LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

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\82X112120W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	59	63	68	rBV	866904	1012526	41.57%	6.277%
2	1.514	68	70	92	rVB	79903	180513	7.41%	1.119%
3	2.123	165	170	179	rBV	47554	65512	2.69%	0.406%
4	2.331	199	204	214	rVV	24260	43306	1.78%	0.268%
5	2.428	214	220	233	rVB	204840	350112	14.37%	2.170%
6	2.611	243	250	258	rVB	12018	24531	1.01%	0.152%
7	2.995	305	313	317	rBV	20048	48968	2.01%	0.304%
8	3.385	367	377	389	rBV2	20511	55170	2.26%	0.342%
9	3.849	445	453	461	rBV2	8684	27796	1.14%	0.172%
10	3.946	461	469	487	rVB	57921	157489	6.47%	0.976%
11	4.306	517	528	544	rBV3	15254	58452	2.40%	0.362%
12	4.452	544	552	571	rVV	35363	114471	4.70%	0.710%
13	4.647	575	584	597	rVB2	8689	28472	1.17%	0.177%
14	5.464	705	718	729	rBV2	168021	482380	19.80%	2.990%
15	5.629	734	745	764	rVB2	303642	872841	35.83%	5.411%
16	6.025	800	810	826	rBV	193298	510849	20.97%	3.167%
17	6.428	866	876	895	rVB	35254	108439	4.45%	0.672%
18	6.671	908	916	930	rVB	33079	89083	3.66%	0.552%
19	6.830	932	942	953	rBV	467879	1116942	45.85%	6.924%
20	6.940	953	960	970	rVB	23870	57882	2.38%	0.359%
21	7.281	1007	1016	1025	rBV2	24766	62838	2.58%	0.390%
22	7.440	1033	1042	1050	rVB2	16039	37258	1.53%	0.231%
23	8.695	1241	1248	1256	rBV	976945	1501518	61.64%	9.308%
24	9.317	1346	1350	1356	rVB	30779	46927	1.93%	0.291%
25	9.598	1392	1396	1404	rBV	241417	400976	16.46%	2.486%
26	9.665	1404	1407	1416	rVB	21071	38767	1.59%	0.240%
27	10.092	1472	1477	1489	rBV	917676	1280832	52.58%	7.940%
28	10.342	1505	1518	1524	rBV	49868	87106	3.58%	0.540%
29	10.683	1569	1574	1583	rVB	22550	34507	1.42%	0.214%
30	10.793	1586	1592	1600	rBV2	16838	28844	1.18%	0.179%
31	11.122	1640	1646	1652	rBV	769972	954398	39.18%	5.917%
32	11.415	1690	1694	1700	rBV	33786	62494	2.57%	0.387%
33	11.652	1729	1733	1737	rVB2	24009	35894	1.47%	0.223%
34	11.793	1751	1756	1763	rVB	101213	125405	5.15%	0.777%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

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\82X112120W.M
Title : SW846 8260

35	11.902	1771	1774	1782	rBV2	40123	65817	2.70%	0.408%
36	12.024	1788	1794	1796	rBV4	21737	43717	1.79%	0.271%
37	12.061	1796	1800	1806	rVV	1001981	1195403	49.07%	7.411%
38	12.128	1806	1811	1816	rVB	30745	44081	1.81%	0.273%
39	12.256	1827	1832	1839	rBV	329261	486556	19.97%	3.016%
40	12.353	1844	1848	1854	rVB4	36421	70135	2.88%	0.435%
41	12.652	1893	1897	1900	rVB	23579	29241	1.20%	0.181%
42	12.890	1932	1936	1940	rVB4	24010	30080	1.23%	0.186%
43	12.957	1940	1947	1951	rVV	20377	32939	1.35%	0.204%
44	13.000	1951	1954	1961	rVB	32427	39462	1.62%	0.245%
45	13.207	1980	1988	1992	rBV2	31614	48725	2.00%	0.302%
46	13.329	2004	2008	2013	rVB2	45005	61715	2.53%	0.383%
47	13.463	2026	2030	2039	rVB2	28686	43258	1.78%	0.268%
48	13.621	2052	2056	2058	rBV3	20869	32731	1.34%	0.203%
49	13.701	2064	2069	2080	rVB5	15923	44005	1.81%	0.273%
50	13.792	2080	2084	2085	rBV2	27671	34977	1.44%	0.217%
51	13.817	2085	2088	2094	rVV	80755	107037	4.39%	0.664%
52	13.884	2094	2099	2106	rVB2	57371	94233	3.87%	0.584%
53	13.957	2106	2111	2124	rBV6	47197	112856	4.63%	0.700%
54	14.268	2154	2162	2166	rBV2	34400	64200	2.64%	0.398%
55	14.518	2199	2203	2208	rVB2	22111	31971	1.31%	0.198%
56	14.676	2222	2229	2233	rBV	109781	159356	6.54%	0.988%
57	14.822	2248	2253	2257	rBV	61852	81842	3.36%	0.507%
58	15.036	2283	2288	2292	rBV3	31738	45066	1.85%	0.279%
59	15.231	2315	2320	2321	rBV	17304	25974	1.07%	0.161%
60	15.249	2321	2323	2327	rVB	25136	28771	1.18%	0.178%
61	15.420	2347	2351	2355	rBV	16774	27697	1.14%	0.172%
62	15.524	2363	2368	2373	rBV	41383	68429	2.81%	0.424%
63	15.664	2385	2391	2394	rBV2	59803	91530	3.76%	0.567%
64	15.700	2394	2397	2402	rVB2	36799	52904	2.17%	0.328%
65	15.889	2420	2428	2438	rVB2	17568	45225	1.86%	0.280%
66	16.023	2443	2450	2465	rBV	1440280	2435879	100.00%	15.101%
67	16.145	2465	2470	2478	rVB2	101585	187513	7.70%	1.162%
68	16.523	2527	2532	2539	rVB4	17003	33963	1.39%	0.211%
69	16.718	2560	2564	2574	rBV3	14922	30055	1.23%	0.186%

