LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

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_U\Method\82U052622W.M
Title : SW846 8260

Signal : TIC: VU048717.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	70	81	91	rBV	69160	92967	1.08%	0.363%
2	1.996	194	204	218	rVB	100547	138691	1.60%	0.541%
3	3.170	550	569	601	rBV	484303	1107224	12.81%	4.318%
4	3.363	609	629	665	rBV	3818443	8642058	100.00%	33.702%
5	3.993	809	825	845	rBV3	35418	91500	1.06%	0.357%
6	5.292	1213	1229	1242	rBV	215058	458893	5.31%	1.790%
7	5.375	1242	1255	1277	rVB	327726	699175	8.09%	2.727%
8	5.703	1342	1357	1368	rBV	220873	449651	5.20%	1.754%
9	5.777	1368	1380	1384	rVV	385532	722694	8.36%	2.818%
10	5.819	1384	1393	1422	rVB	1342279	2984461	34.53%	11.639%
11	6.250	1513	1527	1552	rBV	471666	916456	10.60%	3.574%
12	7.163	1798	1811	1834	rBV2	114013	218463	2.53%	0.852%
13	7.623	1941	1954	1965	rBV	295275	567884	6.57%	2.215%
14	7.687	1965	1974	2001	rVB	158577	348227	4.03%	1.358%
15	7.899	2021	2040	2052	rBV	665654	1167972	13.51%	4.555%
16	7.970	2052	2062	2073	rVV	200994	348417	4.03%	1.359%
17	8.038	2073	2083	2114	rVV	302740	599465	6.94%	2.338%
18	8.266	2143	2154	2166	rVB	53382	91715	1.06%	0.358%
19	8.716	2275	2294	2309	rBV	320854	627988	7.27%	2.449%
20	8.825	2312	2328	2355	rVB5	52381	127093	1.47%	0.496%
21	9.340	2475	2488	2501	rBV3	82352	184416	2.13%	0.719%
22	9.417	2501	2512	2527	rVV	681961	1201805	13.91%	4.687%
23	9.488	2527	2534	2550	rVB2	67439	141557	1.64%	0.552%
24	9.571	2550	2560	2570	rBV	126610	213678	2.47%	0.833%
25	9.693	2587	2598	2609	rBV	271962	456072	5.28%	1.779%
26	10.102	2711	2725	2740	rBV	217185	359477	4.16%	1.402%
27	10.542	2852	2862	2878	rVB2	86920	152874	1.77%	0.596%
28	10.632	2878	2890	2909	rBV	626946	1046607	12.11%	4.082%
29	10.722	2909	2918	2938	rVB4	36412	94204	1.09%	0.367%
30	11.468	3140	3150	3163	rVB2	56336	91857	1.06%	0.358%
31	11.812	3244	3257	3274	rBV	804255	1298785	15.03%	5.065%

