LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030257.D
Acq On : 28 Jul 2022 02:00
Operator : JC/MD
Sample : N3898-04 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

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\82X072522W.M
Title : SW846 8260

Signal : TIC: VX030257.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	71	rBV	224265	264926	8.40%	1.618%
2	2.392	207	214	223	rBV	74979	132718	4.21%	0.811%
3	2.953	297	306	315	rBV2	24389	60922	1.93%	0.372%
4	4.385	531	541	562	rBV	41368	132489	4.20%	0.809%
5	4.580	564	573	588	rVB3	19124	64492	2.05%	0.394%
6	5.391	695	706	720	rBV	133174	387049	12.27%	2.364%
7	5.556	723	733	746	rVB	141247	406786	12.90%	2.484%
8	5.964	788	800	812	rBV	161486	421702	13.37%	2.576%
9	6.763	923	931	941	rBV	232824	578288	18.34%	3.532%
10	6.879	941	950	970	rVB	1344674	3153243	100.00%	19.258%
11	7.214	997	1005	1014	rBV	227618	483130	15.32%	2.951%
12	7.830	1099	1106	1116	rVB	32977	65871	2.09%	0.402%
13	8.580	1222	1229	1235	rBV	33430	63792	2.02%	0.390%
14	8.653	1235	1241	1247	rVV	749960	1163975	36.91%	7.109%
15	8.720	1247	1252	1264	rVB	732702	1142527	36.23%	6.978%
16	9.000	1288	1298	1310	rVB	74654	125606	3.98%	0.767%
17	9.525	1374	1384	1387	rBV5	21494	41957	1.33%	0.256%
18	9.592	1387	1395	1396	rBV	179562	415640	13.18%	2.539%
19	10.055	1466	1471	1481	rVV	575377	764021	24.23%	4.666%
20	10.195	1490	1494	1499	rVB	65791	87738	2.78%	0.536%
21	10.305	1504	1512	1518	rVV	287550	421412	13.36%	2.574%
22	10.366	1518	1522	1524	rVV3	30973	42434	1.35%	0.259%
23	10.403	1524	1528	1533	rVB	73681	96246	3.05%	0.588%
24	10.646	1563	1568	1579	rVV2	100816	155306	4.93%	0.949%
25	10.768	1582	1588	1595	rVV2	34121	54757	1.74%	0.334%
26	10.860	1599	1603	1615	rVB3	31218	52700	1.67%	0.322%
27	11.085	1634	1640	1646	rBV	604465	769810	24.41%	4.702%
28	11.482	1700	1705	1708	rBV	67571	85922	2.72%	0.525%
29	11.518	1708	1711	1715	rVB	54073	62580	1.98%	0.382%
30	11.561	1715	1718	1723	rBV2	21212	32565	1.03%	0.199%
31	11.689	1736	1739	1746	rVB	36824	47287	1.50%	0.289%
32	11.841	1761	1764	1768	rBV2	36760	51223	1.62%	0.313%
33	12.024	1790	1794	1802	rVB	757369	905744	28.72%	5.532%
34	12.146	1809	1814	1821	rVB	34672	55642	1.76%	0.340%
35	12.219	1821	1826	1831	rBV	68706	110415	3.50%	0.674%
36	12.305	1835	1840	1846	rVB7	15922	39517	1.25%	0.241%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

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\82X072522W.M
Title : SW846 8260

37	12.469	1862	1867	1871	rVB2	72271	97805	3.10%	0.597%
38	12.518	1871	1875	1879	rBV	47879	60742	1.93%	0.371%
39	12.585	1879	1886	1891	rVV3	42584	101211	3.21%	0.618%
40	12.768	1911	1916	1919	rBV	56371	78910	2.50%	0.482%
41	12.799	1919	1921	1927	rVV4	29133	45965	1.46%	0.281%
42	12.860	1927	1931	1935	rVB2	24953	33264	1.05%	0.203%
43	13.018	1953	1957	1965	rVB5	19138	35720	1.13%	0.218%
44	13.097	1965	1970	1974	rBV4	31117	62592	1.99%	0.382%
45	13.164	1974	1981	1985	rVB6	35234	72327	2.29%	0.442%
46	13.280	1994	2000	2004	rBV	74868	118217	3.75%	0.722%
47	13.323	2004	2007	2013	rVB	76330	95898	3.04%	0.586%
48	13.420	2019	2023	2031	rVV4	51616	94922	3.01%	0.580%
49	13.603	2049	2053	2058	rBV2	83967	121759	3.86%	0.744%
50	13.701	2064	2069	2076	rVB6	23568	59724	1.89%	0.365%
51	13.774	2076	2081	2088	rVB2	31076	64237	2.04%	0.392%
52	13.841	2088	2092	2095	rBV4	22400	34571	1.10%	0.211%
53	14.036	2120	2124	2132	rBV4	47267	132463	4.20%	0.809%
54	14.103	2132	2135	2143	rVV	63533	98119	3.11%	0.599%
55	14.195	2148	2150	2154	rVV3	30310	38040	1.21%	0.232%
56	14.371	2174	2179	2184	rBV	179435	240639	7.63%	1.470%
57	14.426	2184	2188	2191	rBV4	21911	39440	1.25%	0.241%
58	14.640	2215	2223	2226	rBV5	42406	89755	2.85%	0.548%
59	14.743	2235	2240	2245	rBV4	122315	210971	6.69%	1.288%
60	14.835	2252	2255	2257	rBV	44328	44986	1.43%	0.275%
61	14.865	2257	2260	2266	rVB	127319	157911	5.01%	0.964%
62	15.054	2284	2291	2294	rBV7	13888	36020	1.14%	0.220%
63	15.097	2294	2298	2302	rVV	71853	90936	2.88%	0.555%
64	15.140	2302	2305	2307	rVV2	26779	35388	1.12%	0.216%
65	15.176	2307	2311	2315	rVV	247384	344815	10.94%	2.106%
66	15.213	2315	2317	2325	rVB5	55698	121680	3.86%	0.743%
67	15.487	2357	2362	2370	rBV4	55906	119447	3.79%	0.730%
68	15.609	2378	2382	2384	rBV4	22495	34519	1.09%	0.211%
69	15.646	2385	2388	2392	rVB2	66161	91106	2.89%	0.556%
70	15.761	2403	2407	2414	rVB2	72813	122091	3.87%	0.746%
71	15.914	2429	2432	2442	rVB5	35580	75943	2.41%	0.464%
72	16.085	2454	2460	2468	rVB6	52904	130848	4.15%	0.799%