Sum of corrected areas: 16130841

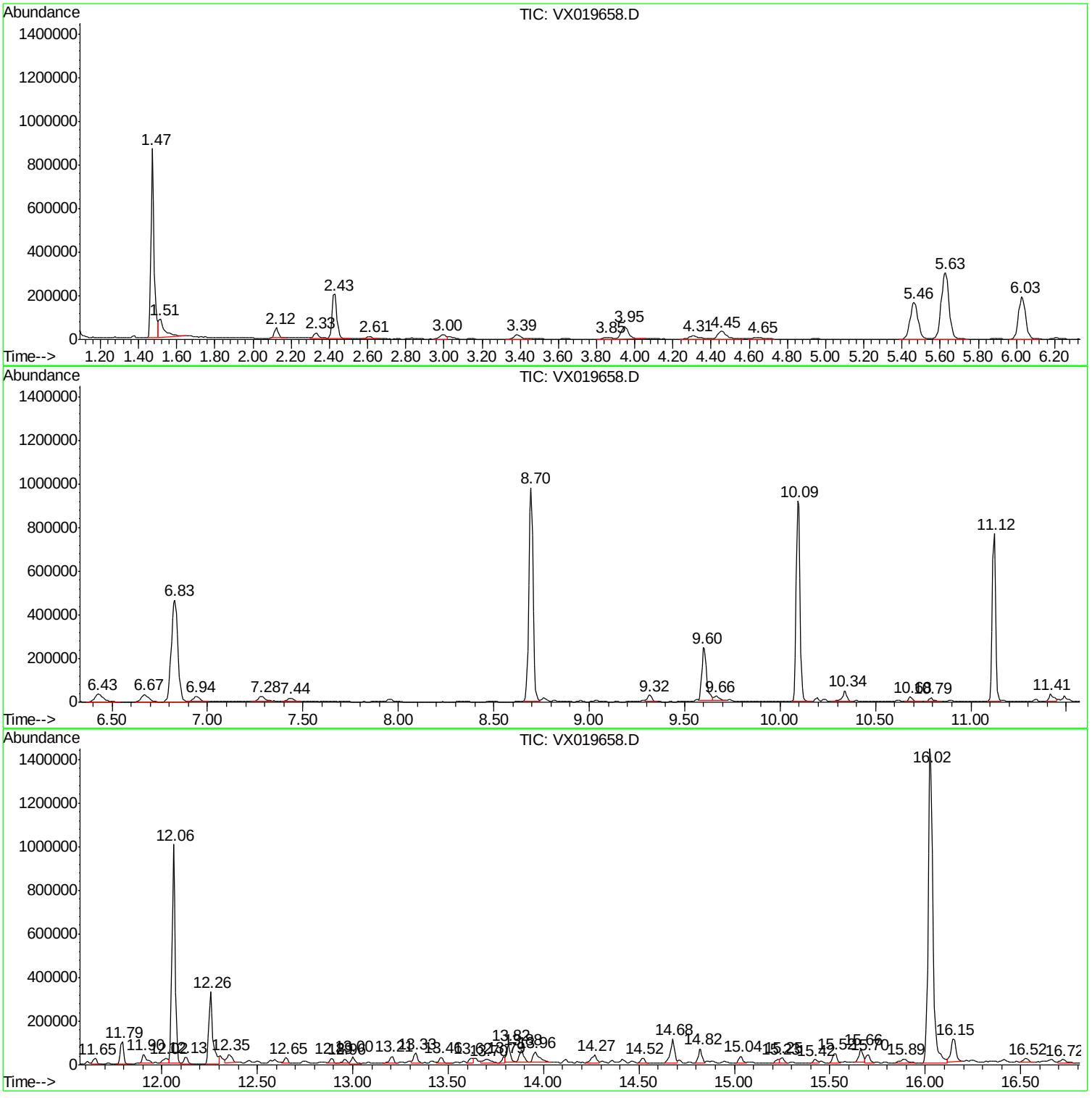
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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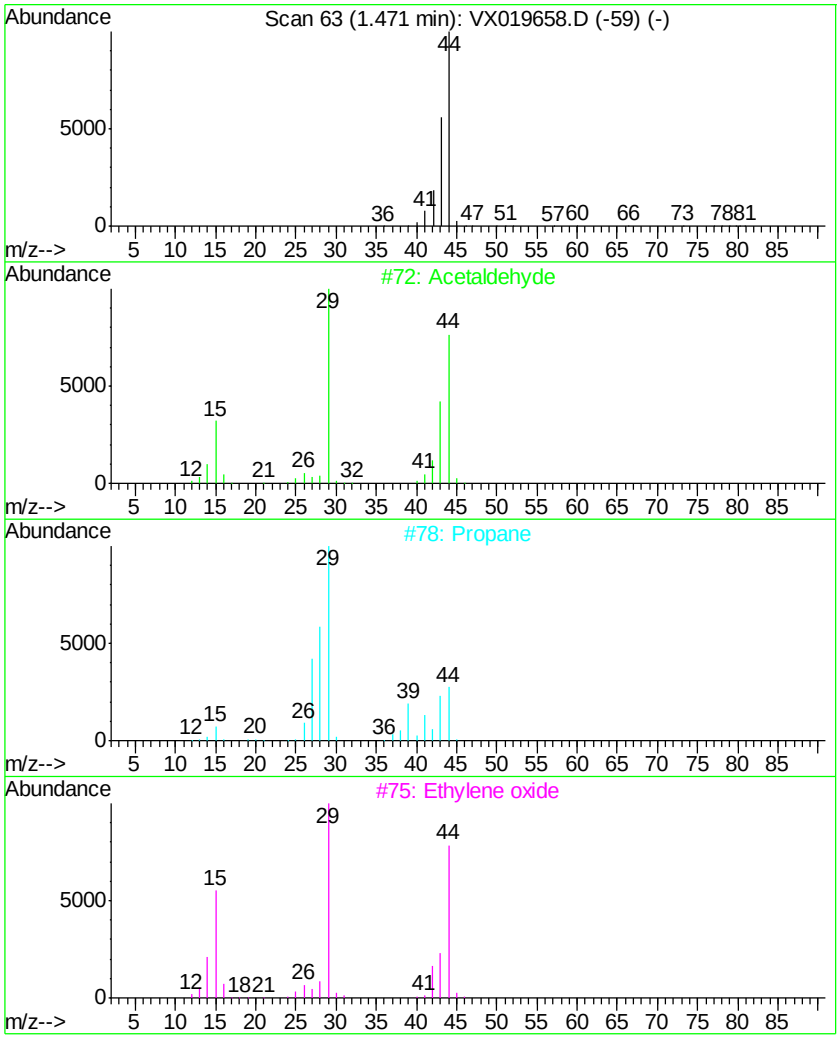
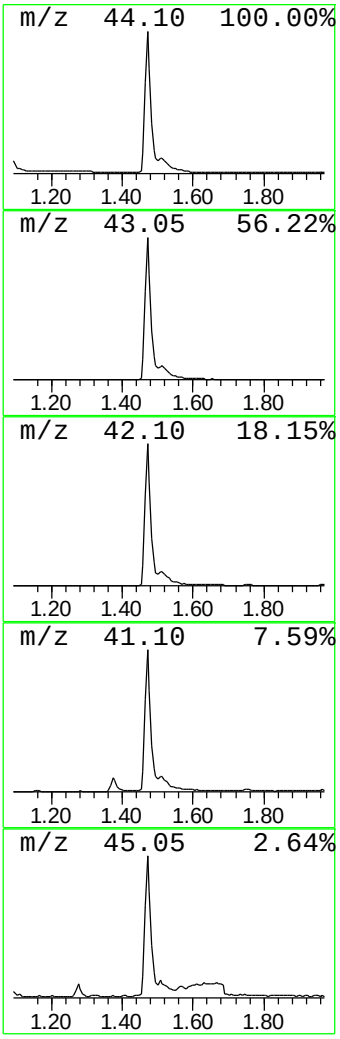
Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	58.00 ug/l	1012530	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
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	1,2-Propanediamine	74	C3H10N2	000078-90-0	