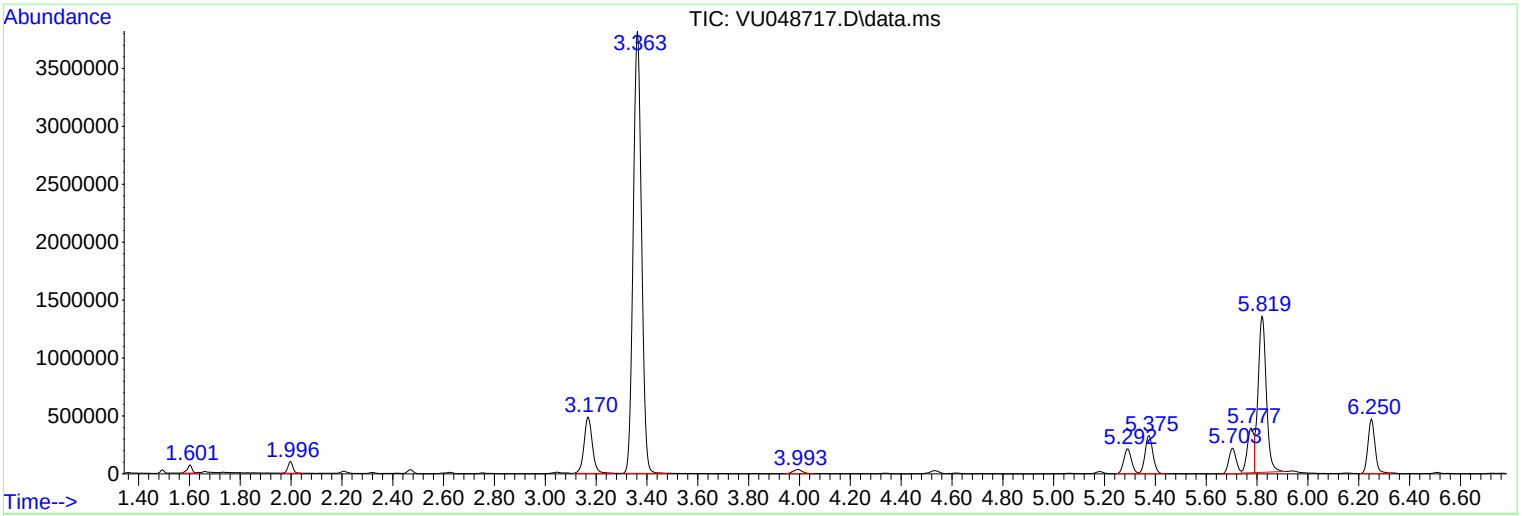
Sum of corrected areas: 25642326

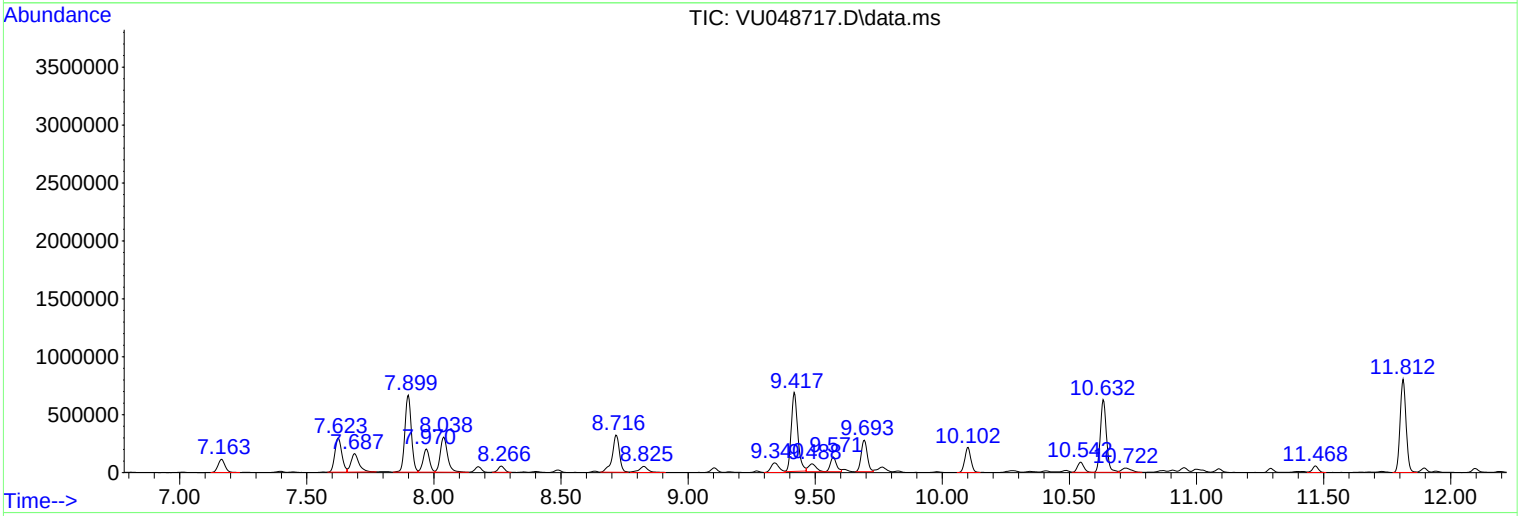
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