Sum of corrected areas: 16373413

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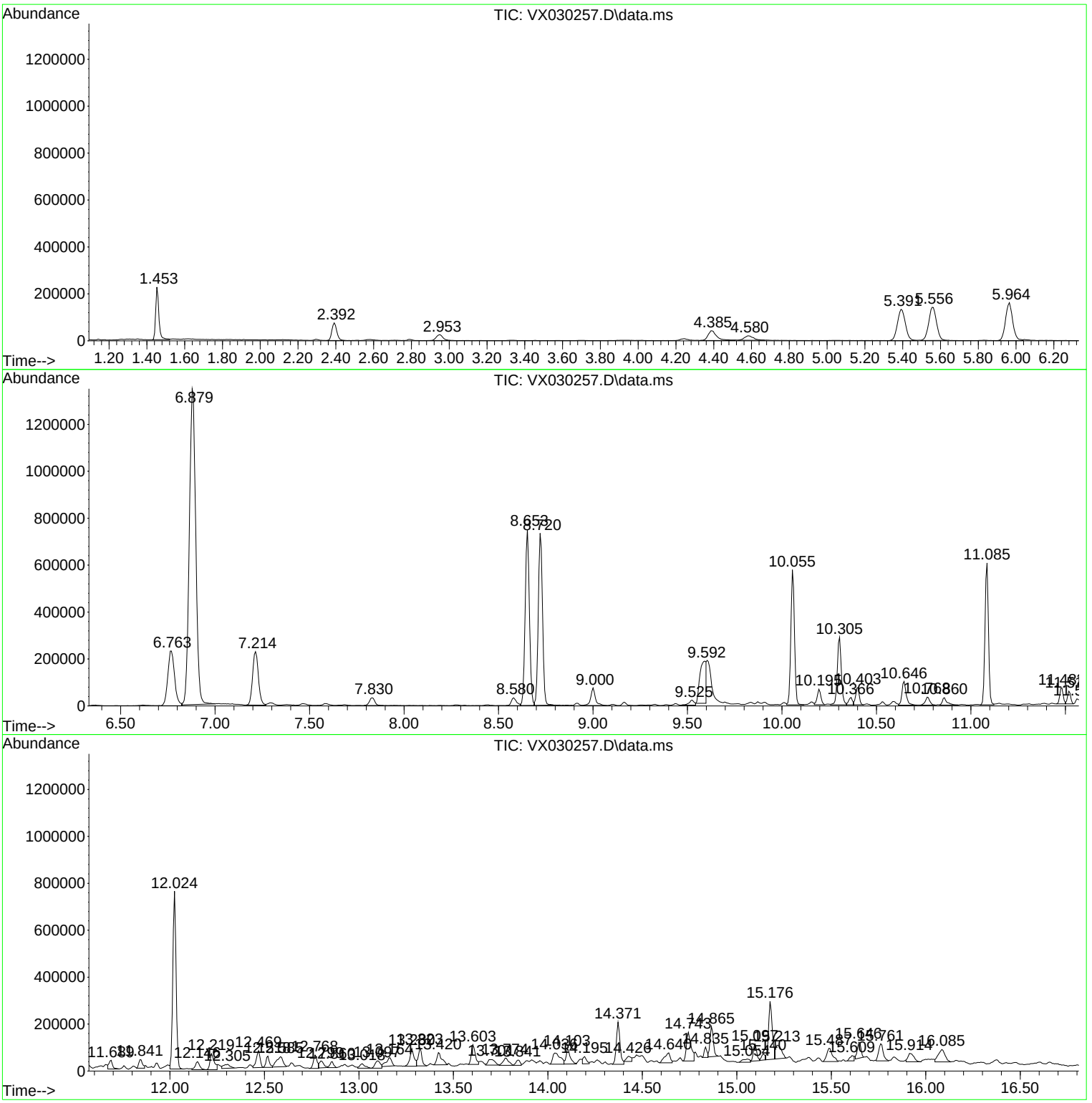
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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



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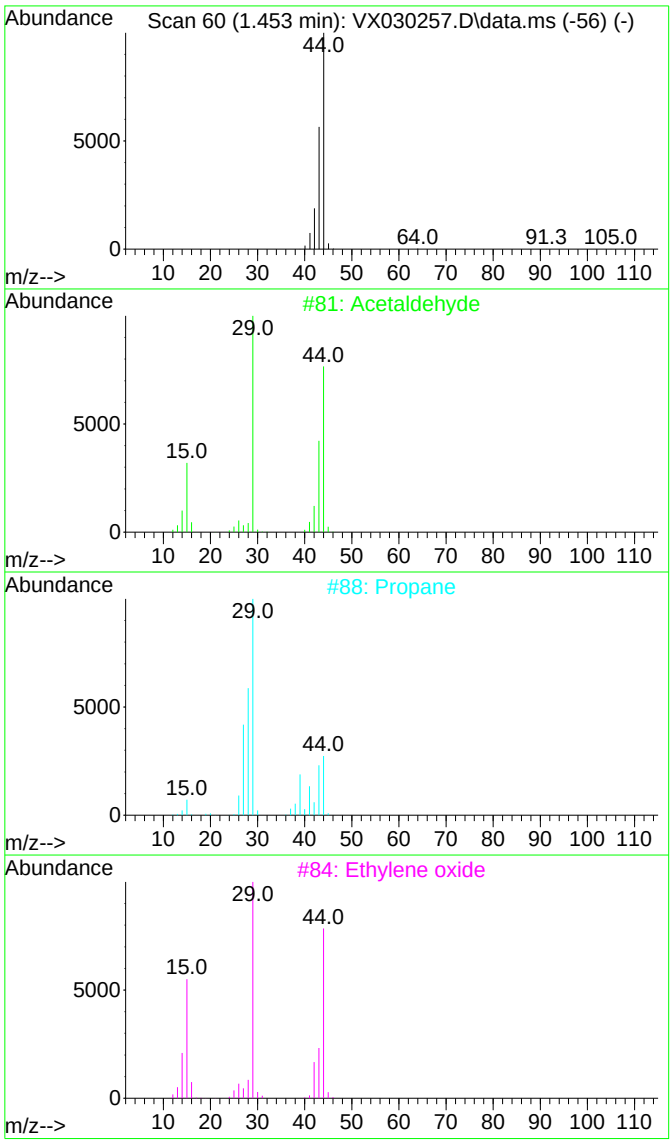
Quant Title : SW846 8260