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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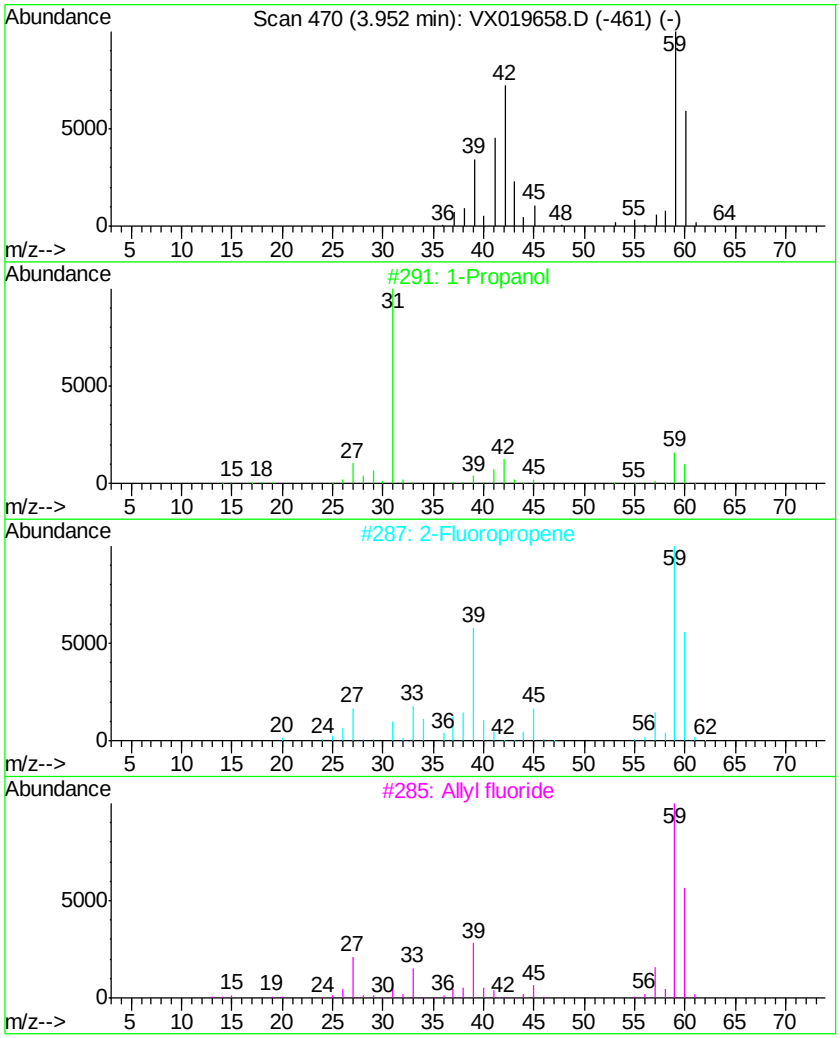
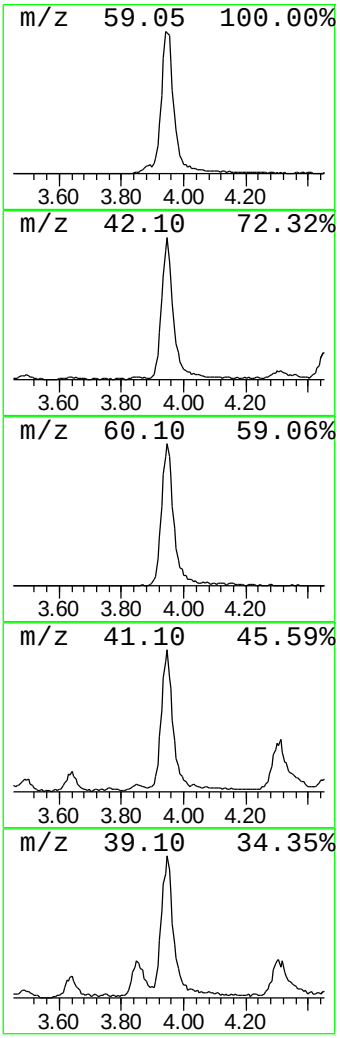
Peak Number 3 1-Propanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.95	9.02 ug/l	157489	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	2-Fluoropropene	60	C3H5F	001184-60-7	47
3	Allyl fluoride	60	C3H5F	000818-92-8	47
4	Isoxazolidine, 5-ethyl-2,4-dimet...	129	C7H15NO	056728-14-4	28
5	Isoxazolidine, 4-ethyl-2,5-dimet...	129	C7H15NO	056728-13-3	23