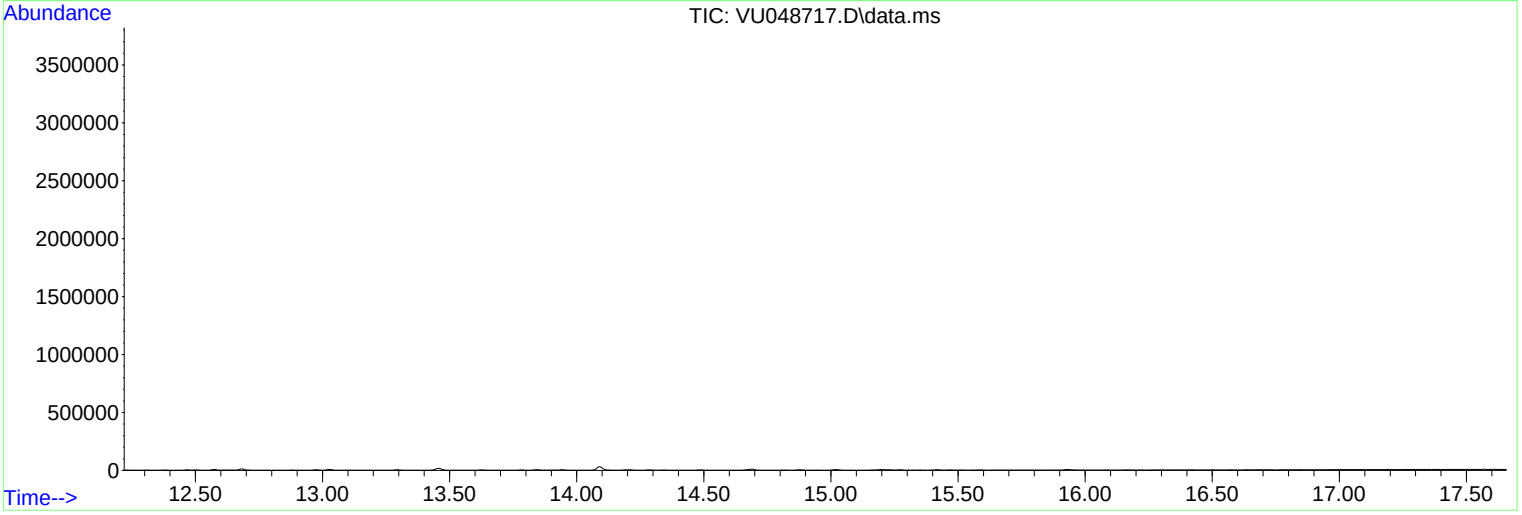
Instrument :
MSVOA_U
ClientSampleId :
TW-17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

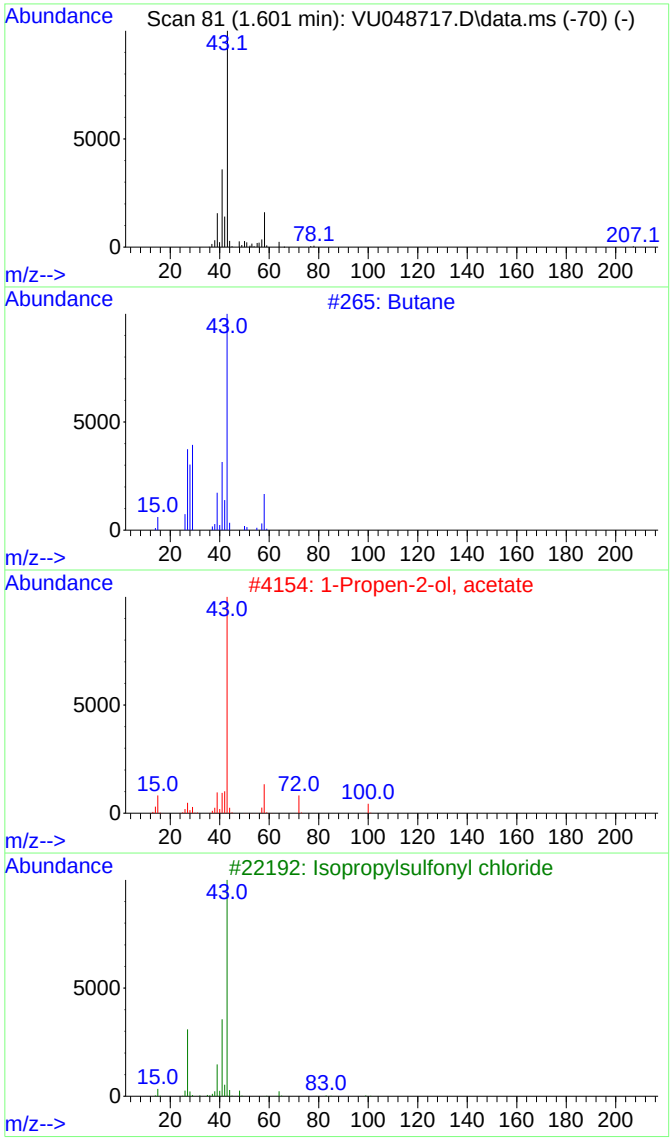
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

