.D
Acq On : 09 Mar 2021 15:50
Operator : JC/MD
Sample : M1578-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.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
Butanal	4.299	274.9	ug/l	3108660	1	5.629	565337	50.0
1-Butanol	7.265	13.0	ug/l	217449	2	6.829	834299	50.0
Pentanal	7.635	11.7	ug/l	194427	2	6.829	834299	50.0
1-Pentanol	9.277	11.3	ug/l	246019	3	10.094	1092280	50.0
Butanoic acid, ...	11.724	19.9	ug/l	434465	4	12.059	1094320	50.0
4-Heptanol, 2,6...	11.906	13.4	ug/l	293066	4	12.059	1094320	50.0
1-Hexanol, 2-et...	12.253	78.3	ug/l	1714140	4	12.059	1094320	50.0
6-tert-Butyl-2,...	14.607	26.2	ug/l	574311	4	12.059	1094320	50.0
2,5-Cyclohexadi...	16.025	141.3	ug/l	3093070	4	12.059	1094320	50.0