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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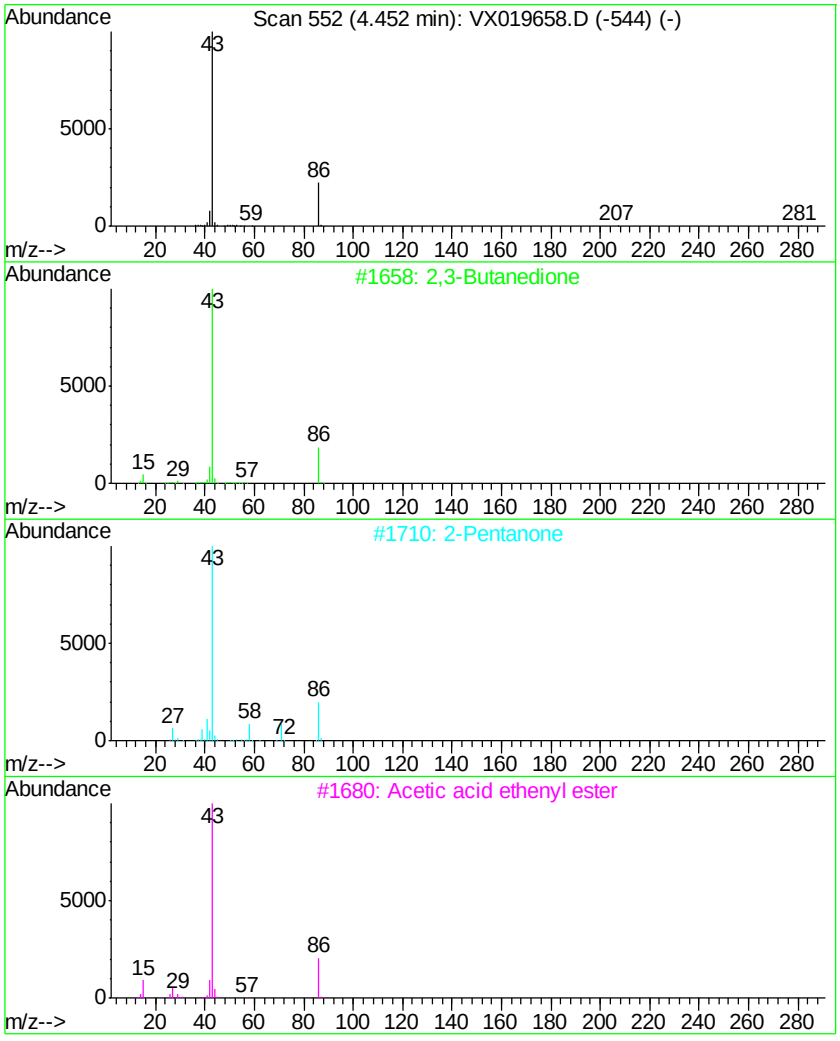
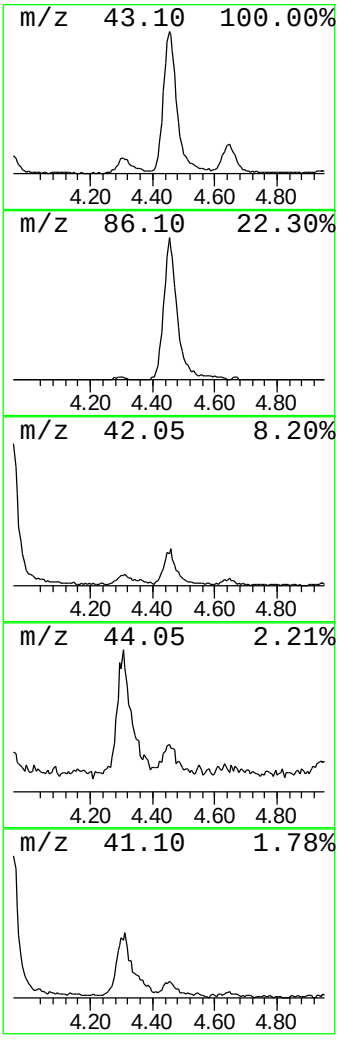
Peak Number 4 2,3-Butanedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	6.56 ug/l	114471	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	64
2	2-Pentanone	86	C5H10O	000107-87-9	64
3	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	45