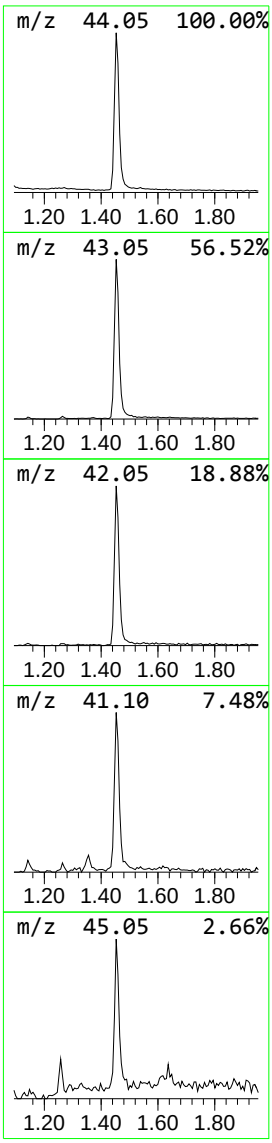
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.453	32.56 ug/l	264926	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





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Data File : VX030257.D
Acq On : 28 Jul 2022 02:00
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

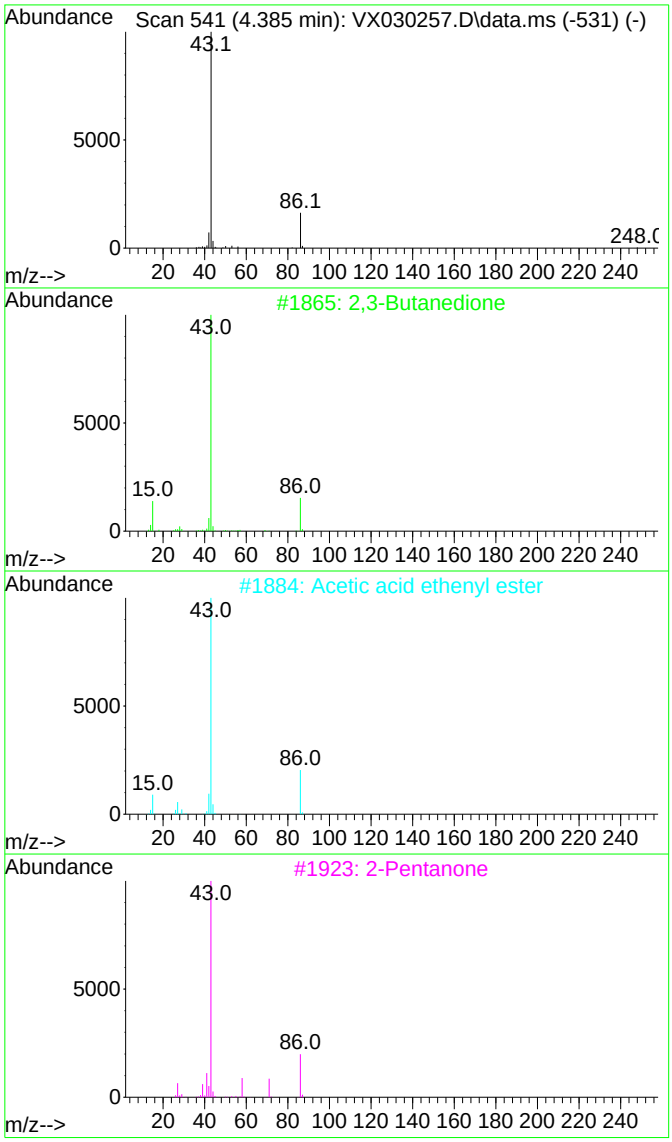
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

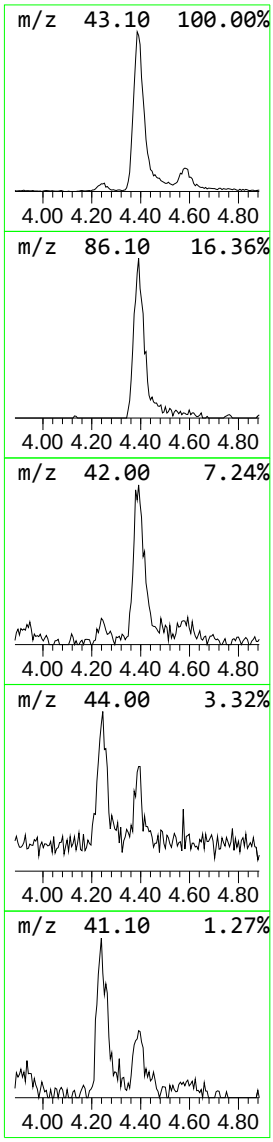
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,3-Butanedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.385	16.28 ug/l	132489	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	64
2	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	59
3	2-Pentanone	86	C5H10O	000107-87-9	50
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
5	2-Propanone, 1-(acetyloxy)-	116	C5H8O3	000592-20-1	9





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Operator : JC/MD
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ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

