LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029627.D
Acq On : 20 Jun 2022 16:49
Operator : JC/MD
Sample : N3391-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M15848

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\82X061822W.M
Title : SW846 8260

Signal : TIC: VX029627.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	16	rVB2	40753	37687	2.96%	0.283%
2	1.355	41	44	49	rVB2	25556	27808	2.18%	0.209%
3	1.453	56	60	65	rBV	31776	33605	2.64%	0.252%
4	2.294	193	198	206	rBV	14787	22429	1.76%	0.168%
5	2.379	206	212	224	rBV	294390	501908	39.40%	3.765%
6	2.556	230	241	255	rBV	46196	117817	9.25%	0.884%
7	2.971	296	309	321	rBV	51112	135451	10.63%	1.016%
8	3.331	358	368	380	rBV	17202	40216	3.16%	0.302%
9	4.227	504	515	523	rBV4	19731	64353	5.05%	0.483%
10	4.562	560	570	594	rBV	63796	182430	14.32%	1.368%
11	5.019	636	645	661	rBV3	10795	39300	3.08%	0.295%
12	5.391	694	706	719	rBV	141527	408829	32.09%	3.067%
13	5.556	721	733	749	rVB	261975	744604	58.45%	5.585%
14	5.958	788	799	810	rBV	150646	401537	31.52%	3.012%
15	6.245	837	846	856	rBV4	18684	55045	4.32%	0.413%
16	6.348	858	863	881	rVB5	6729	22288	1.75%	0.167%
17	6.635	896	910	922	rBV	261837	672065	52.75%	5.041%
18	6.763	922	931	946	rVB	391123	940194	73.80%	7.052%
19	6.958	954	963	979	rBV	271921	632448	49.64%	4.744%
20	7.129	979	991	998	rVB6	6282	22654	1.78%	0.170%
21	7.403	1027	1036	1039	rBV4	10928	29338	2.30%	0.220%
22	7.458	1039	1045	1061	rVV2	160290	394390	30.96%	2.958%
23	7.586	1061	1066	1071	rVV3	9478	21093	1.66%	0.158%
24	7.647	1071	1076	1086	rVB	8895	18942	1.49%	0.142%
25	7.903	1112	1118	1133	rVB2	58243	127260	9.99%	0.955%
26	8.427	1199	1204	1212	rBV2	11032	19872	1.56%	0.149%
27	8.506	1212	1217	1223	rVV	50498	81536	6.40%	0.612%
28	8.573	1223	1228	1233	rVV	119694	197761	15.52%	1.483%
29	8.653	1233	1241	1247	rVV	793110	1274010	100.00%	9.556%
30	8.714	1247	1251	1261	rVV	41015	72830	5.72%	0.546%
31	8.805	1261	1266	1283	rVB	84549	156841	12.31%	1.176%
32	8.945	1283	1289	1295	rBV	40393	63880	5.01%	0.479%
33	9.012	1295	1300	1301	rVV	11886	17765	1.39%	0.133%
34	9.031	1301	1303	1310	rVB2	15955	23607	1.85%	0.177%
35	9.183	1321	1328	1332	rBV5	7487	14220	1.12%	0.107%
36	9.244	1332	1338	1345	rVV	58239	94489	7.42%	0.709%

LSC Area Percent Report

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Sample : N3391-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : M15848

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

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Peak separation: 5

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Title : SW846 8260

37	9.311	1345	1349	1357	rVB	19005	28560	2.24%	0.214%
38	9.439	1364	1370	1377	rBV3	95718	183174	14.38%	1.374%
39	9.524	1377	1384	1387	rBV4	19458	30953	2.43%	0.232%
40	9.640	1397	1403	1407	rVB5	10132	21911	1.72%	0.164%
41	9.707	1407	1414	1421	rVB2	23826	52308	4.11%	0.392%
42	9.799	1424	1429	1431	rBV	13232	19415	1.52%	0.146%
43	9.835	1431	1435	1445	rVB	79656	110577	8.68%	0.829%
44	9.945	1448	1453	1461	rBV	135046	197932	15.54%	1.485%
45	10.055	1461	1471	1477	rBV	782046	1085679	85.22%	8.144%
46	10.104	1477	1479	1483	rVB2	12392	13569	1.07%	0.102%
47	10.146	1483	1486	1490	rVB	15475	16190	1.27%	0.121%
48	10.213	1490	1497	1503	rBV	112885	176535	13.86%	1.324%
49	10.274	1503	1507	1514	rVB	85370	114528	8.99%	0.859%
50	10.378	1519	1524	1528	rBV2	90647	141575	11.11%	1.062%
51	10.415	1528	1530	1537	rVB	45893	54676	4.29%	0.410%
52	10.506	1537	1545	1548	rBV4	13874	26783	2.10%	0.201%
53	10.549	1548	1552	1556	rVB2	12017	16299	1.28%	0.122%
54	10.597	1556	1560	1565	rVB3	12362	19678	1.54%	0.148%
55	10.652	1565	1569	1572	rBV3	10863	15101	1.19%	0.113%
56	10.689	1572	1575	1581	rVB2	14323	19267	1.51%	0.145%
57	10.768	1581	1588	1594	rBV	48669	78519	6.16%	0.589%
58	10.878	1599	1606	1614	rBV6	37031	106079	8.33%	0.796%
59	11.036	1625	1632	1635	rBV3	18015	38810	3.05%	0.291%
60	11.085	1635	1640	1649	rVB	600654	786823	61.76%	5.902%
61	11.171	1649	1654	1661	rVB4	42714	81856	6.43%	0.614%
62	11.280	1668	1672	1673	rBV2	10355	13108	1.03%	0.098%
63	11.360	1680	1685	1690	rVB3	9875	19236	1.51%	0.144%
64	11.414	1690	1694	1695	rBV3	11861	14902	1.17%	0.112%
65	11.481	1699	1705	1711	rVV	44274	80610	6.33%	0.605%
66	11.561	1715	1718	1722	rVB2	23385	30632	2.40%	0.230%
67	11.658	1729	1734	1738	rBV5	9973	18724	1.47%	0.140%
68	11.707	1738	1742	1746	rVV3	16409	26533	2.08%	0.199%
69	11.756	1746	1750	1754	rVB3	16270	24361	1.91%	0.183%
70	11.841	1760	1764	1767	rBV2	14081	17748	1.39%	0.133%
71	11.878	1767	1770	1772	rVV2	12596	17986	1.41%	0.135%
72	11.902	1772	1774	1782	rVV8	14556	35123	2.76%	0.263%
73	11.975	1782	1786	1789	rVV	39371	50209	3.94%	0.377%
74	12.024	1789	1794	1802	rVB	798636	956572	75.08%	7.175%
75	12.122	1806	1810	1814	rBV5	16099	27406	2.15%	0.206%
76	12.219	1822	1826	1833	rBV	110668	148929	11.69%	1.117%