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7
5	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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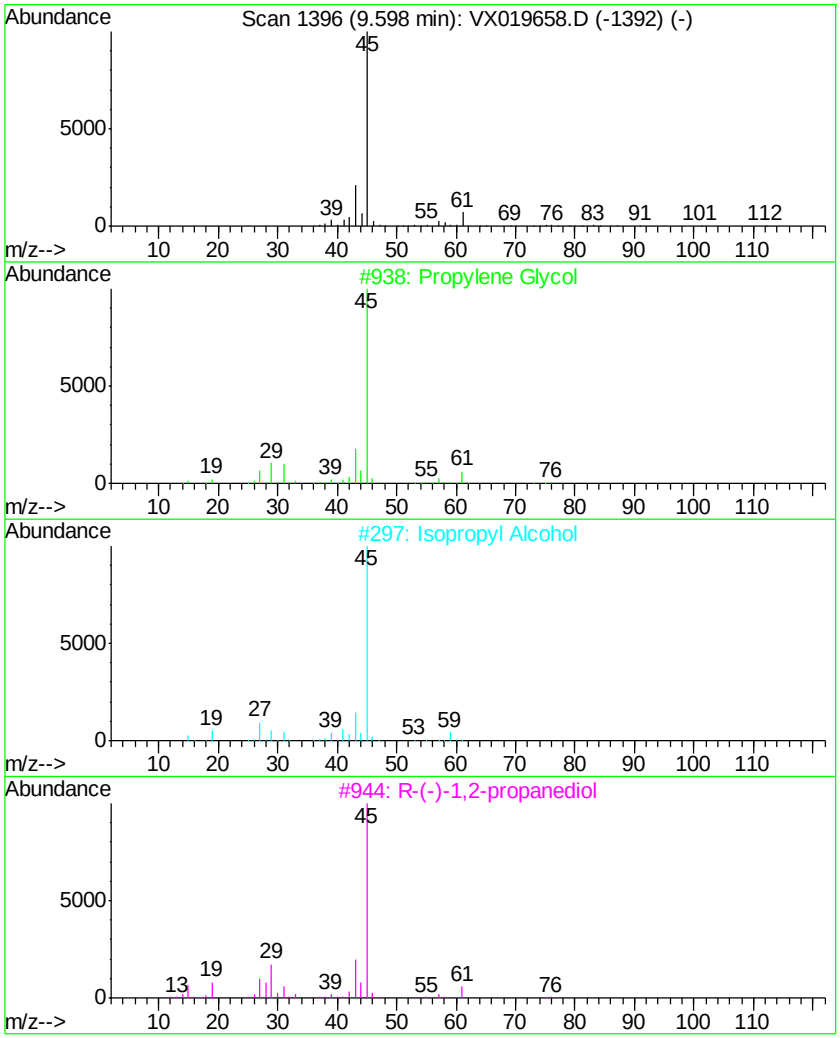
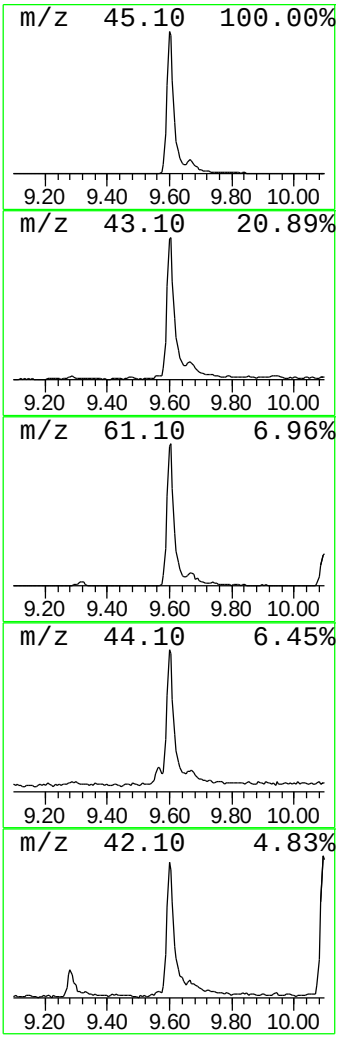
Peak Number 5 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	15.65 ug/l	400976	Chlorobenzene-d5	10.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	72
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	12