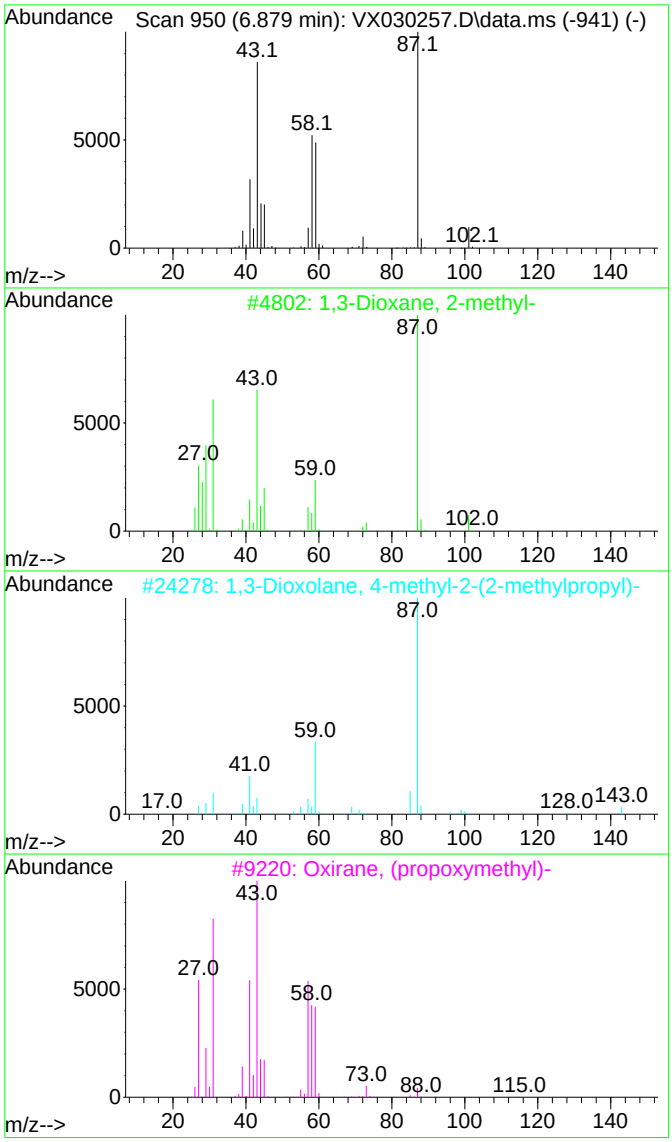
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

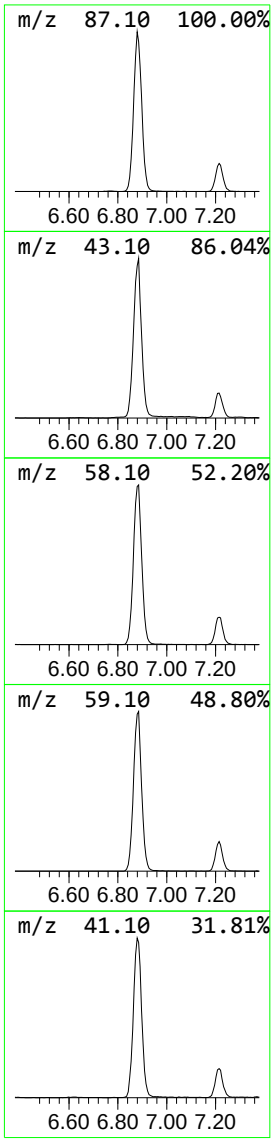
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	272.64 ug/l	3153240	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	59
2	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	37
3	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
4	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	36
5	Monomethyl malonate	118	C4H6O4	016695-14-0	33





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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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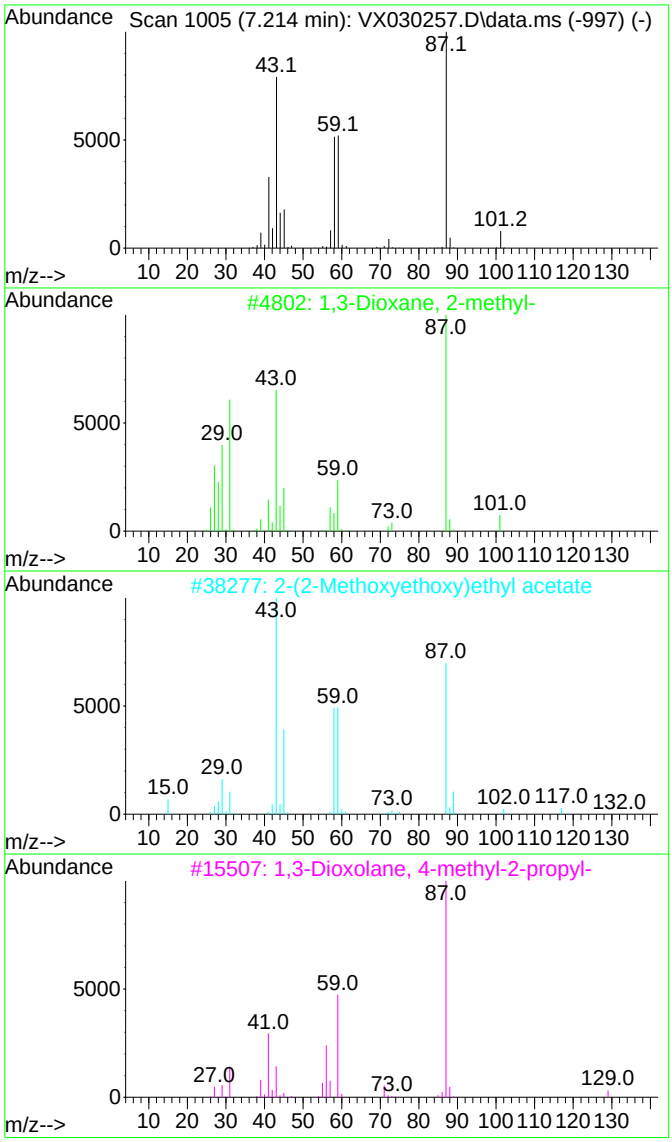
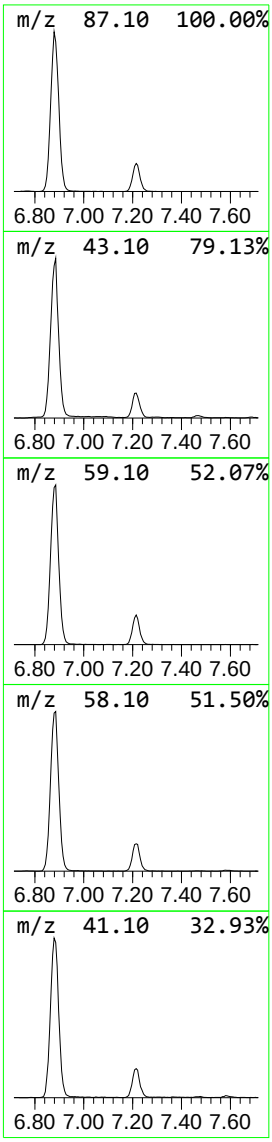
****

