LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR061720WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.636	81	92	105	rBV2	129213	186273	14.63%	1.618%
2	1.771	128	134	142	rVB2	20090	26850	2.11%	0.233%
3	1.954	183	191	200	rBV	101511	129426	10.17%	1.124%
4	2.118	236	242	245	rBV3	14643	20153	1.58%	0.175%
5	2.610	385	395	408	rVB	276251	442854	34.79%	3.848%
6	4.552	976	999	1016	rBV4	34210	110612	8.69%	0.961%
7	4.797	1049	1075	1118	rBV	93399	459735	36.12%	3.994%
8	5.144	1166	1183	1199	rBV	190464	426189	33.48%	3.703%
9	5.797	1367	1386	1404	rBV2	422910	993773	78.07%	8.634%
10	6.311	1533	1546	1566	rVB	331961	609367	47.87%	5.294%
11	6.748	1670	1682	1700	rVV	241084	477237	37.49%	4.146%
12	6.944	1732	1743	1753	rBV4	9625	16666	1.31%	0.145%
13	7.227	1807	1831	1860	rBV	149842	327775	25.75%	2.848%
14	7.607	1935	1949	1969	rBV	125721	220144	17.29%	1.913%
15	7.848	2013	2024	2029	rBV3	14603	26212	2.06%	0.228%
16	7.890	2030	2037	2040	rVV3	18993	30077	2.36%	0.261%
17	7.935	2041	2051	2065	rVB	457730	776267	60.98%	6.744%
18	8.083	2087	2097	2108	rBV3	11178	18963	1.49%	0.165%
19	8.214	2123	2138	2150	rBV	85272	140977	11.07%	1.225%
20	8.530	2217	2236	2245	rBV4	15002	35385	2.78%	0.307%
21	8.587	2245	2254	2264	rBV8	9623	14807	1.16%	0.129%
22	8.674	2264	2281	2293	rBV	713205	1272964	100.00%	11.060%
23	8.819	2317	2326	2335	rVB3	22263	34952	2.75%	0.304%
24	9.443	2506	2520	2538	rBV	477854	795154	62.46%	6.908%
25	9.661	2570	2588	2597	rBV2	44965	77585	6.09%	0.674%
26	9.790	2613	2628	2646	rBV6	18648	44553	3.50%	0.387%
27	9.944	2664	2676	2687	rBV5	14928	25487	2.00%	0.221%
28	10.256	2759	2773	2781	rBV3	15464	25882	2.03%	0.225%
29	10.365	2796	2807	2820	rBV9	12416	24431	1.92%	0.212%
30	10.703	2905	2912	2923	rVB7	9559	16421	1.29%	0.143%
31	10.774	2923	2934	2950	rBV	217216	347596	27.31%	3.020%
32	10.906	2957	2975	2986	rBV9	9875	24459	1.92%	0.213%
33	10.983	2990	2999	3010	rVV2	11935	20278	1.59%	0.176%
34	11.066	3012	3025	3035	rVB10	6819	17099	1.34%	0.149%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR061720WMA.M
Title : TRACE VOA SOM01.0

35	11.481	3147	3154	3163	rBV8	9070	14483	1.14%	0.126%
36	11.587	3174	3187	3199	rBV2	28695	47007	3.69%	0.408%
37	11.700	3214	3222	3231	rVB4	30199	46392	3.64%	0.403%
38	11.825	3248	3261	3275	rVB	519488	816876	64.17%	7.097%
39	12.076	3324	3339	3359	rBV	93398	216980	17.05%	1.885%
40	12.205	3367	3379	3394	rVB	521378	825002	64.81%	7.168%
41	12.336	3412	3420	3427	rBV	13026	18869	1.48%	0.164%
42	12.793	3551	3562	3571	rBV2	63536	97442	7.65%	0.847%
43	12.906	3590	3597	3606	rVB3	22093	32746	2.57%	0.285%
44	13.166	3666	3678	3687	rVB5	6531	13591	1.07%	0.118%
45	14.015	3932	3942	3950	rBV6	14727	21830	1.71%	0.190%
46	14.227	3996	4008	4023	rBV	224468	350292	27.52%	3.043%
47	14.352	4039	4047	4061	rVB4	20075	33322	2.62%	0.290%
48	14.925	4216	4225	4234	rVB4	18841	29039	2.28%	0.252%
49	15.044	4254	4262	4270	rBV6	17521	26695	2.10%	0.232%
50	15.504	4396	4405	4417	rBV3	11119	16150	1.27%	0.140%
51	15.600	4426	4435	4440	rBV7	9591	14195	1.12%	0.123%
52	15.639	4441	4447	4456	rVV4	11968	18879	1.48%	0.164%
53	15.745	4470	4480	4493	rVB5	30039	56939	4.47%	0.495%
54	16.195	4607	4620	4631	rBV3	53359	87923	6.91%	0.764%
55	16.413	4679	4688	4697	rVB6	14514	22243	1.75%	0.193%
56	16.838	4810	4820	4831	rBV2	110590	178451	14.02%	1.550%
57	16.960	4847	4858	4871	rBV2	175764	307894	24.19%	2.675%