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Title : SW846 8260

77	12.280	1834	1836	1842	rVB6	13050	21242	1.67%	0.159%
78	12.426	1855	1860	1871	rBV4	19304	55787	4.38%	0.418%
79	12.518	1871	1875	1878	rVV2	22133	31734	2.49%	0.238%
80	12.585	1882	1886	1894	rVV4	17289	32621	2.56%	0.245%
81	12.664	1895	1899	1907	rVB2	38872	67876	5.33%	0.509%
82	12.804	1917	1922	1933	rVB	89124	153175	12.02%	1.149%
83	13.164	1978	1981	1985	rVB	15734	18331	1.44%	0.138%
84	13.420	2020	2023	2029	rVB5	8500	13889	1.09%	0.104%
85	13.512	2034	2038	2044	rBV4	11810	19536	1.53%	0.147%
86	13.591	2047	2051	2060	rBV3	62236	100337	7.88%	0.753%
87	14.646	2217	2224	2228	rBV4	12320	24646	1.93%	0.185%
88	14.755	2238	2242	2244	rBV4	9531	13965	1.10%	0.105%
89	14.932	2267	2271	2278	rBV	20298	34425	2.70%	0.258%
90	15.420	2347	2351	2356	rVB2	18284	27785	2.18%	0.208%
91	15.487	2359	2362	2367	rBV6	6753	13002	1.02%	0.098%
92	15.743	2400	2404	2412	rVB5	19251	31632	2.48%	0.237%
93	15.865	2421	2424	2430	rVB6	11229	17738	1.39%	0.133%
94	16.706	2557	2562	2568	rVB5	12196	24404	1.92%	0.183%

Sum of corrected areas: 13331503

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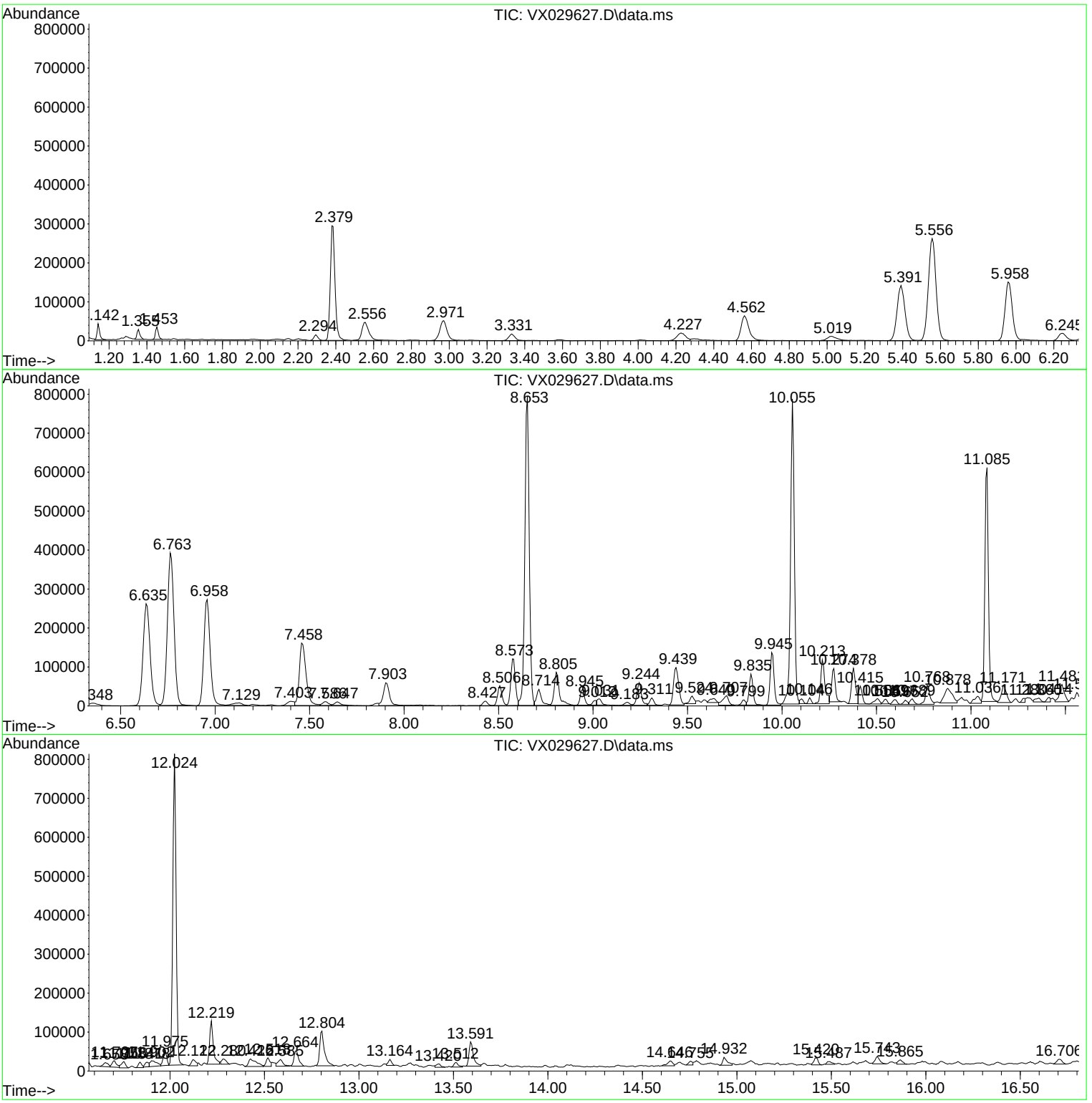
Instrument :
MSVOA_X
ClientSampleId :
M15848