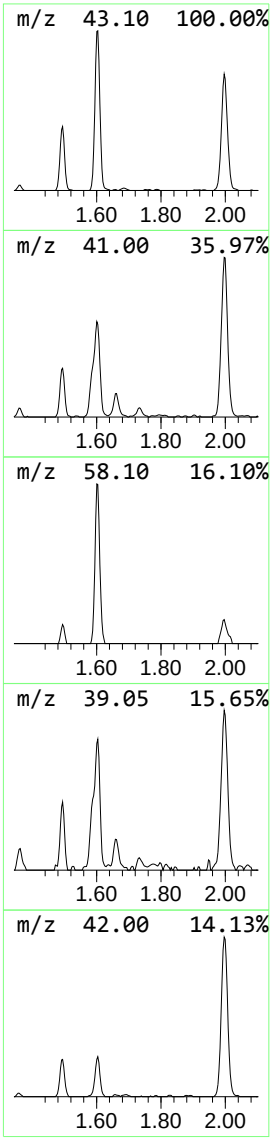
****

Peak Number 1 Butane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.601	6.65 ug/l	92967	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	50
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	37
4	Acetone	58	C3H6O	000067-64-1	9
5	1-Propanesulfonyl chloride	142	C3H7ClO2S	010147-36-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

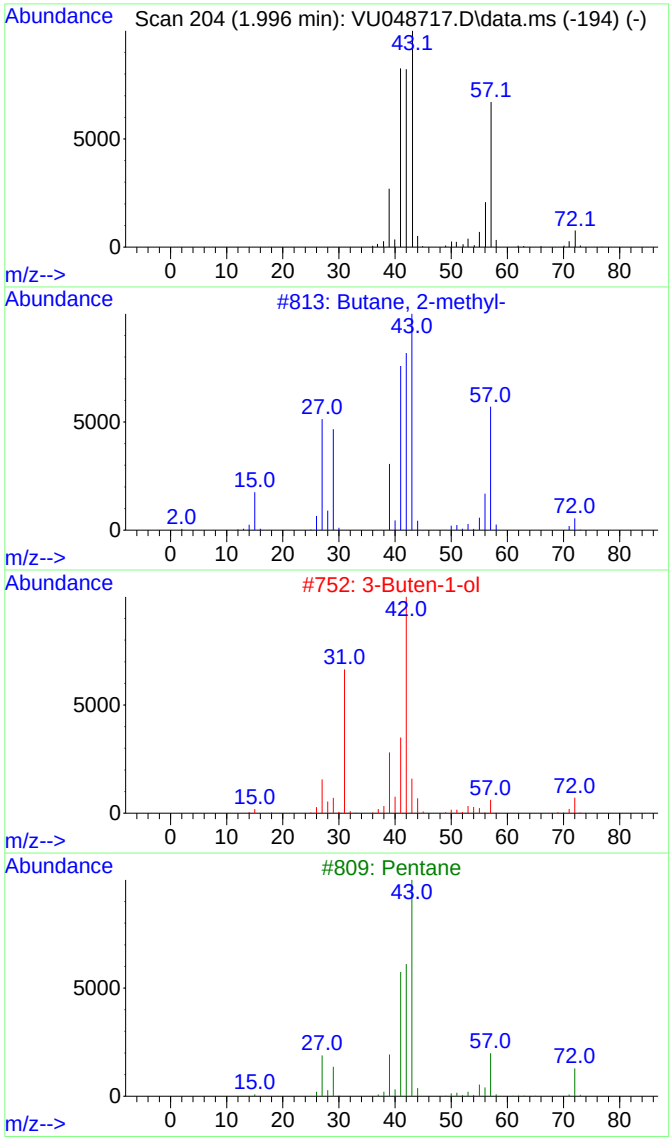
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