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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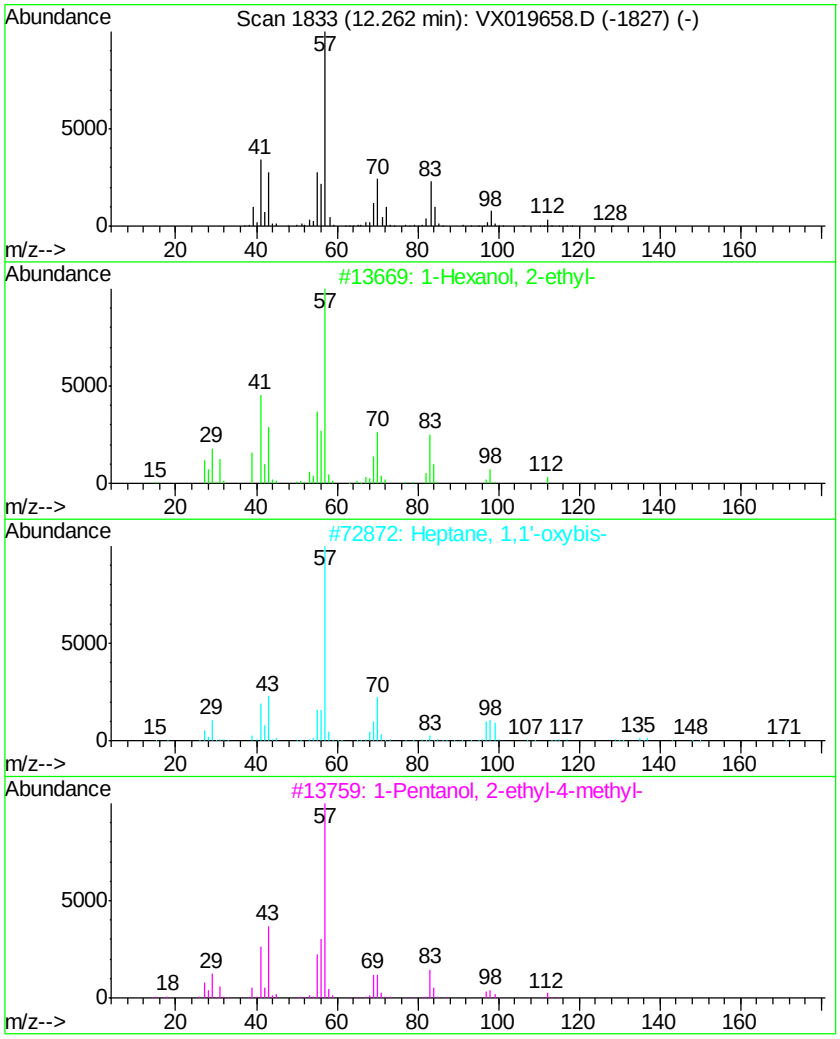
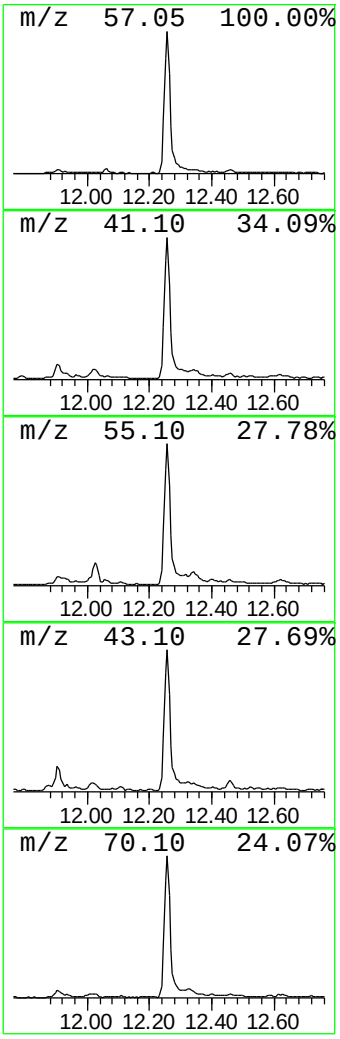
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	20.35 ug/l	486556	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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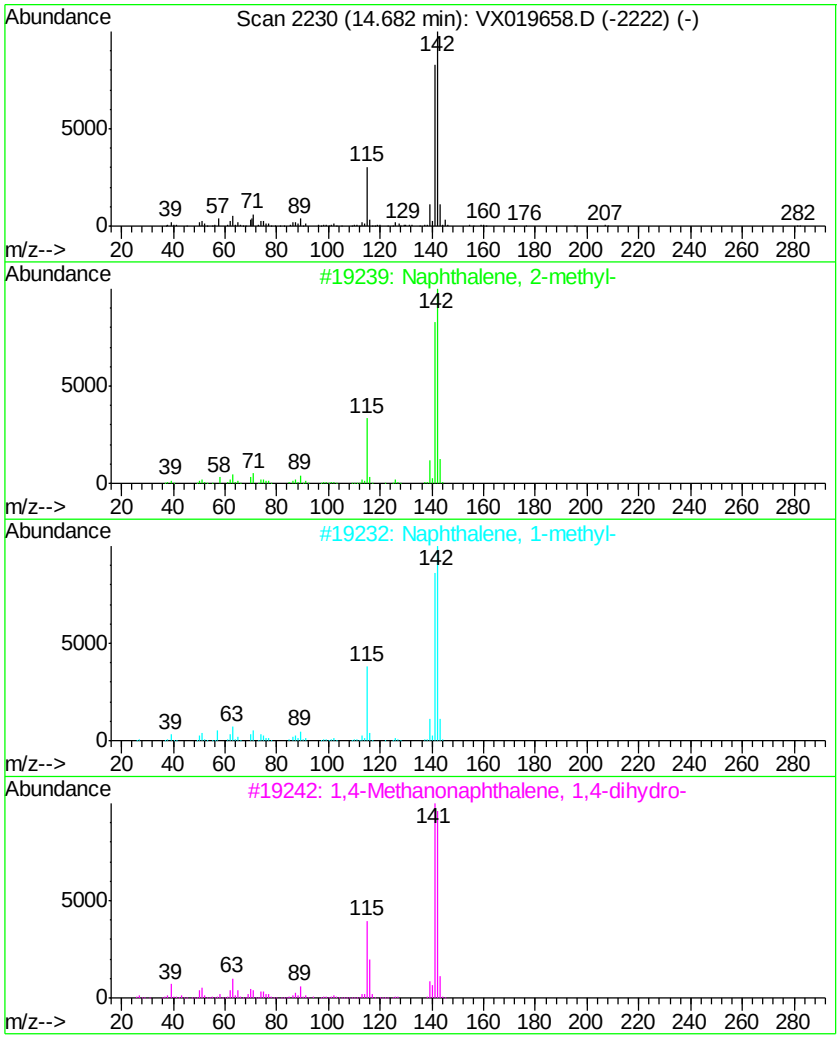
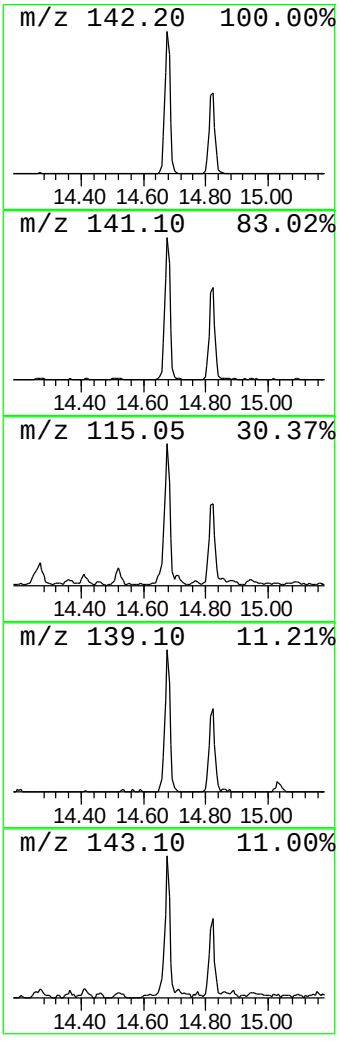
Peak Number 7 Naphthalene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.68	6.67 ug/l	159356	1,4-Dichlorobenzene-d4	12.06