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

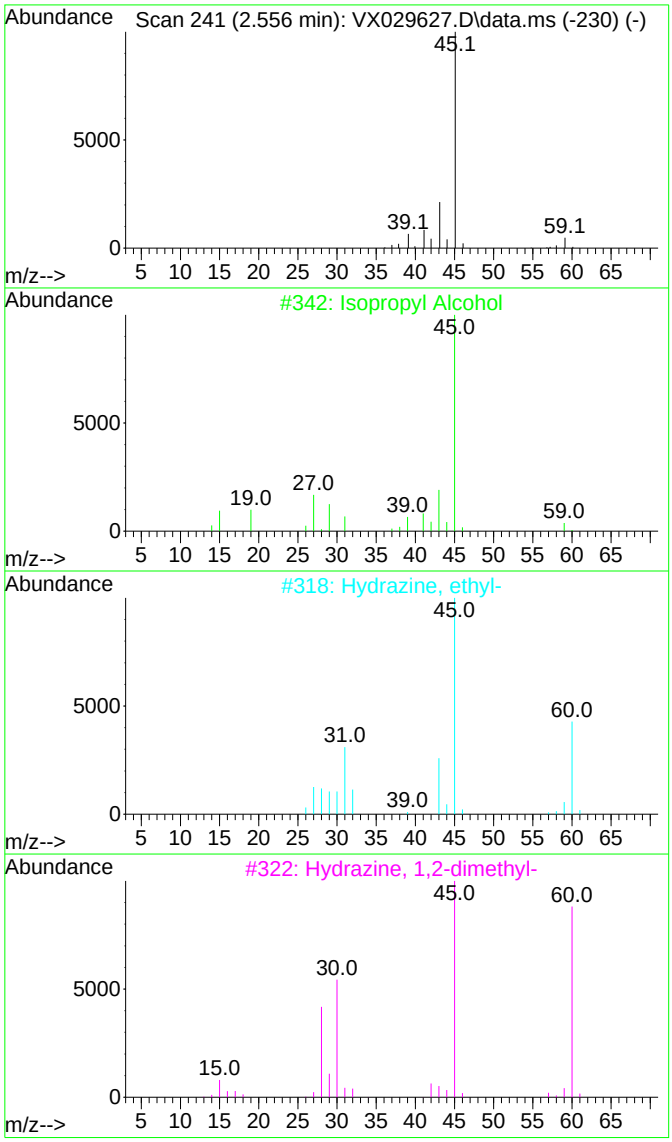
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

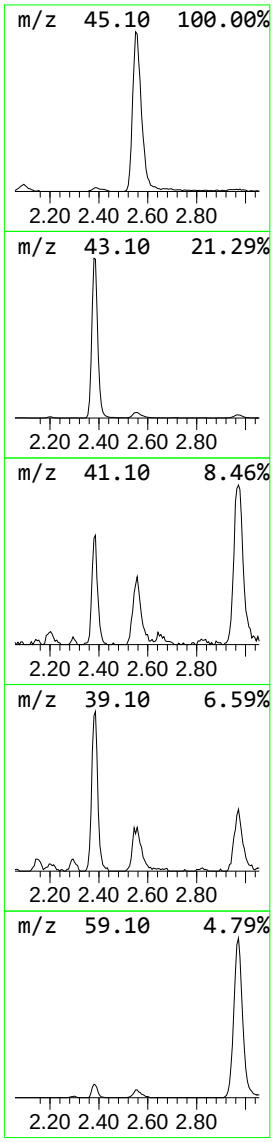
****

Peak Number 1 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.556	7.91 ug/l	117817	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Formamide	45	CH3NO	000075-12-7	5
5	2-Butanol	74	C4H10O	000078-92-2	4





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M15848

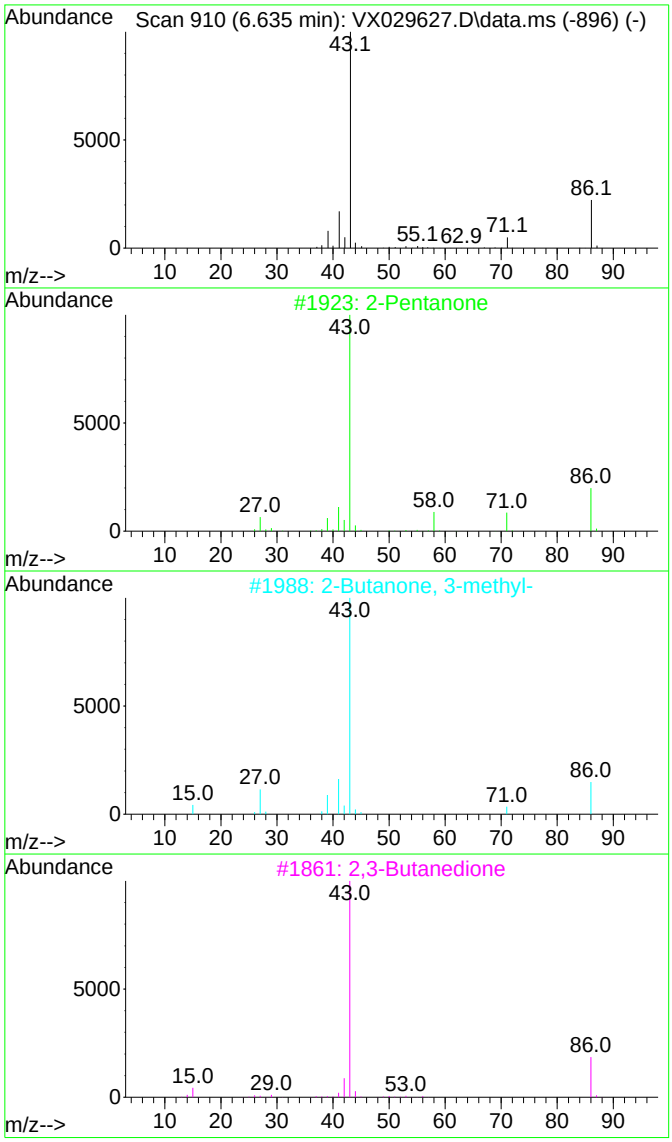
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