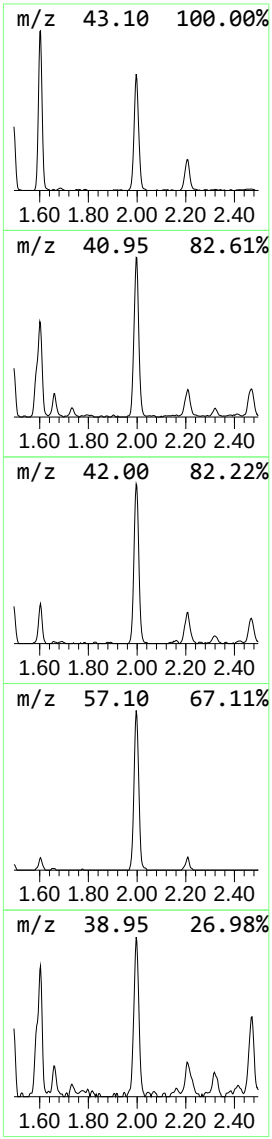
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.996	9.92 ug/l	138691	Pentafluorobenzene	5.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	49
3	Pentane	72	C5H12	000109-66-0	42
4	1-Butene	56	C4H8	000106-98-9	10
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

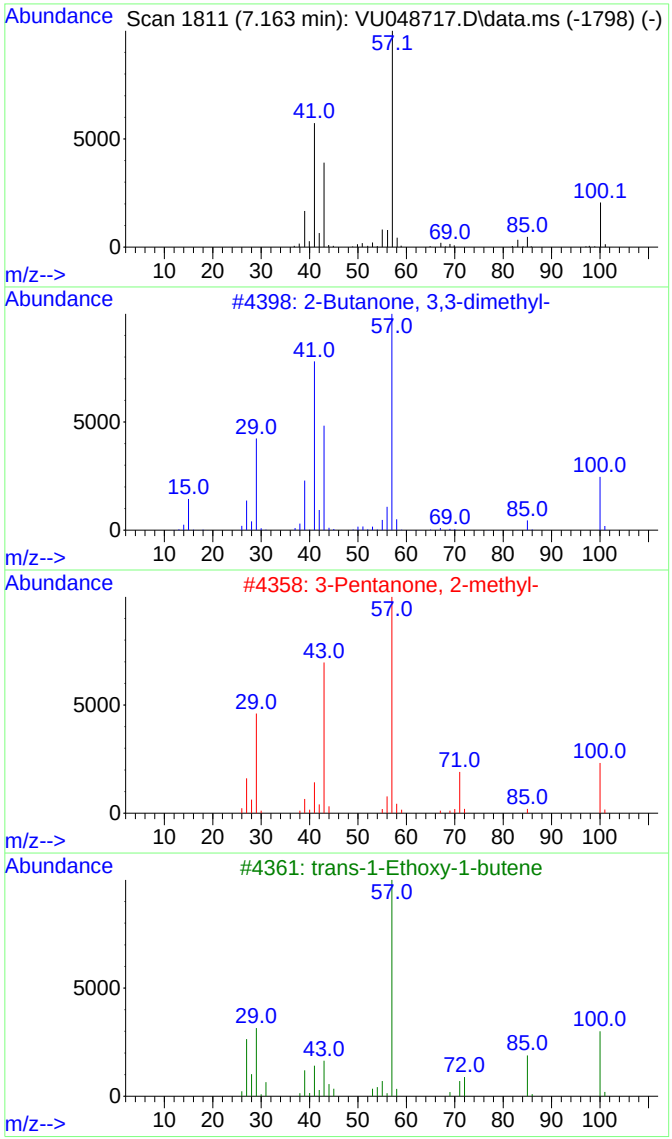
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