Peak Number 4 unknown7.214 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	41.77 ug/l	483130	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	49
2	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	40
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	38
4	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38





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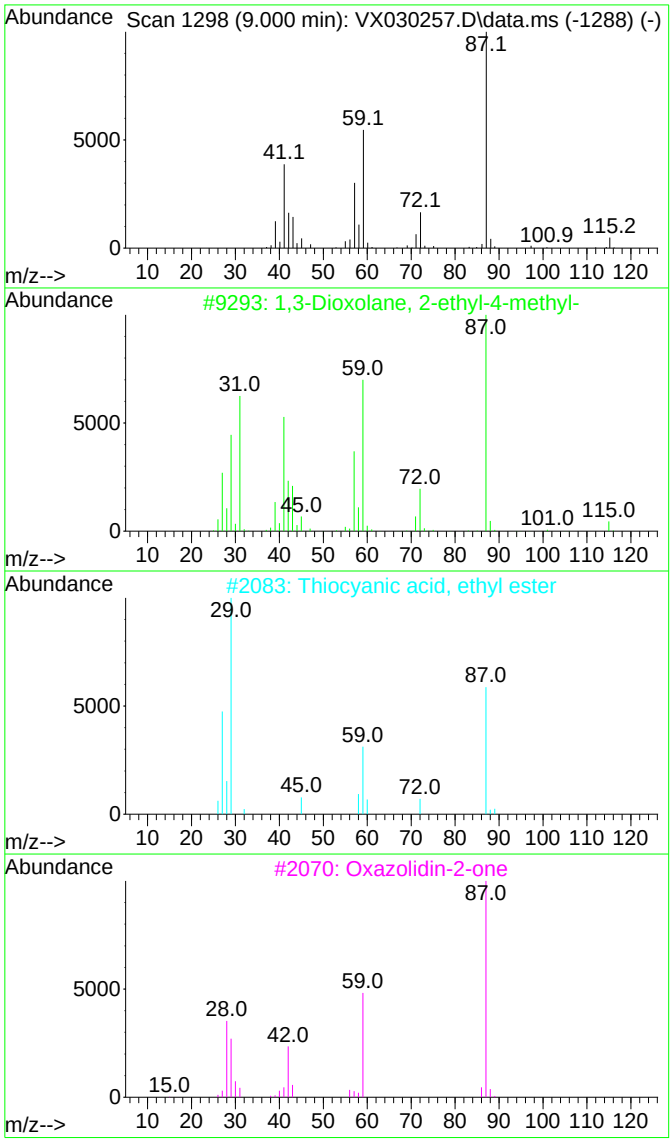
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

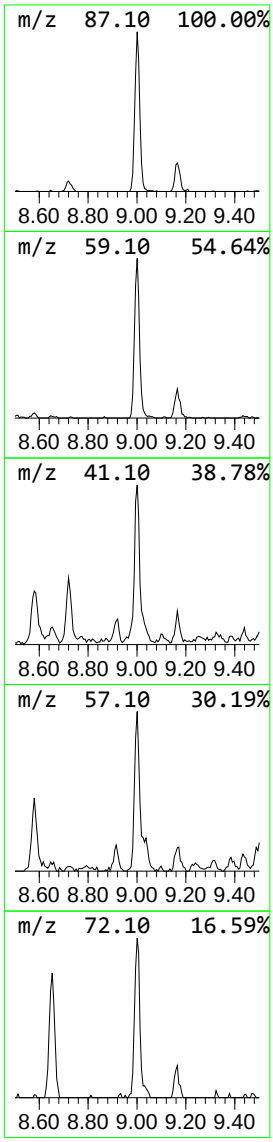
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.000	8.22 ug/l	125606	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	95
2	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	72
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	47





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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

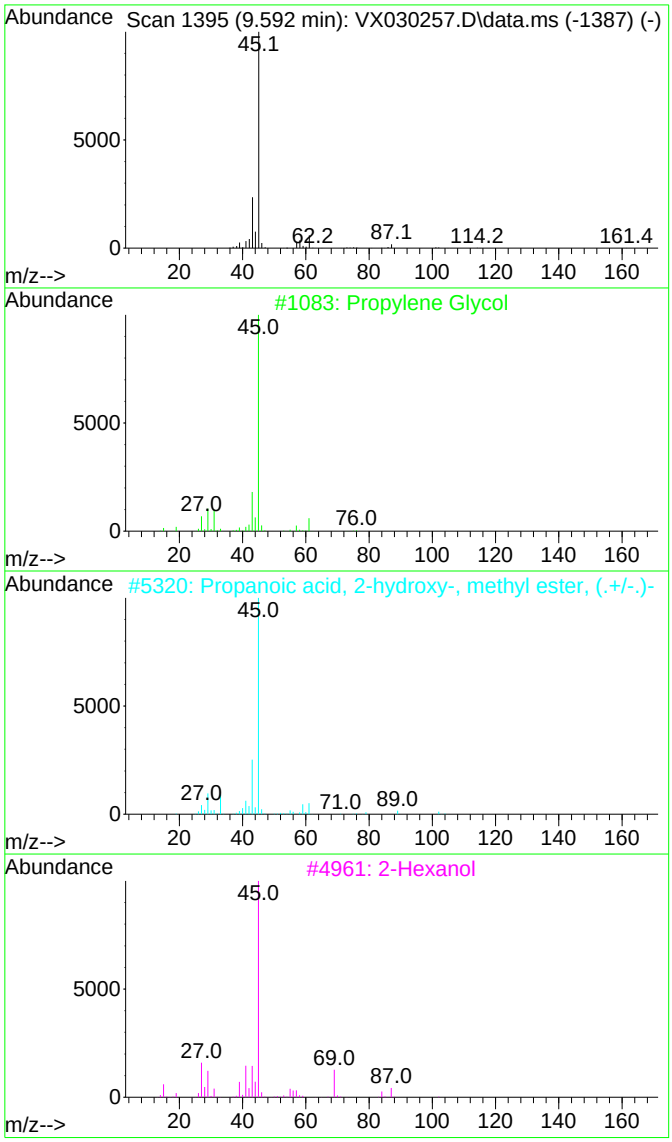
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