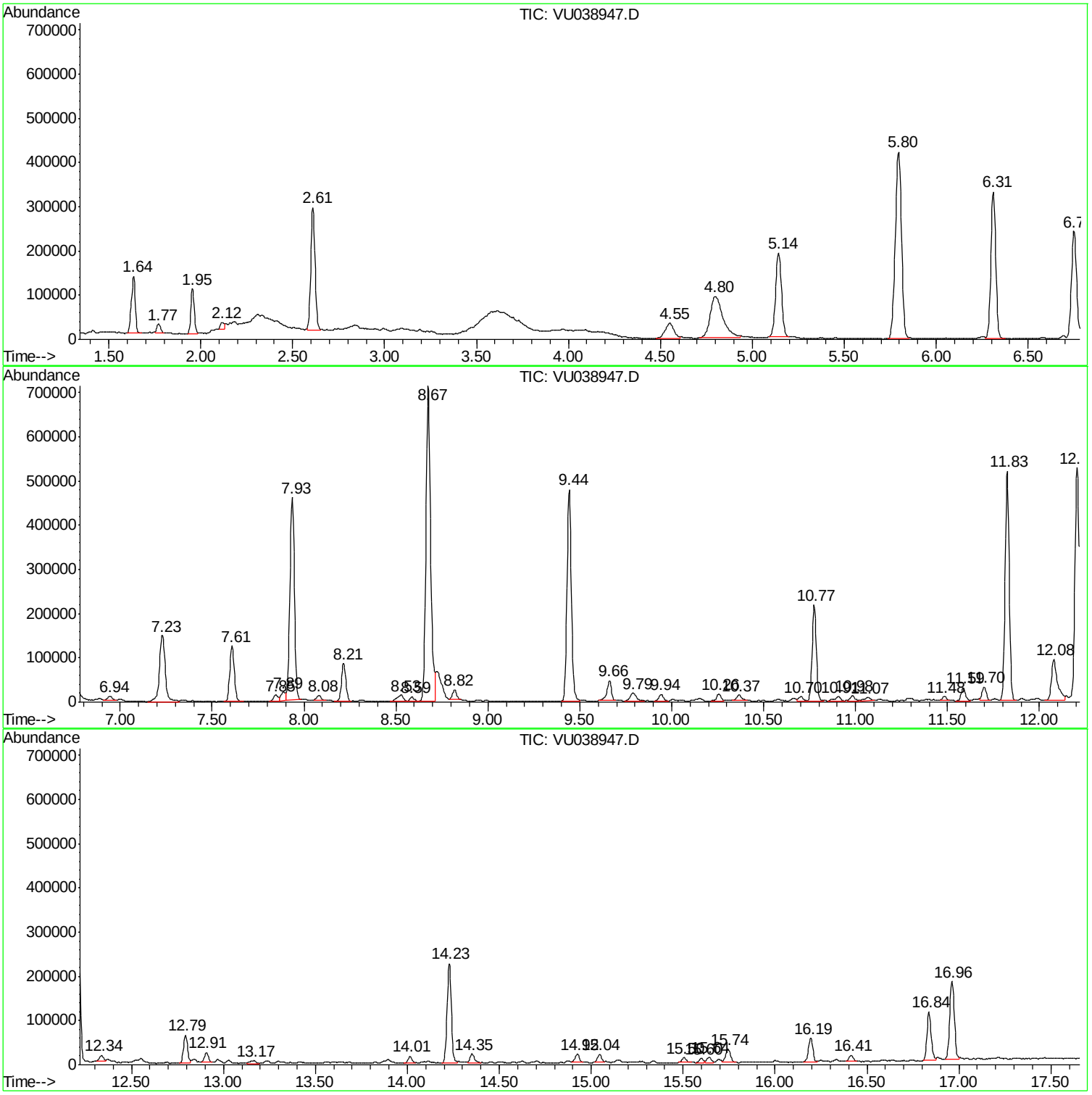
Sum of corrected areas: 11509843

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

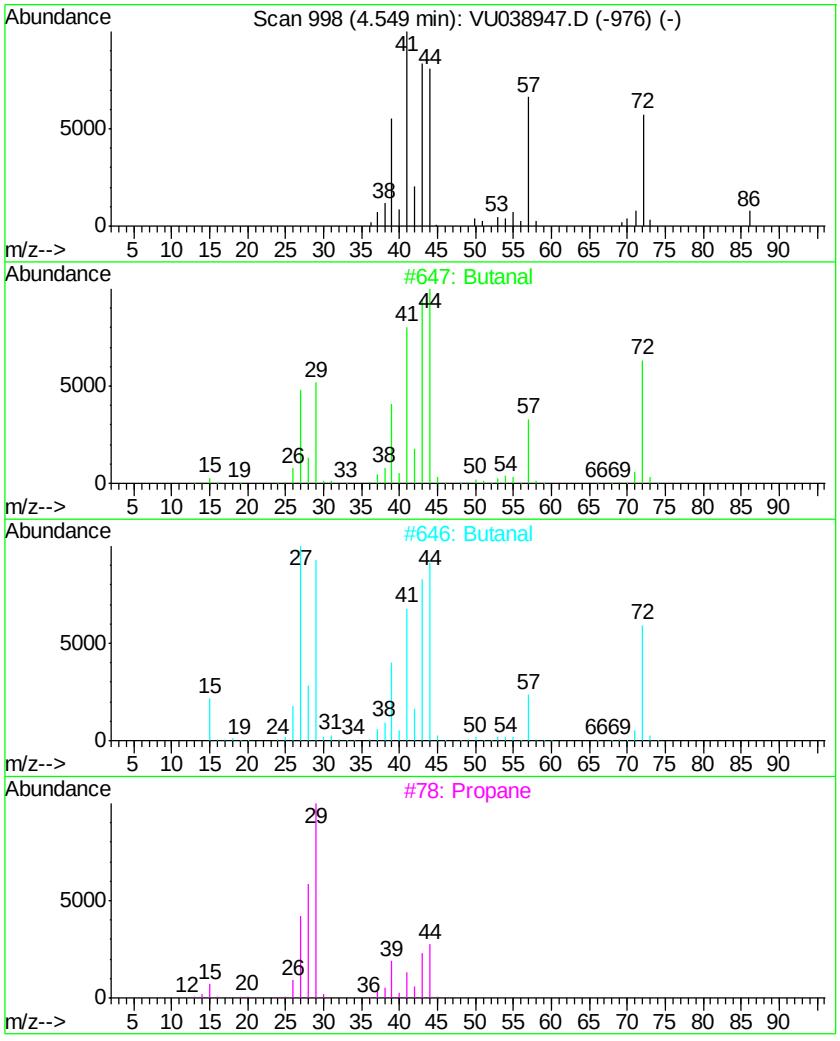
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