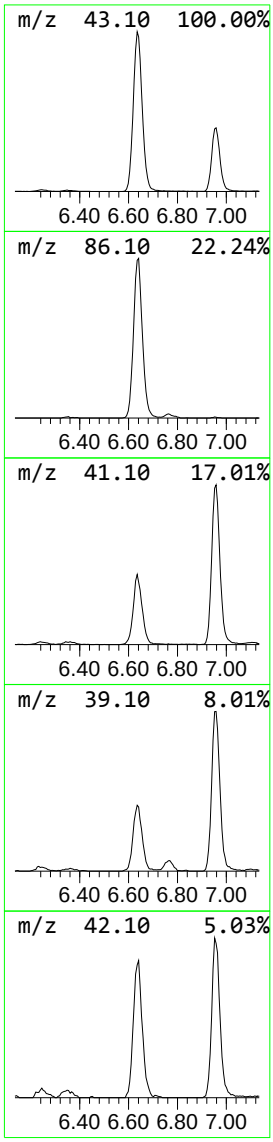
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.635	35.74 ug/l	672065	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	80
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
3	2,3-Butanedione	86	C4H6O2	000431-03-8	53
4	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	38
5	2-Imidazolidinone	86	C3H6N2O	000120-93-4	7





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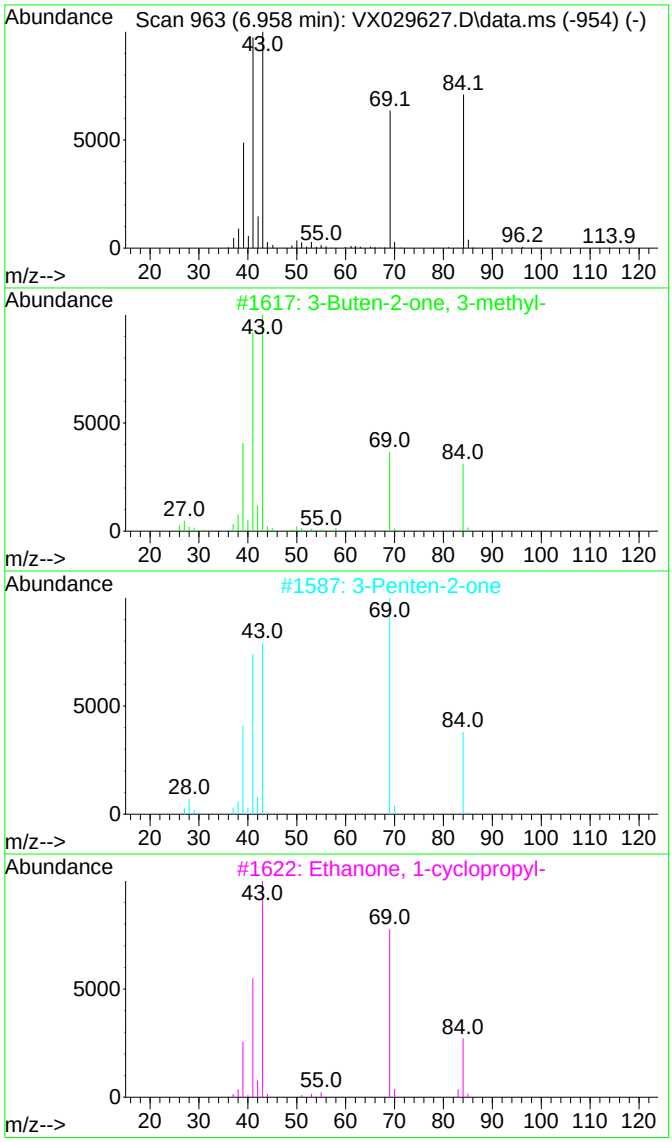
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

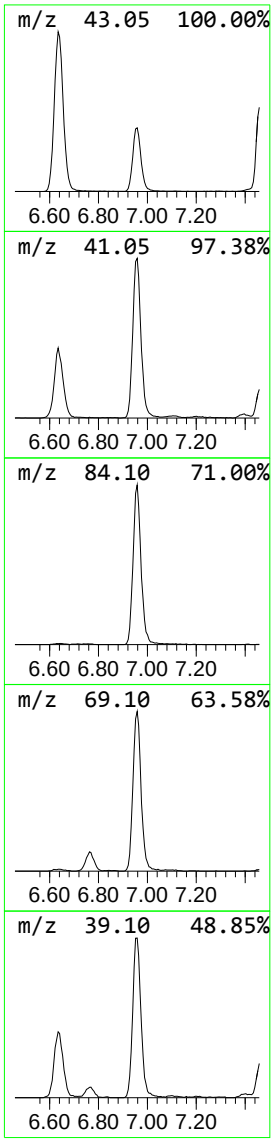
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Buten-2-one, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.958	33.63 ug/l	632448	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2	3-Penten-2-one	84	C5H8O	000625-33-2	90
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	72
4	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	50
5	Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	40





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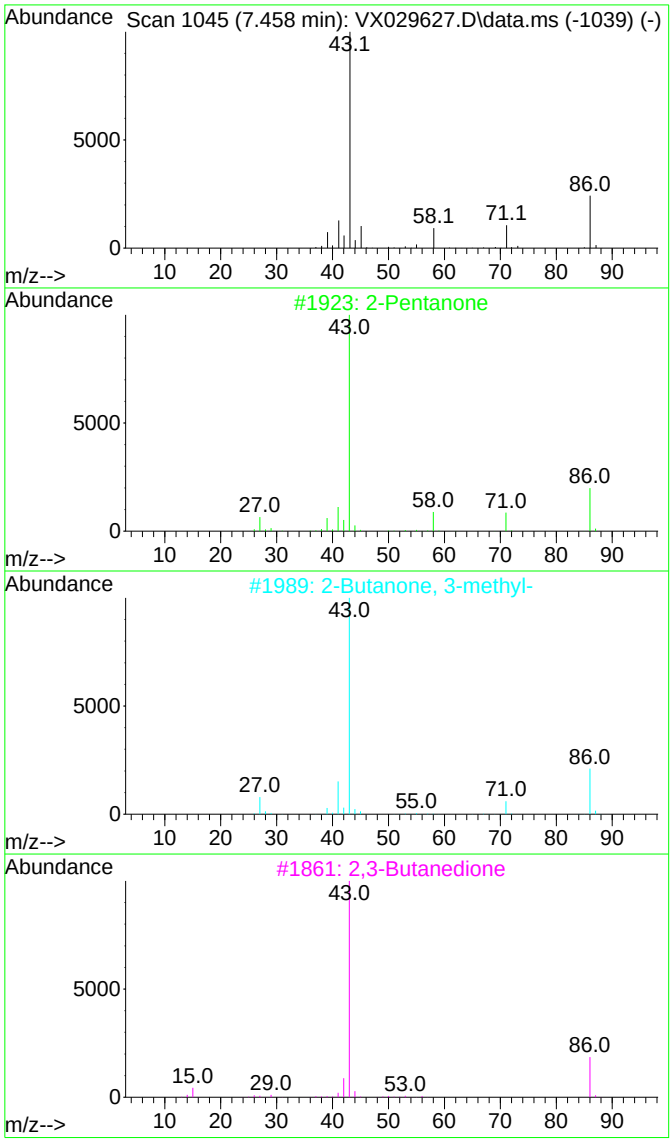
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