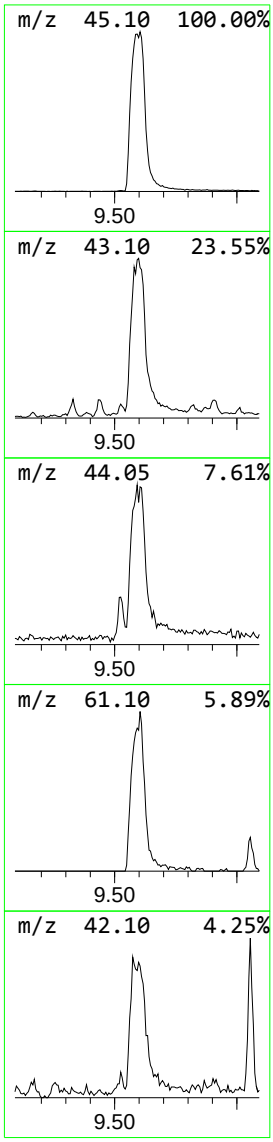
****

Peak Number 6 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	27.20 ug/l	415640	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	72
2	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
3	2-Hexanol	102	C6H14O	000626-93-7	40
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

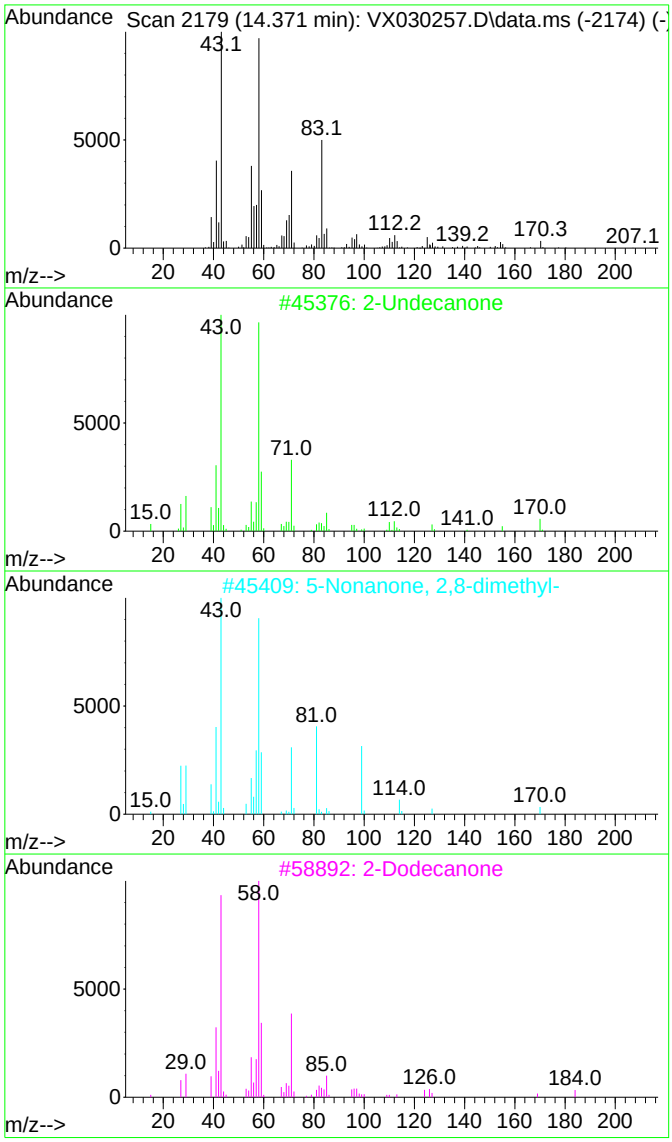
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

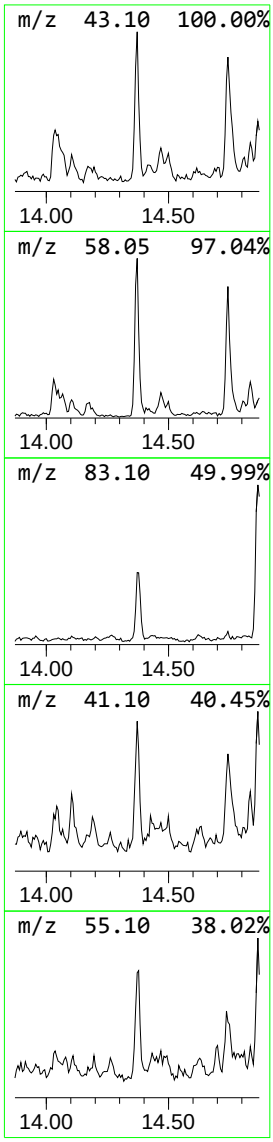
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Undecanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.371	13.28 ug/l	240639	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecanone	170	C11H22O	000112-12-9	64
2	5-Nonanone, 2,8-dimethyl-	170	C11H22O	002050-99-9	49
3	2-Dodecanone	184	C12H24O	006175-49-1	49
4	2-Nonanone	142	C9H18O	000821-55-6	47
5	2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030257.D
Acq On : 28 Jul 2022 02:00
Operator : JC/MD
Sample : N3898-04 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