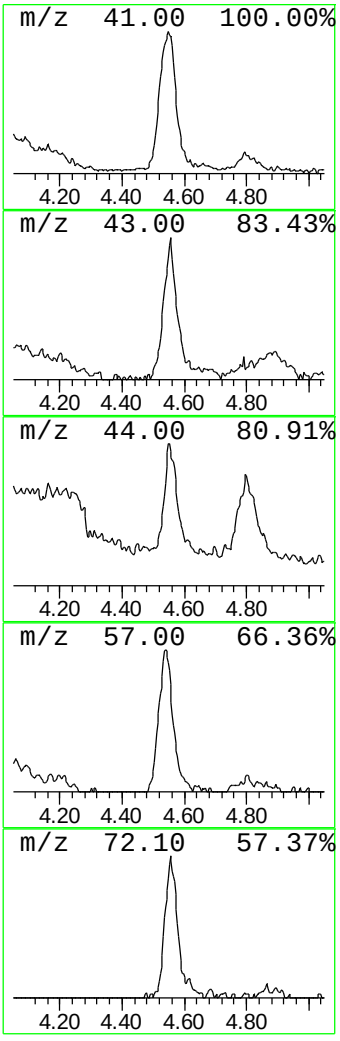
****

Peak Number 1 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	0.91 ug/L	110612	1,4-Difluorobenzene	6.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	81
2	Butanal	72	C4H8O	000123-72-8	53
3	Propane	44	C3H8	000074-98-6	43
4	Propane	44	C3H8	000074-98-6	40
5	Butanal	72	C4H8O	000123-72-8	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

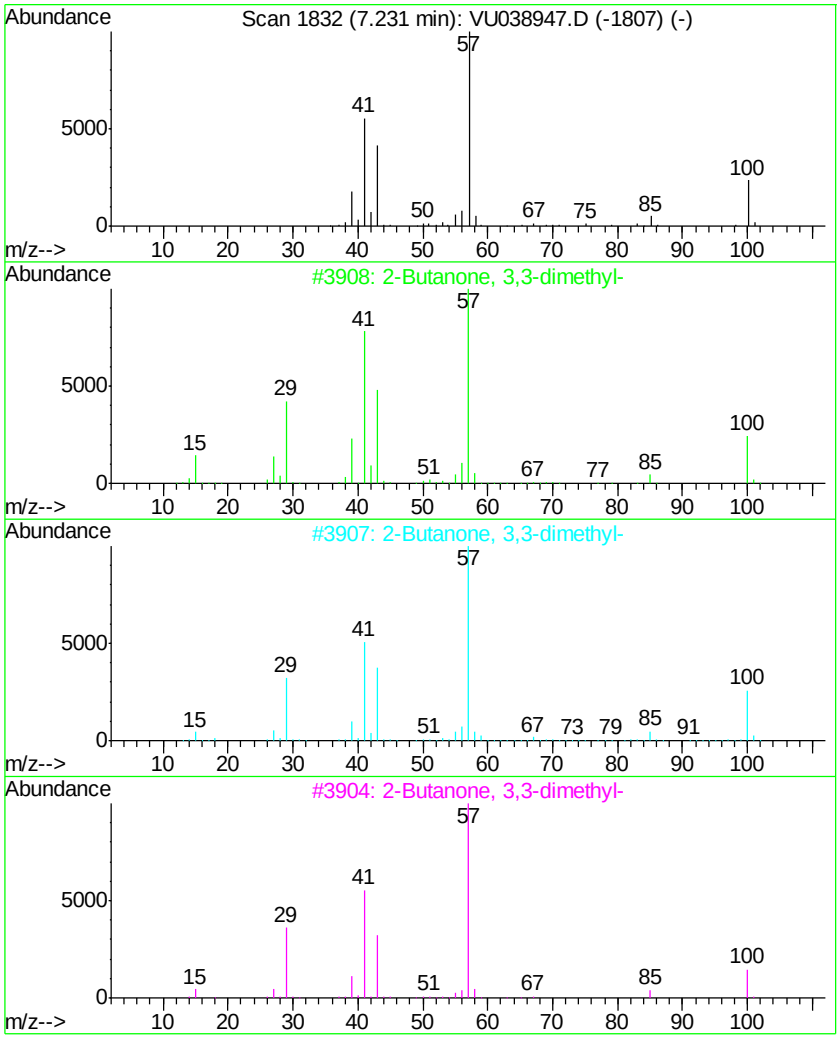
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