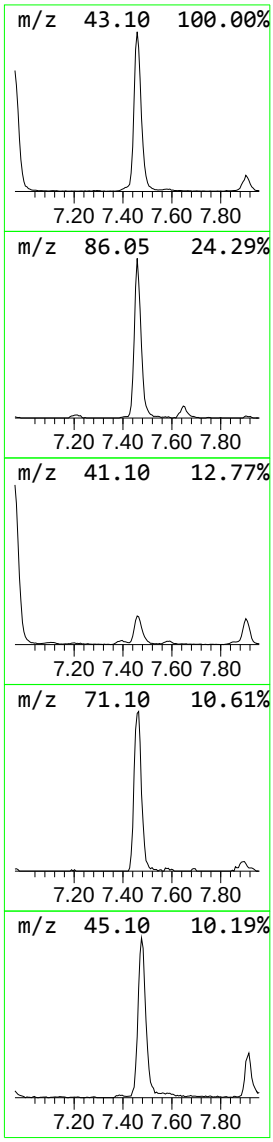
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butanone, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	20.97 ug/l	394390	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	72
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
3	2,3-Butanedione	86	C4H6O2	000431-03-8	49
4	2-Propanone, methylhydrazone	86	C4H10N2	005771-02-8	9
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M15848

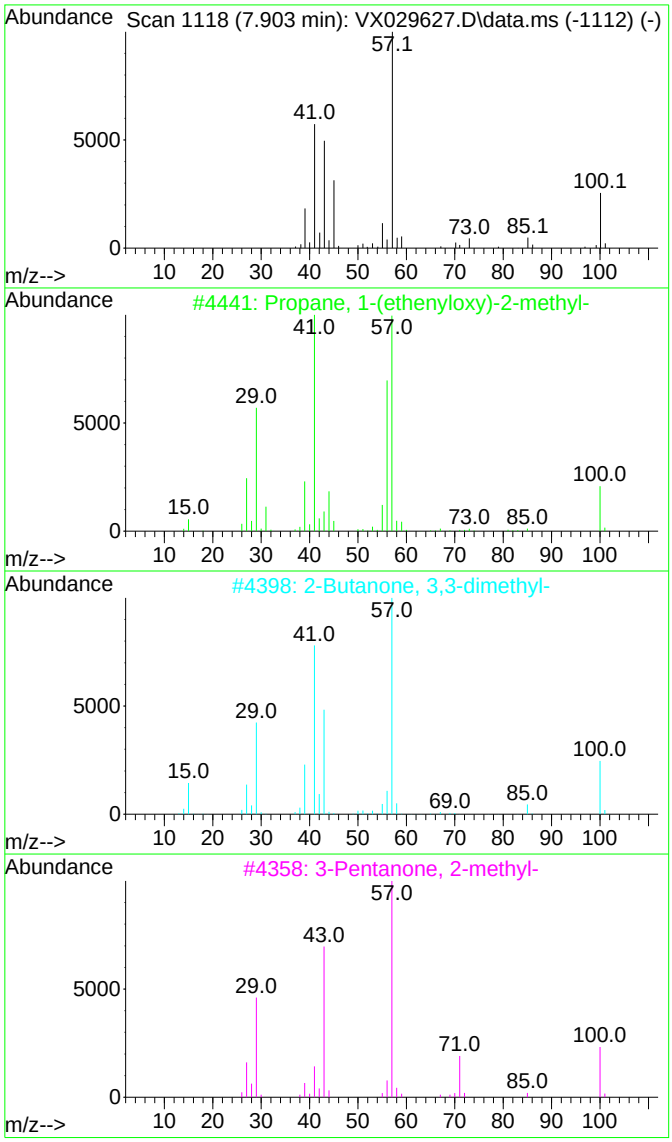
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

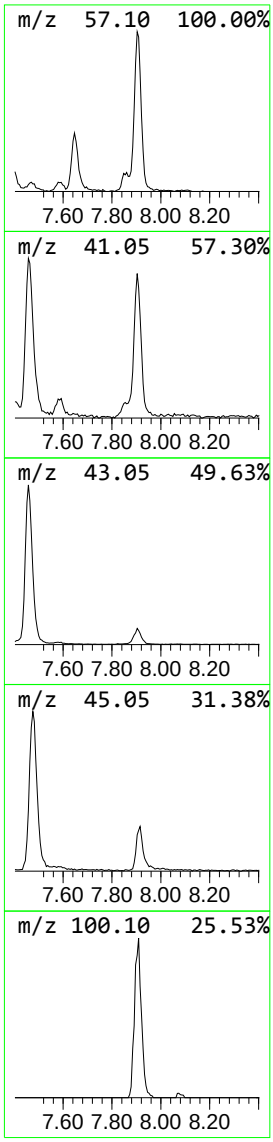
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propane, 1-(ethenyloxy)-2-m... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.903	6.77 ug/l	127260	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-(ethenyloxy)-2-methyl-	100	C6H12O	000109-53-5	50
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	46
3	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	43
4	3-Hexanone	100	C6H12O	000589-38-8	43
5	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	37