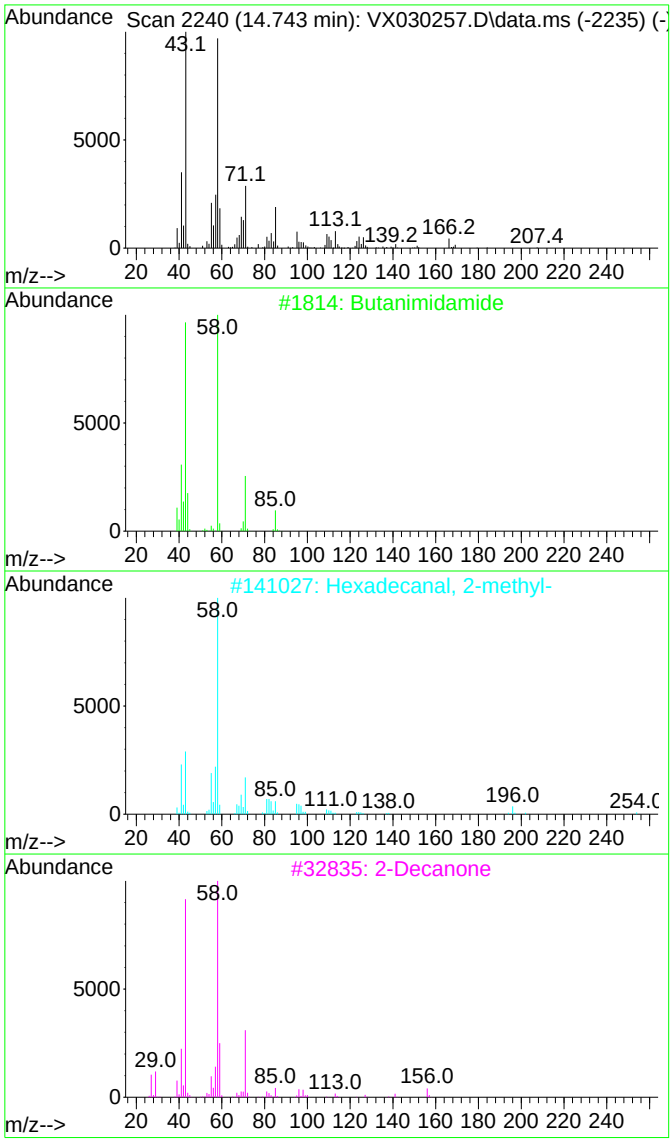
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

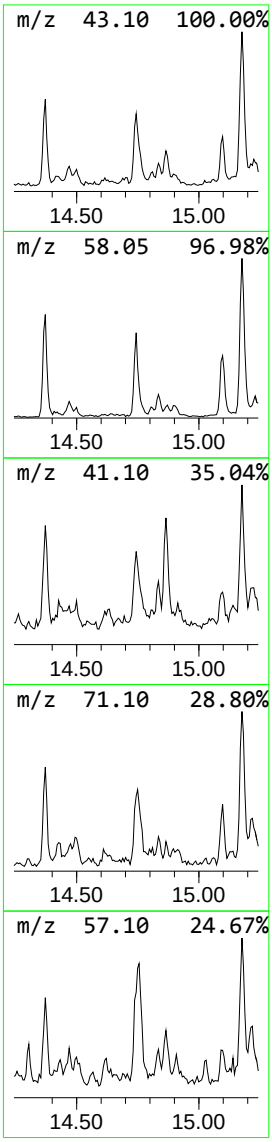
****

Peak Number 8 Butanimidamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.743	11.65 ug/l	210971	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanimidamide	86	C4H10N2	000107-90-4	64
2	Hexadecanal, 2-methyl-	254	C17H34O	055019-46-0	64
3	2-Decanone	156	C10H20O	000693-54-9	53
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	53
5	2-Dodecanone	184	C12H24O	006175-49-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030257.D
Acq On : 28 Jul 2022 02:00
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

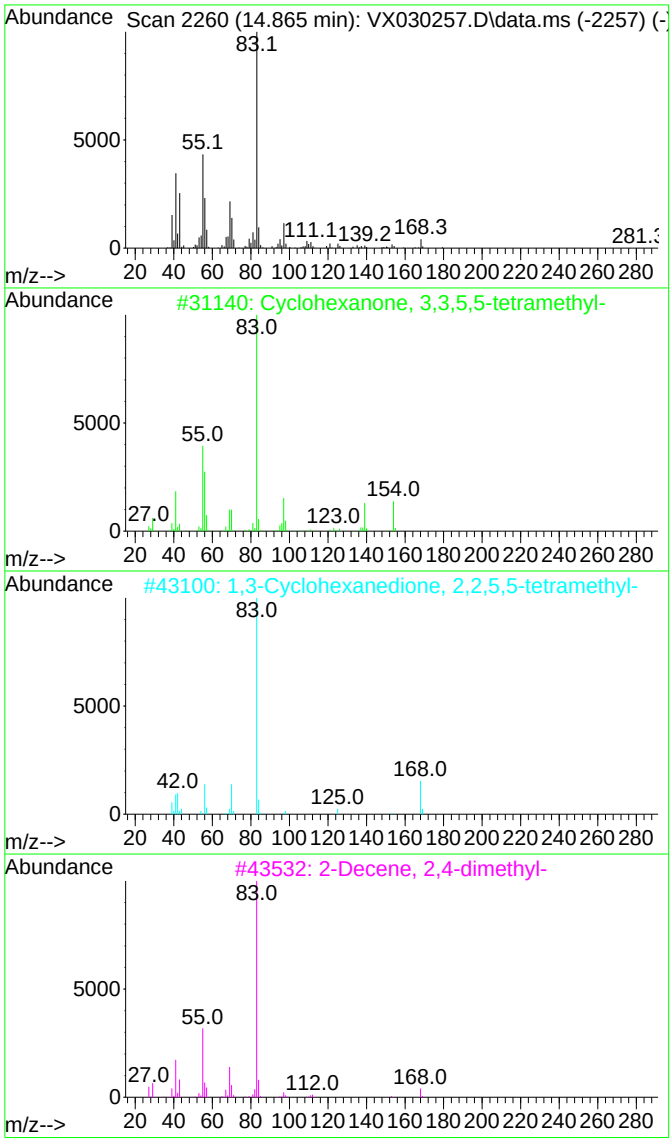
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