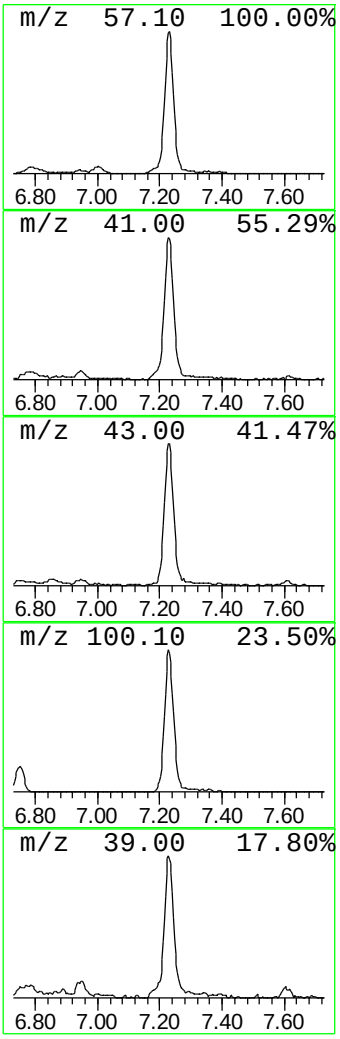
****

Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	2.69 ug/L	327775	1,4-Difluorobenzene	6.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	91
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	87
3	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	72
4	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64
5	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

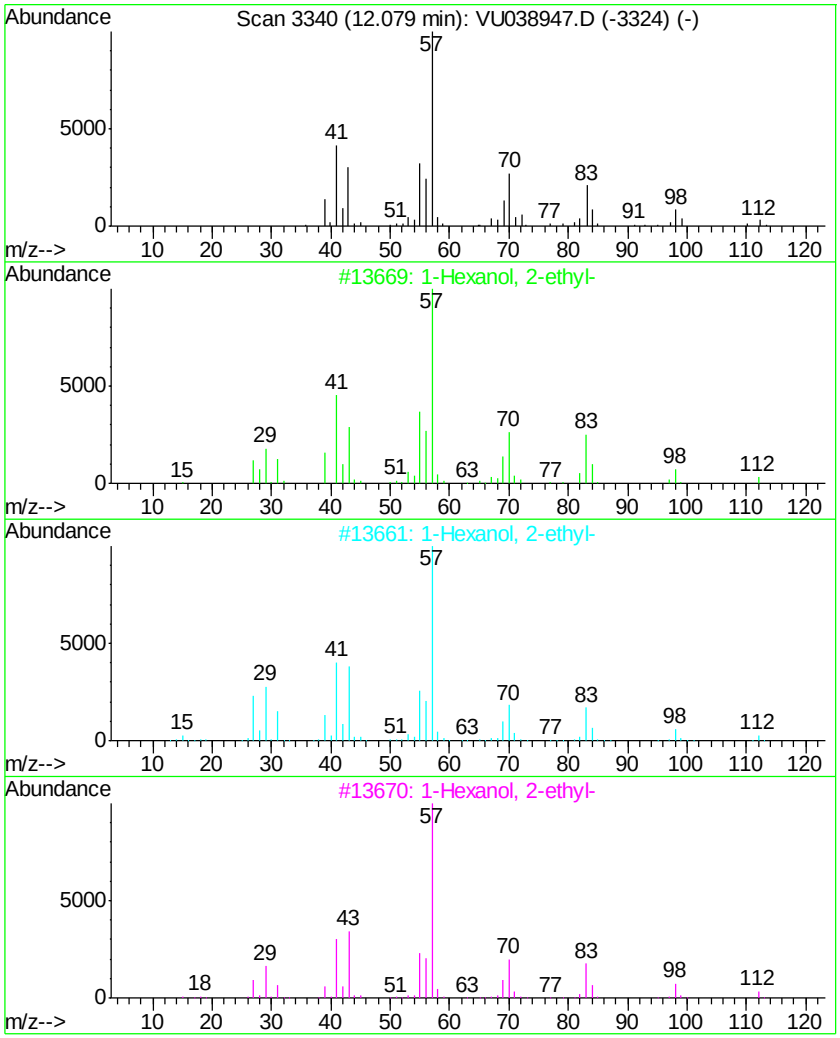
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

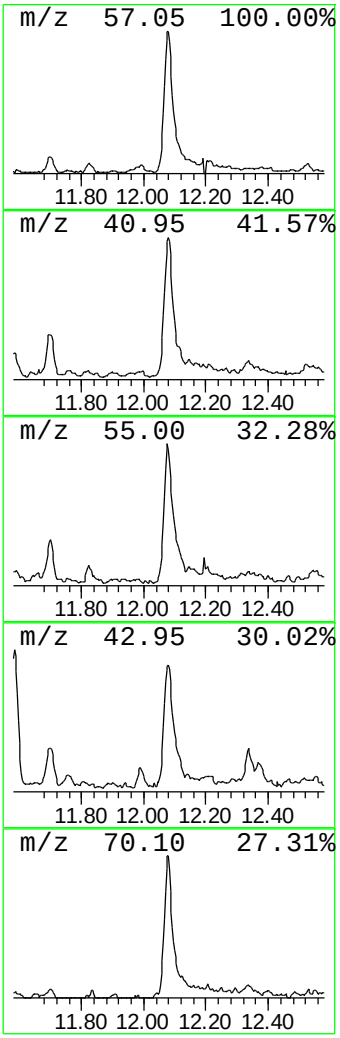
****

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	1.33 ug/L	216980	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