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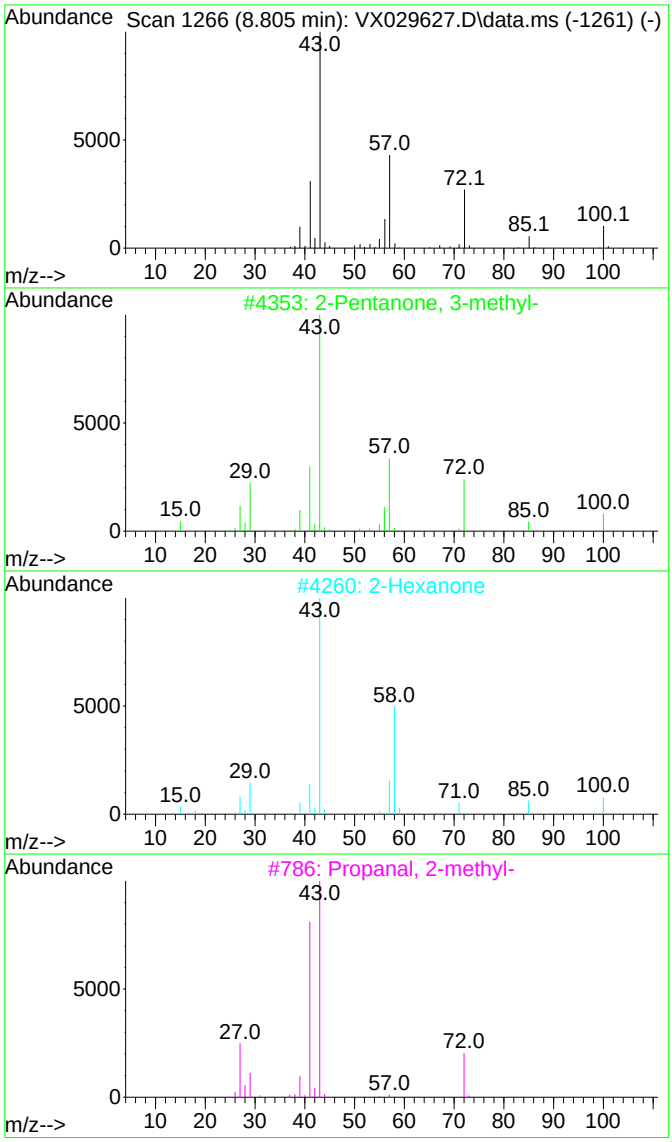
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

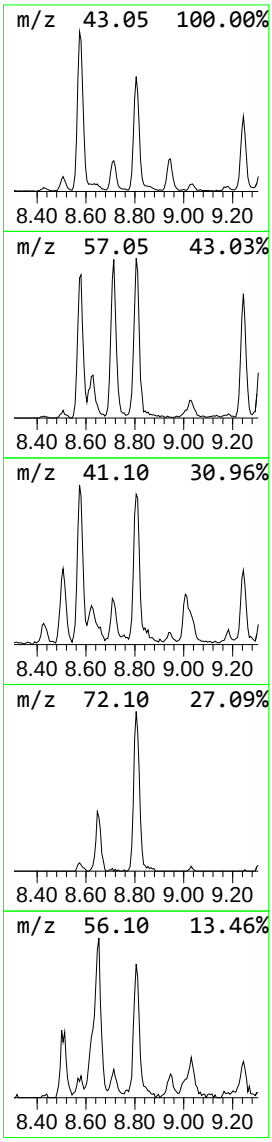
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Pentanone, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.805	7.22 ug/l	156841	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	91
2	2-Hexanone	100	C6H12O	000591-78-6	47
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4	2-Butanone	72	C4H8O	000078-93-3	43
5	Pyruvic acid, butyl ester	144	C7H12O3	020279-44-1	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029627.D
Acq On : 20 Jun 2022 16:49
Operator : JC/MD
Sample : N3391-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M15848

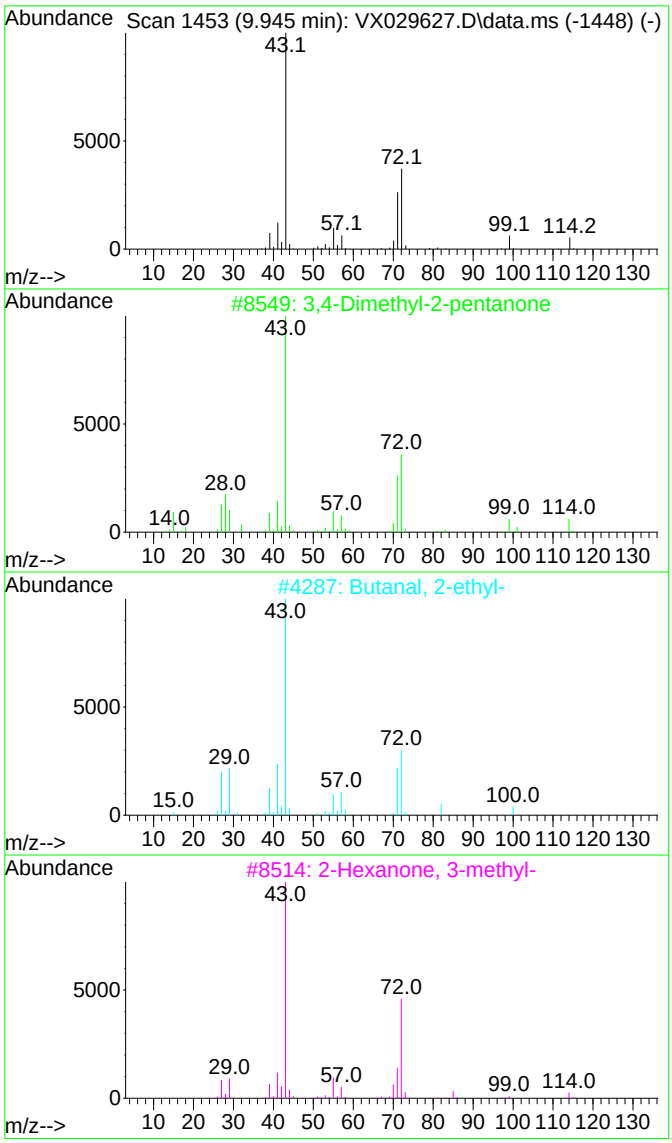
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

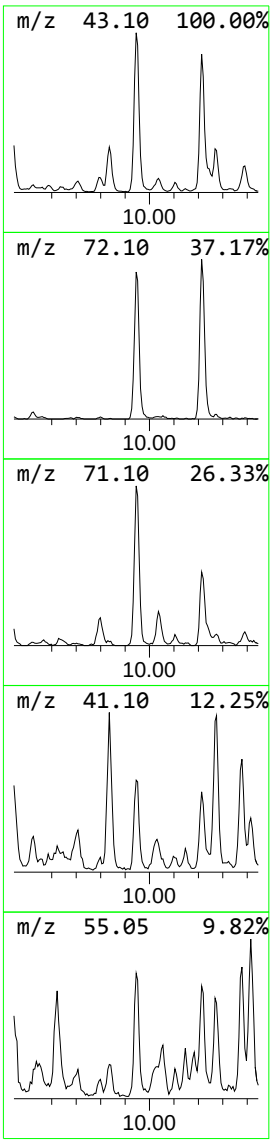
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3,4-Dimethyl-2-pentanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.945	9.12 ug/l	197932	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	91
2	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	42
3	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	37
4	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	36
5	1-Methylallyl acetate	114	C6H10O2	006737-11-7	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029627.D
Acq On : 20 Jun 2022 16:49
Operator : JC/MD
Sample : N3391-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M15848