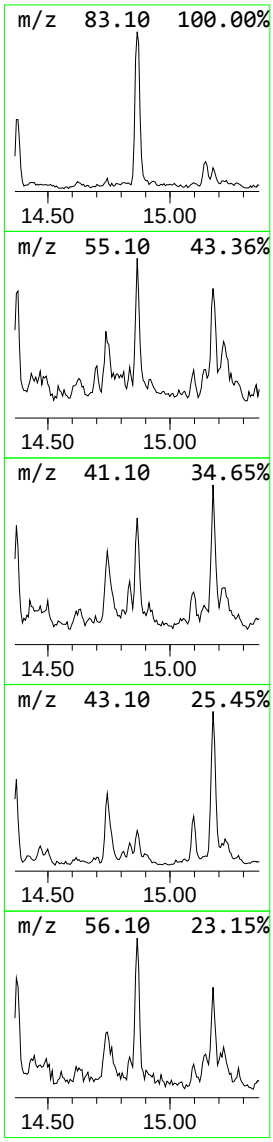
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclohexanone, 3,3,5,5-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.865	8.72 ug/l	157911	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3,3,5,5-tetramethyl-	154	C10H18O	014376-79-5	78
2	1,3-Cyclohexanedione, 2,2,5,5-te...	168	C10H16O2	000702-50-1	64
3	2-Decene, 2,4-dimethyl-	168	C12H24	074421-03-7	64
4	Cyclohexane, eicosyl-	364	C26H52	004443-55-4	64
5	3,3-Dimethylcyclohexanone	126	C8H14O	002979-19-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030257.D
Acq On : 28 Jul 2022 02:00
Operator : JC/MD
Sample : N3898-04 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

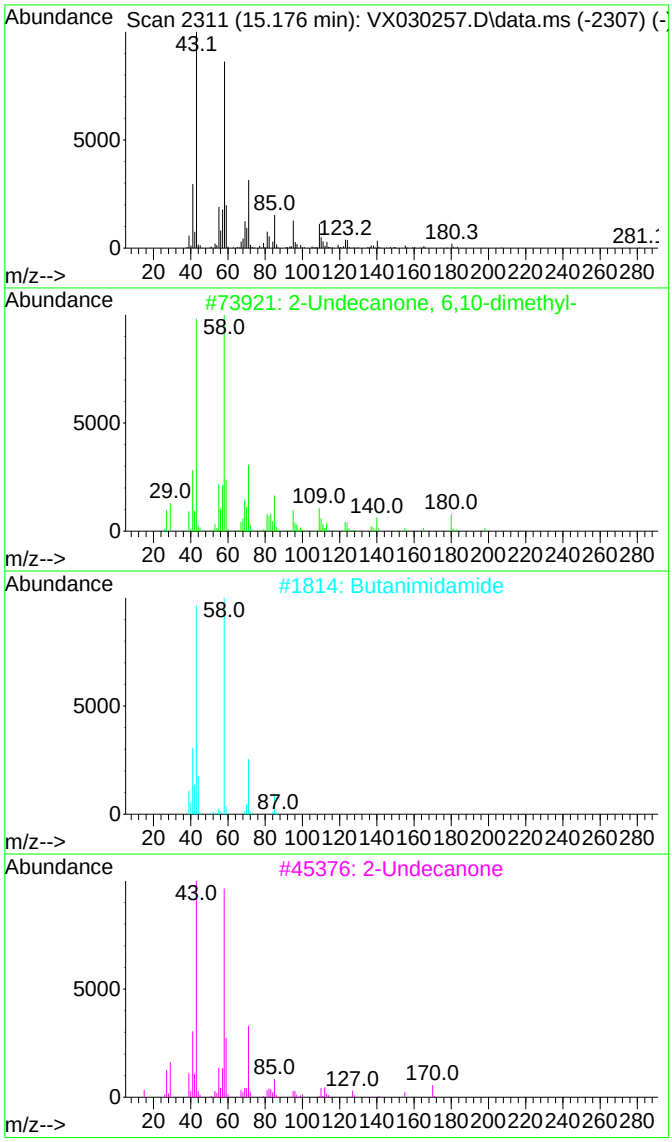
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

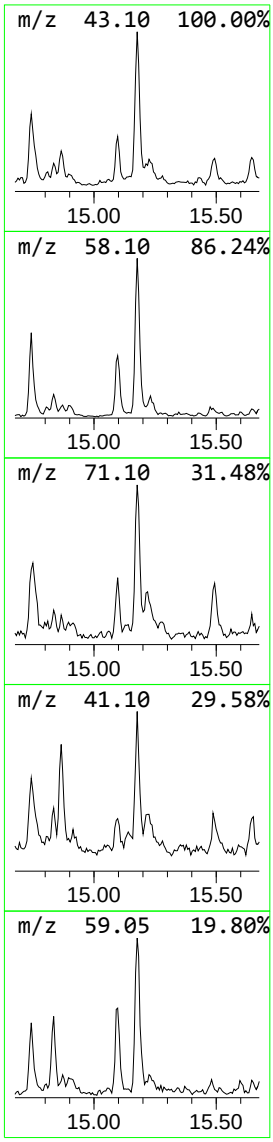
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Undecanone, 6,10-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.176	19.03 ug/l	344815	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecanone, 6,10-dimethyl-	198	C13H26O	001604-34-8	59
2	Butanimidamide	86	C4H10N2	000107-90-4	52
3	2-Undecanone	170	C11H22O	000112-12-9	45
4	6-Methyl-2-tridecanone	212	C14H28O	073105-73-4	45
5	5-Hepten-2-amine, N,6-dimethyl-	141	C9H19N	000503-01-5	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072722\
Data File : VX030257.D
Acq On : 28 Jul 2022 02:00
Operator : JC/MD
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ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
61422-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.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
Acetaldehyde	1.453	32.6	ug/l	264926	1	5.562	406786	50.0
2,3-Butanedione	4.385	16.3	ug/l	132489	1	5.562	406786	50.0
1,3-Dioxane, 2-...	6.879	272.6	ug/l	3153240	2	6.769	578288	50.0
unknown7.214	7.214	41.8	ug/l	483130	2	6.769	578288	50.0
1,3-Dioxolane, ...	9.000	8.2	ug/l	125606	3	10.055	764021	50.0
Propylene Glycol	9.592	27.2	ug/l	415640	3	10.055	764021	50.0
2-Undecanone	14.371	13.3	ug/l	240639	4	12.024	905744	50.0
Butanimidamide	14.743	11.7	ug/l	210971	4	12.024	905744	50.0
Cyclohexanone, ...	14.865	8.7	ug/l	157911	4	12.024	905744	50.0
2-Undecanone, 6...	15.176	19.0	ug/l	344815	4	12.024	905744	50.0