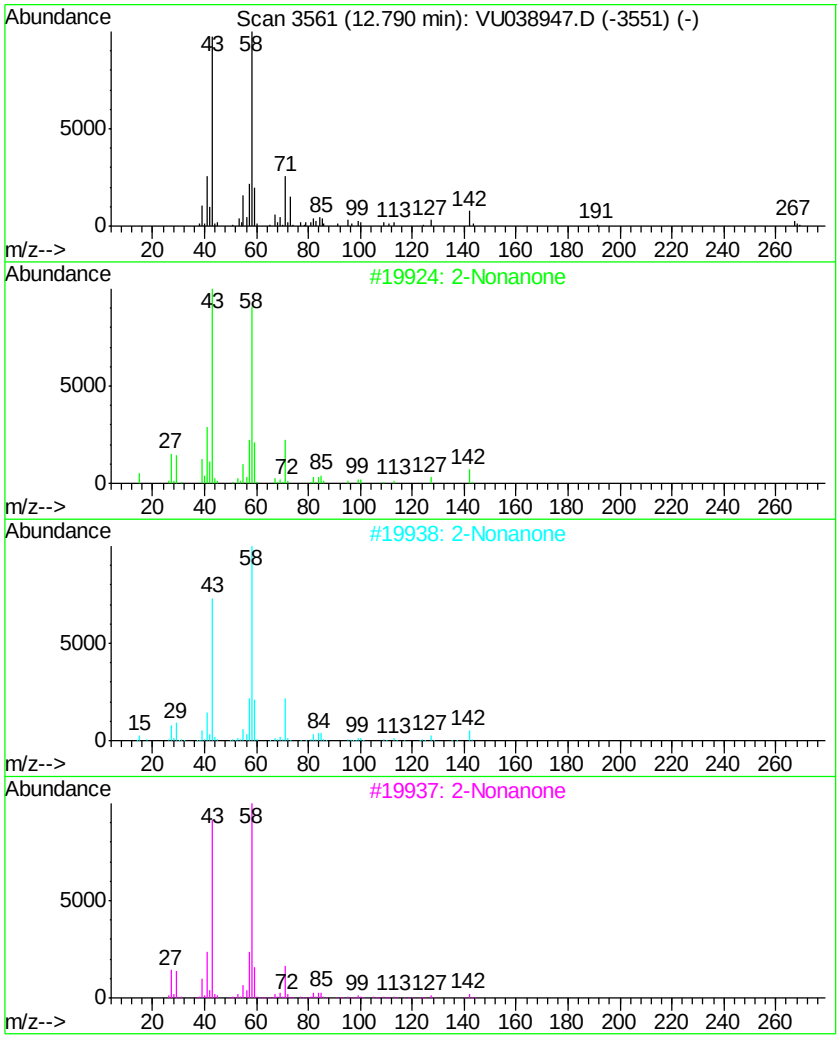
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

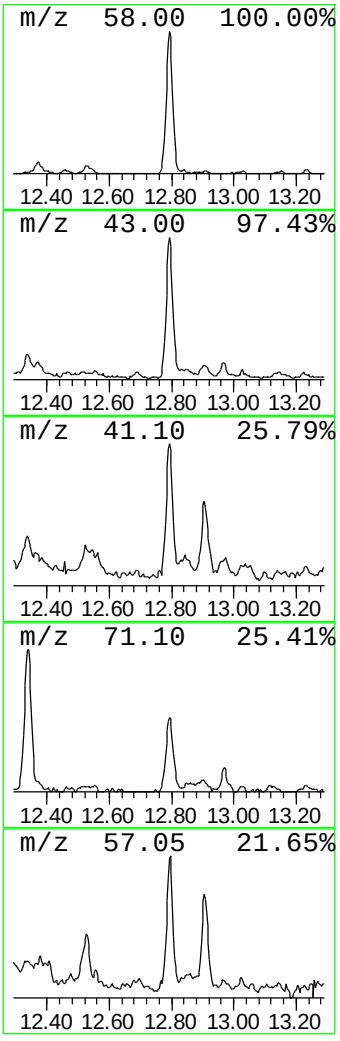
****

Peak Number 5 2-Nonanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	0.60 ug/L	97442	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	94
2	2-Nonanone	142	C9H18O	000821-55-6	93
3	2-Nonanone	142	C9H18O	000821-55-6	87
4	2-Nonanone	142	C9H18O	000821-55-6	68
5	2-Octanone	128	C8H16O	000111-13-7	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

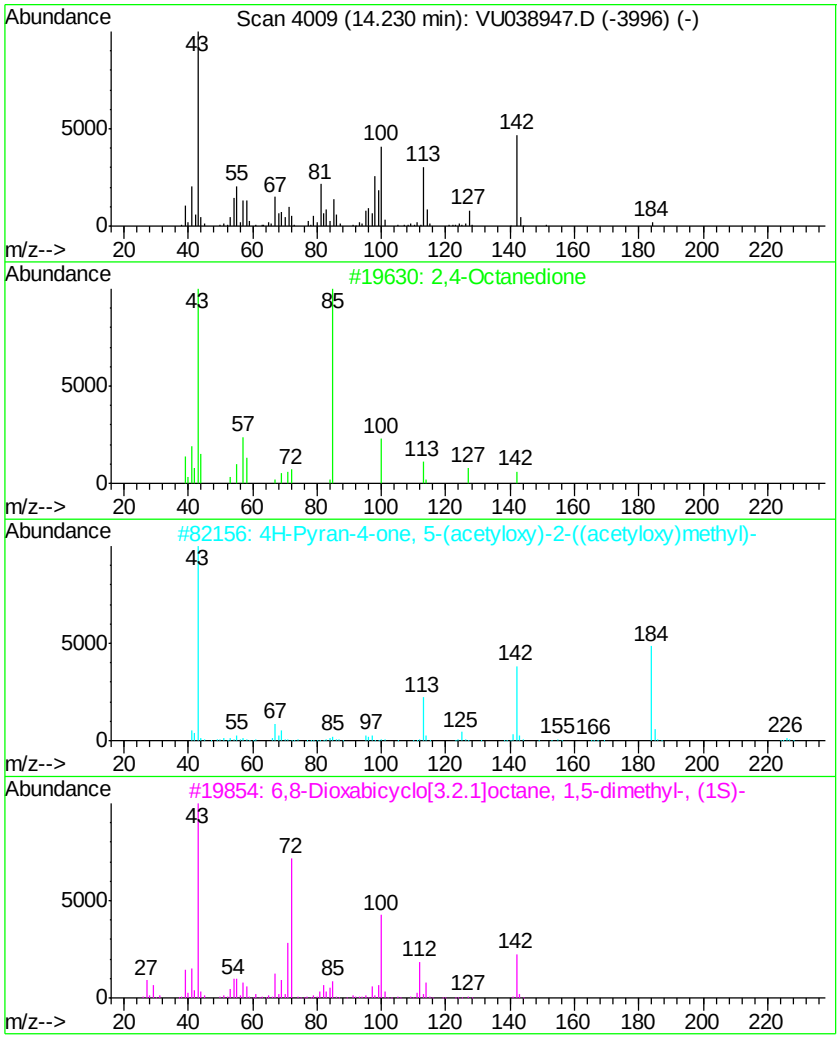
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