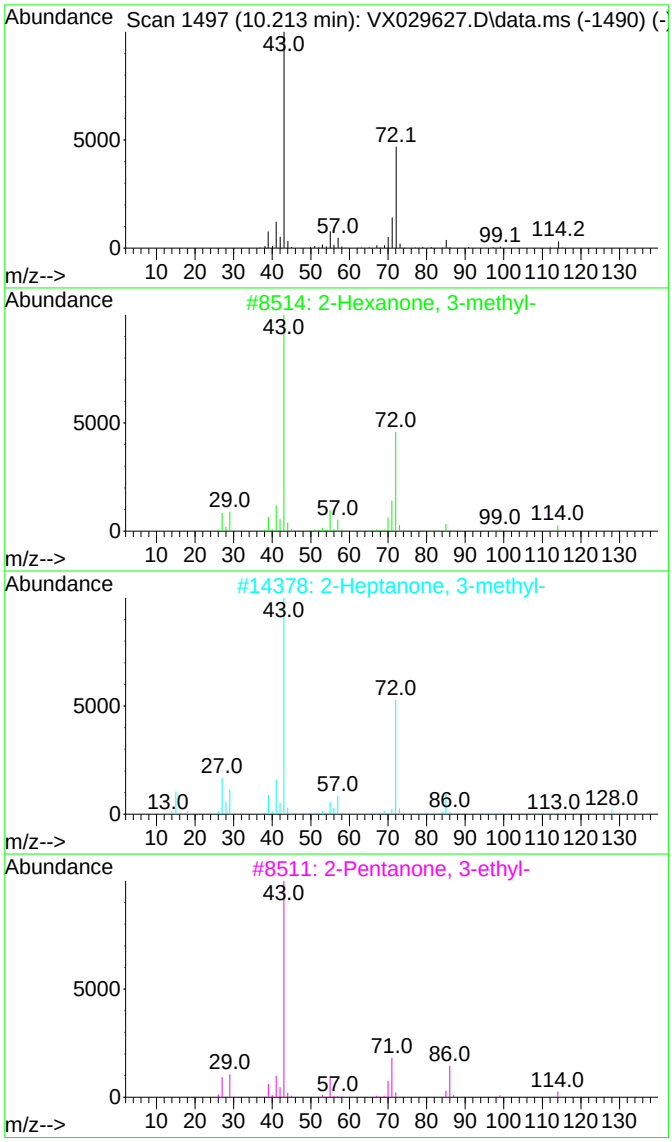
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

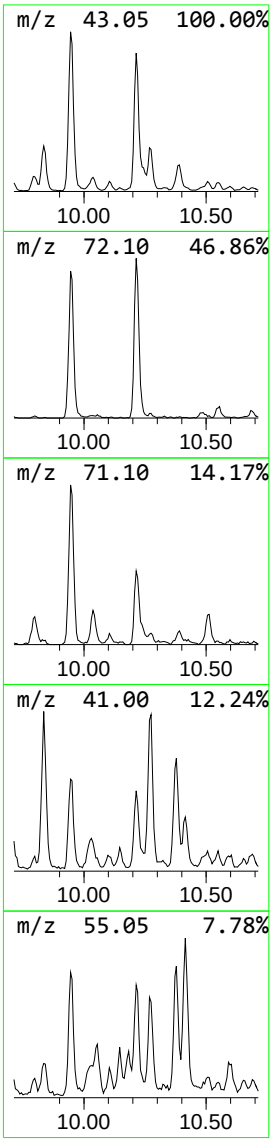
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Hexanone, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.213	8.13 ug/l	176535	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	91
2	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	64
3	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	46
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	40
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029627.D
Acq On : 20 Jun 2022 16:49
Operator : JC/MD
Sample : N3391-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M15848

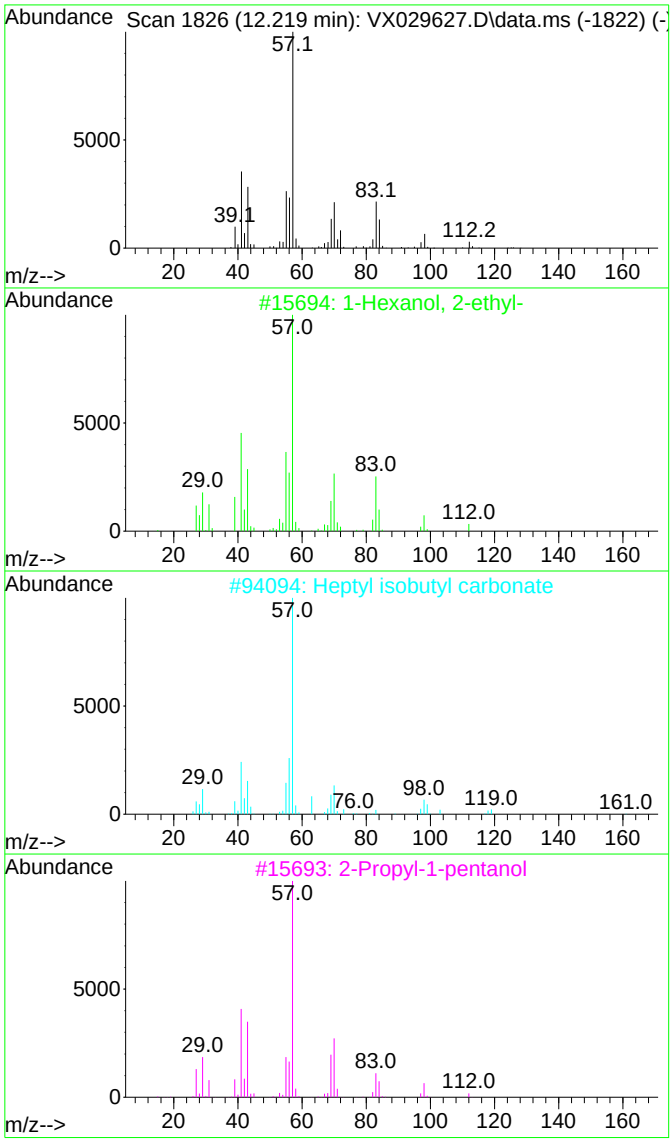
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