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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

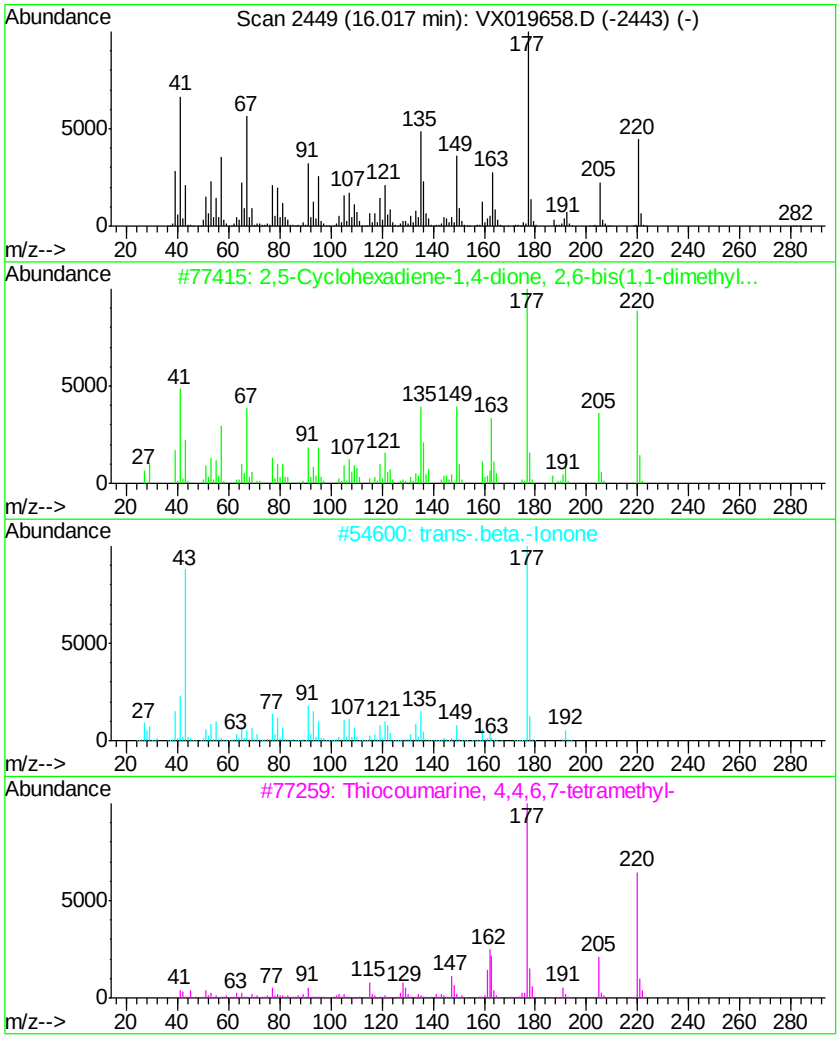
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

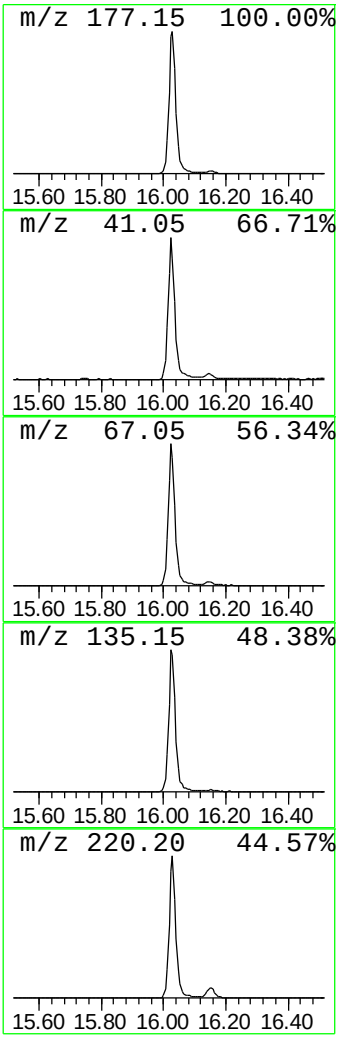
****

Peak Number 8 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	101.89 ug/l	2435880	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2	trans-.beta.-Ionone	192	C13H20O	000079-77-6	38
3	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	38
4	2H-1-Benzopyran, 3,5,6,8a-tetrah...	192	C13H20O	041678-29-9	35
5	1,3,5,7-Tetramethyl-adamantane	192	C14H24	001687-36-1	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