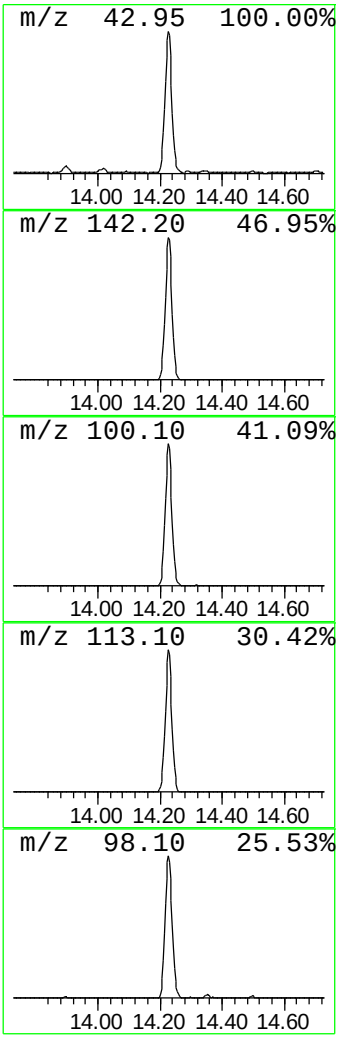
****

Peak Number 6 2,4-Octanedione Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	2.14 ug/L	350292	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Octanedione	142	C8H14O2	014090-87-0	50
2	4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	35
3	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	35
4	Acetamide, N-(4-amino-3-furazanyl)-	142	C4H6N4O2	140706-47-4	23
5	3-n-Propyl-5-methylhexan-2-one	156	C10H20O	1000202-22-8	12





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

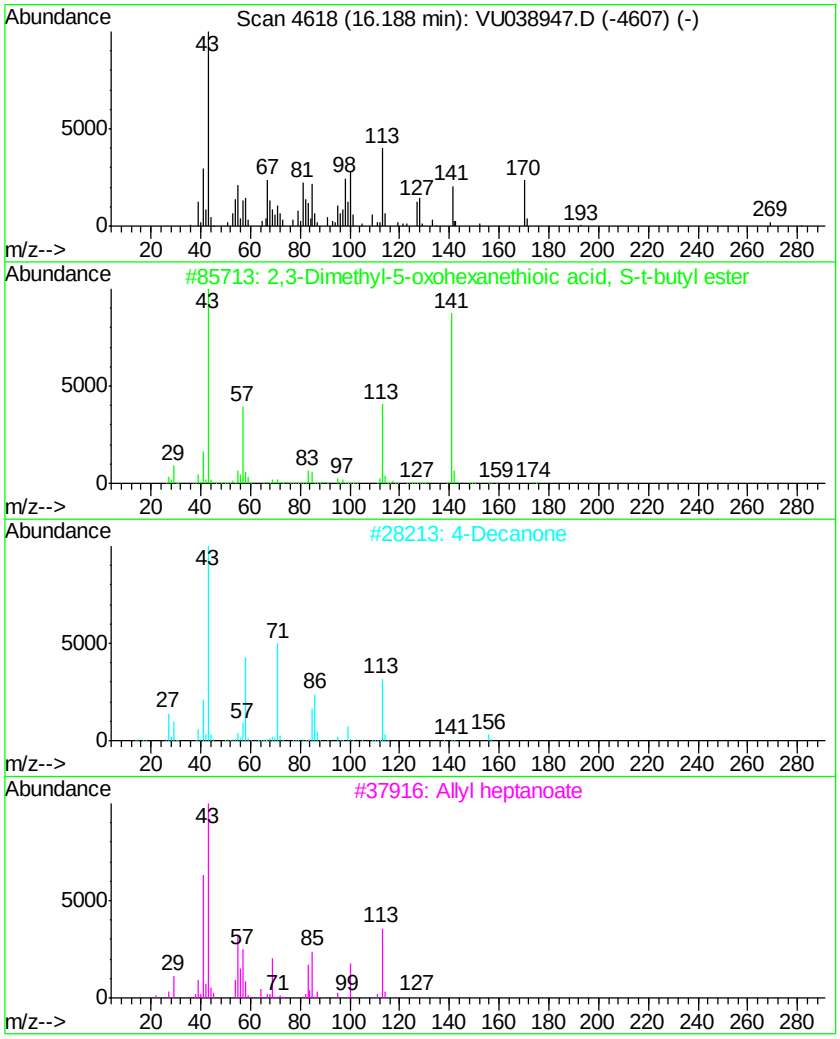
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