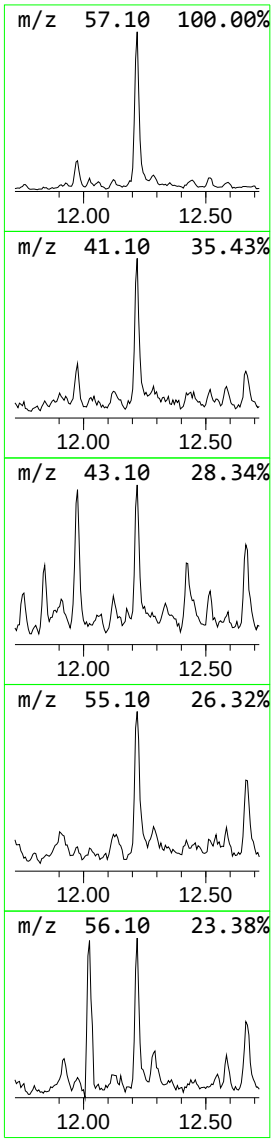
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	7.78 ug/l	148929	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	90
2	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50





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Data File : VX029627.D
Acq On : 20 Jun 2022 16:49
Operator : JC/MD
Sample : N3391-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M15848

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

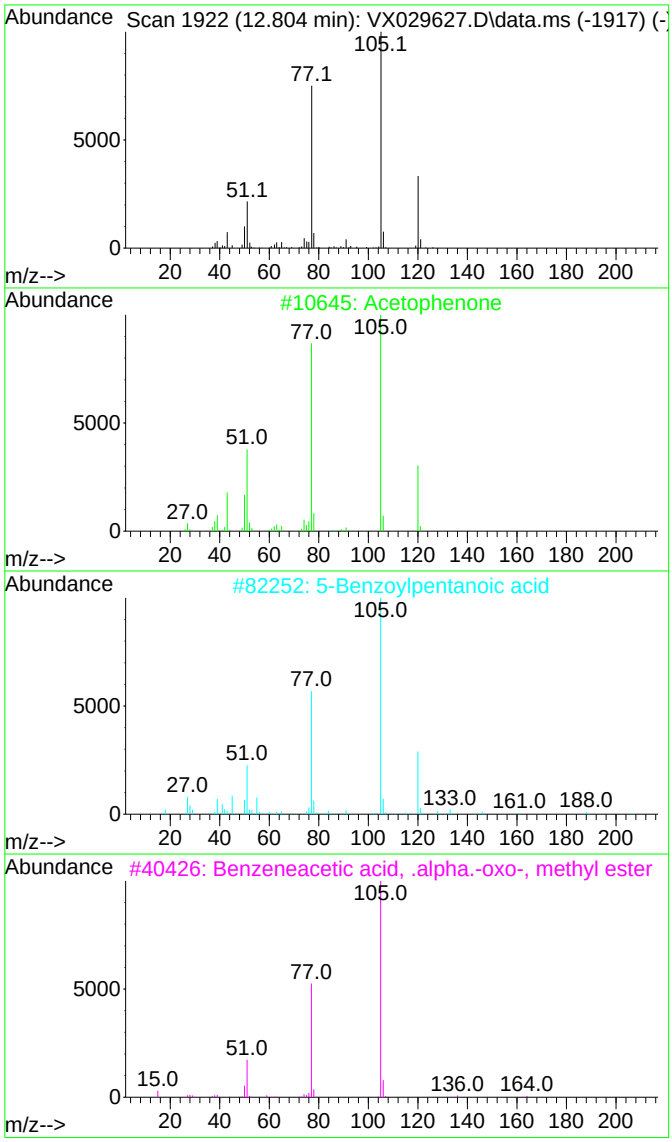
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

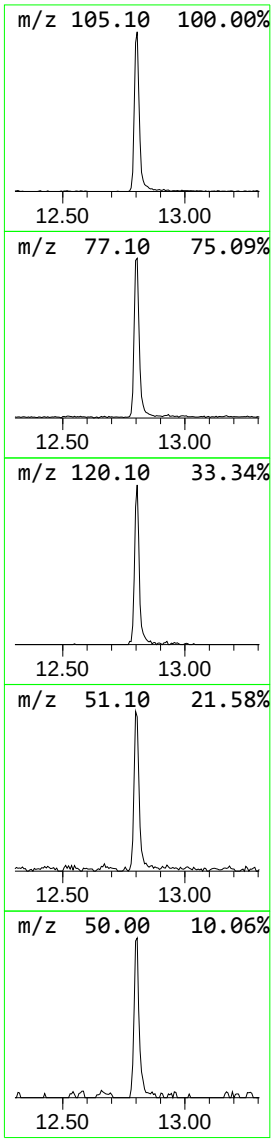
****

Peak Number 10 Acetophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.804	8.01 ug/l	153175	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone	120	C8H8O	000098-86-2	91
2	5-Benzoylpentanoic acid	206	C12H14O3	004144-62-1	72
3	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	64
4	Benzoic acid, 2-(benzoylthio)thi...	341	C17H11NO3S2	1000258-72-7	64
5	Propan-1-one, 3-nitro-1-phenyl-	179	C9H9NO3	062847-52-3	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062022\
Data File : VX029627.D
Acq On : 20 Jun 2022 16:49
Operator : JC/MD
Sample : N3391-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
M15848

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.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
Isopropyl Alcohol	2.556	7.9	ug/l	117817	1	5.556	744604	50.0
2-Pentanone	6.635	35.7	ug/l	672065	2	6.763	940194	50.0
3-Buten-2-one, ...	6.958	33.6	ug/l	632448	2	6.763	940194	50.0
2-Butanone, 3-m...	7.458	21.0	ug/l	394390	2	6.763	940194	50.0
Propane, 1-(eth...	7.903	6.8	ug/l	127260	2	6.763	940194	50.0
2-Pentanone, 3-...	8.805	7.2	ug/l	156841	3	10.055	1085680	50.0
3,4-Dimethyl-2-...	9.945	9.1	ug/l	197932	3	10.055	1085680	50.0
2-Hexanone, 3-m...	10.213	8.1	ug/l	176535	3	10.055	1085680	50.0
1-Hexanol, 2-et...	12.219	7.8	ug/l	148929	4	12.024	956572	50.0
Acetophenone	12.804	8.0	ug/l	153175	4	12.024	956572	50.0