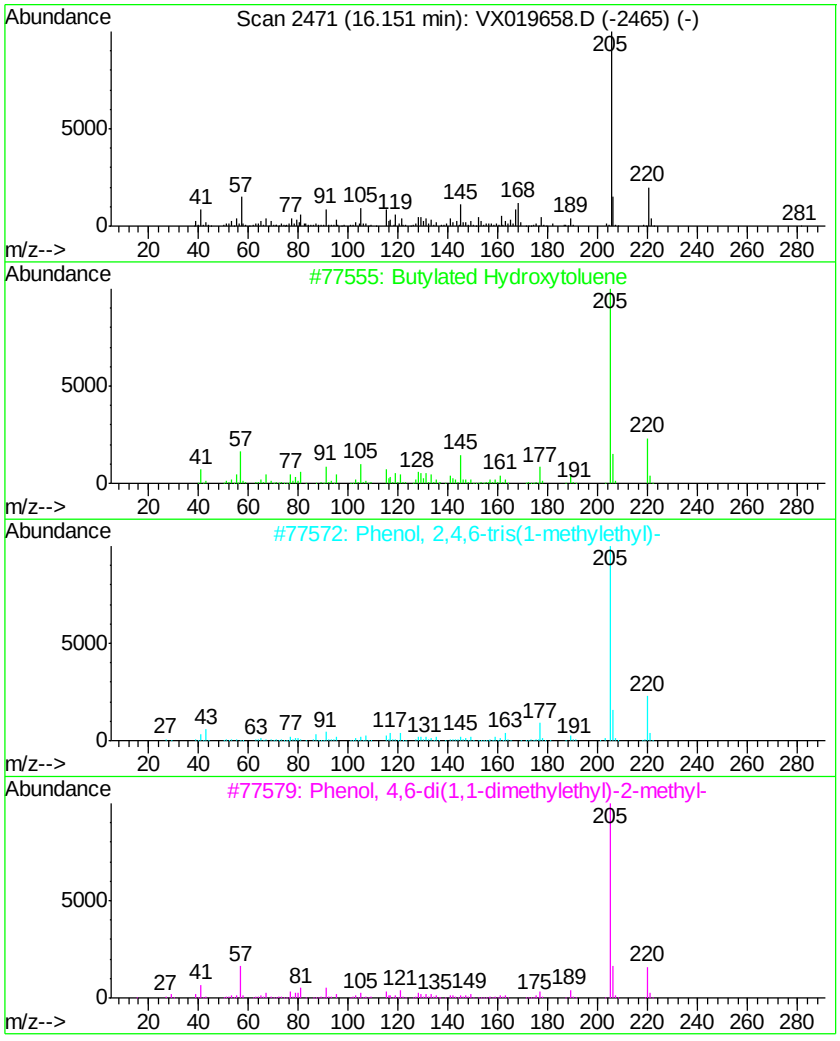
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

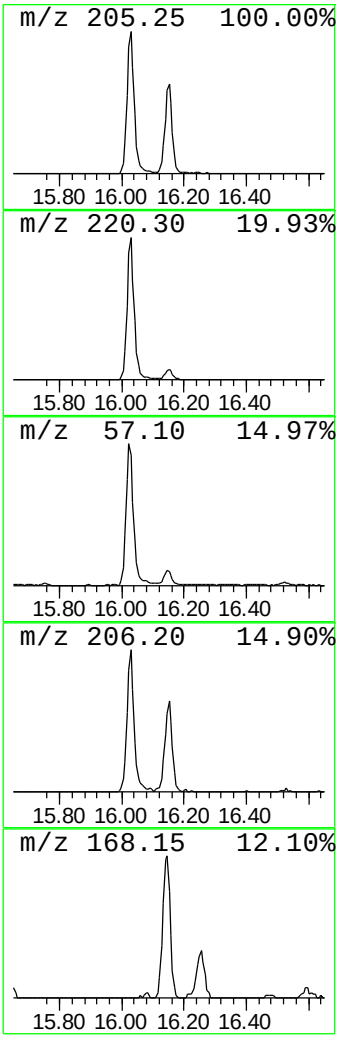
****

Peak Number 9 Butylated Hydroxytoluene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	7.84 ug/l	187513	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2	Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	76
3	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	76
4	Trimethyl-3,4-methylenedioxychro...	220	C13H16O3	1000378-97-7	53
5	Propanoic acid, 2-methyl-3-[4-t-...	220	C14H20O2	1000131-87-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112520\
Data File : VX019658.D
Acq On : 25 Nov 2020 15:55
Operator : JC/MD
Sample : L4841-03 5X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 16881

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.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
Acetaldehyde	1.47	58.0	ug/l	1012530	1	5.63	872841	50.0
1-Propanol	3.95	9.0	ug/l	157489	1	5.63	872841	50.0
2,3-Butanedione	4.45	6.6	ug/l	114471	1	5.63	872841	50.0
Propylene Glycol	9.60	15.7	ug/l	400976	3	10.09	1280830	50.0
1-Hexanol, 2-ethyl-	12.26	20.4	ug/l	486556	4	12.06	1195400	50.0
Naphthalene, 2-me...	14.68	6.7	ug/l	159356	4	12.06	1195400	50.0
2,5-Cyclohexadien...	16.02	101.9	ug/l	2435880	4	12.06	1195400	50.0
Butylated Hydroxy...	16.15	7.8	ug/l	187513	4	12.06	1195400	50.0