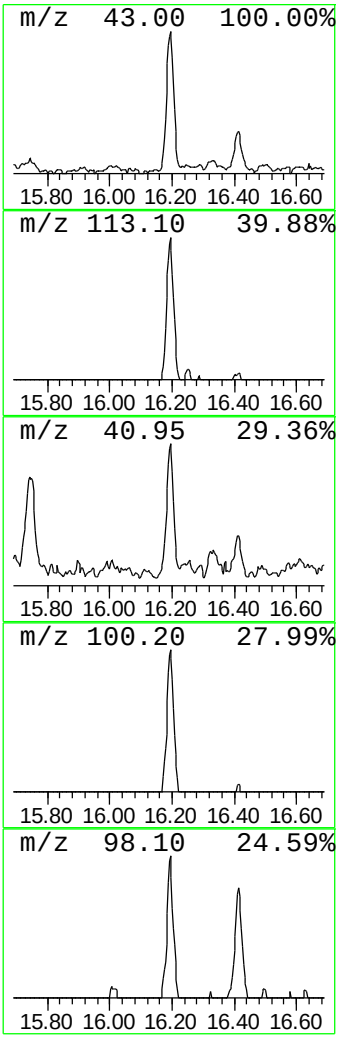
****

Peak Number 7 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	0.54 ug/L	87923	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethyl-5-oxohexanethioic a...	230	C12H22O2S	1000186-90-3	22
2	4-Decanone	156	C10H20O	000624-16-8	16
3	Allyl heptanoate	170	C10H18O2	000142-19-8	16
4	3,4-Diethoxy-3-cyclobutene-1,2-d...	170	C8H10O4	005231-87-8	16
5	1-Acetyl-5,5-dimethyl-2,4-dioxoi...	170	C7H10N2O3	006341-67-9	16





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

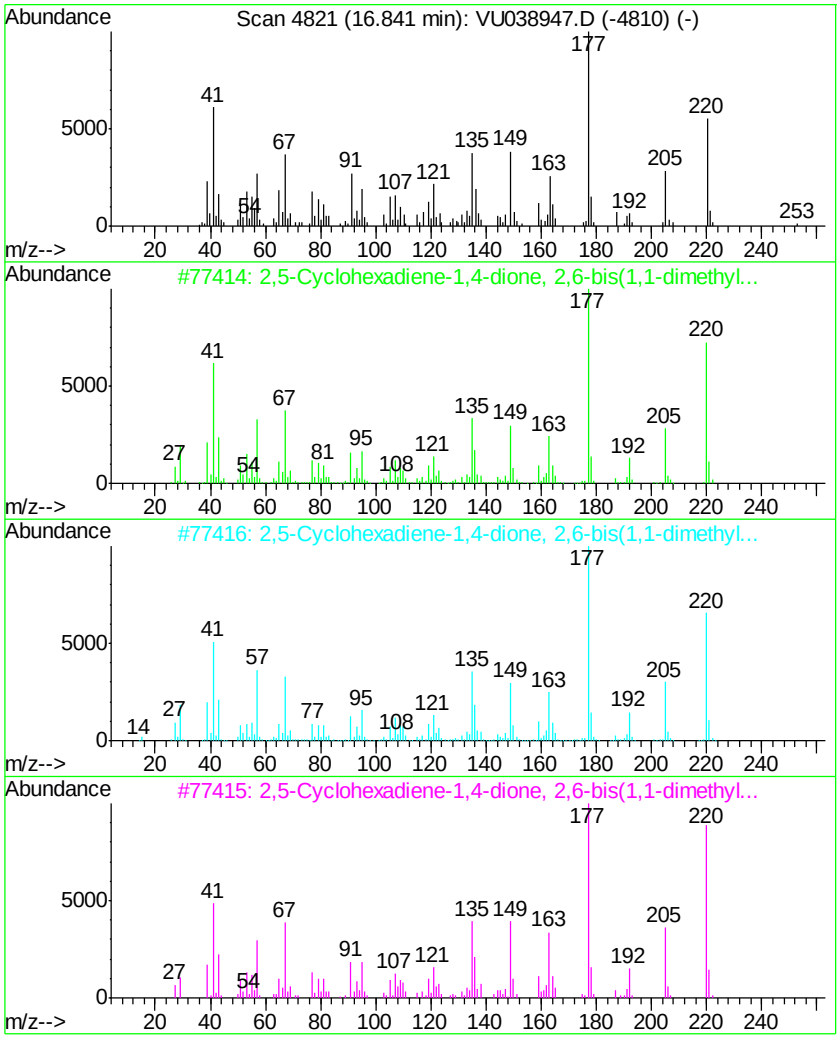
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

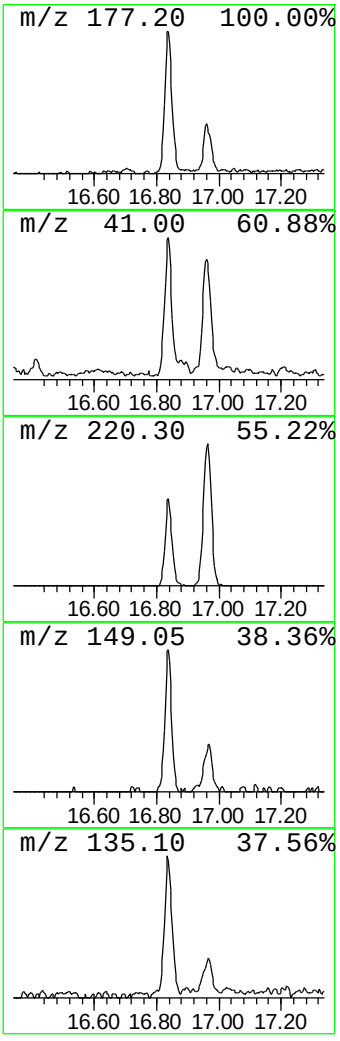
****

Peak Number 8 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	1.09 ug/L	178451	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	90
4	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	43
5	2H-1-Benzopyran, 3,5,6,8a-tetrah...	192	C13H20O	041678-29-9	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

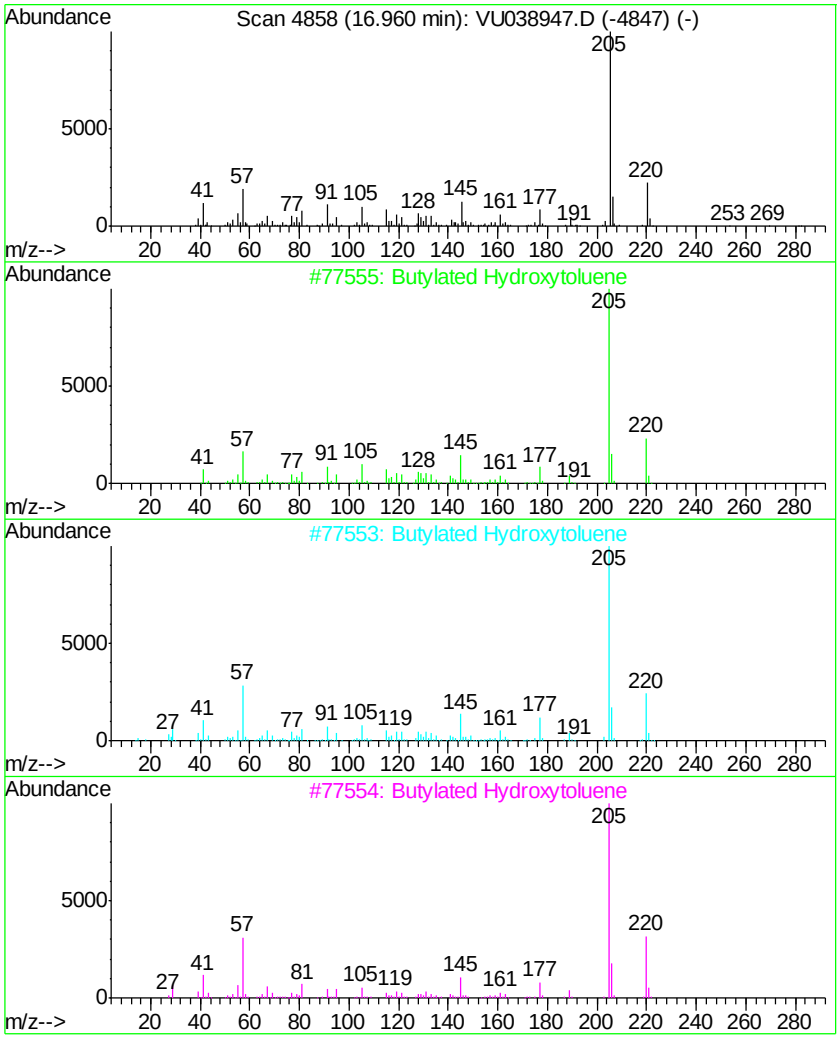
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

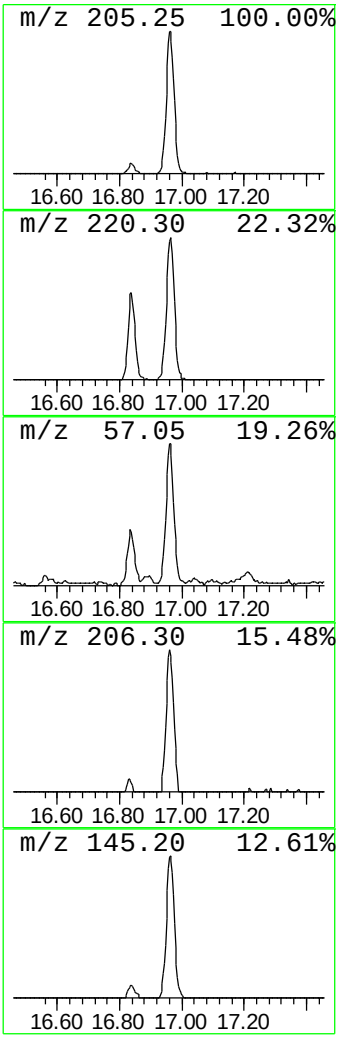
****

Peak Number 9 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	1.88 ug/L	307894	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038947.D
Acq On : 17 Jun 2020 16:30
Operator : SY/MD
Sample : L3040-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L10

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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	4.55	0.9	ug/L	110612	1	6.31	609367	5.0
2-Butanone, 3,3-d...	7.23	2.7	ug/L	327775	1	6.31	609367	5.0
1-Hexanol, 2-ethyl-	12.08	1.3	ug/L	216980	3	11.83	816876	5.0
2-Nonanone	12.79	0.6	ug/L	97442	3	11.83	816876	5.0
2,4-Octanedione	14.23	2.1	ug/L	350292	3	11.83	816876	5.0
unknown-01	16.19	0.5	ug/L	87923	3	11.83	816876	5.0
2,5-Cyclohexadien...	16.84	1.1	ug/L	178451	3	11.83	816876	5.0
Butylated Hydroxy...	16.96	1.9	ug/L	307894	3	11.83	816876	5.0