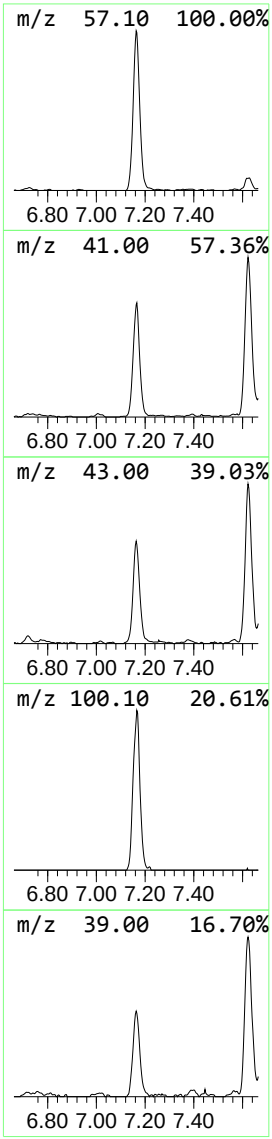
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.163	11.92 ug/l	218463	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	90
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72
3	trans-1-Ethoxy-1-butene	100	C6H12O	1000139-43-9	40
4	cis-1-Ethoxy-1-butene	100	C6H12O	1000139-43-8	40
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

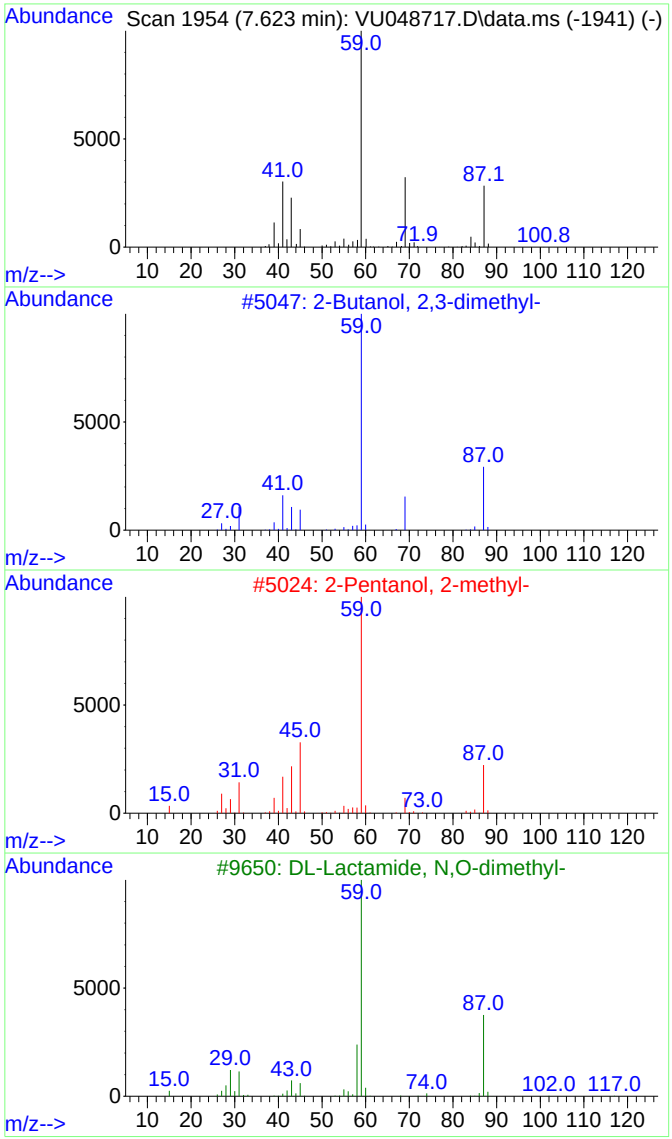
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

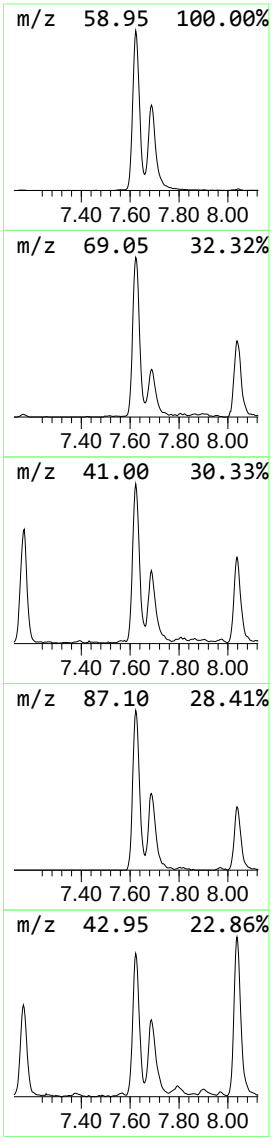
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butanol, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.623	30.98 ug/l	567884	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
3	DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	56
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	56
5	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

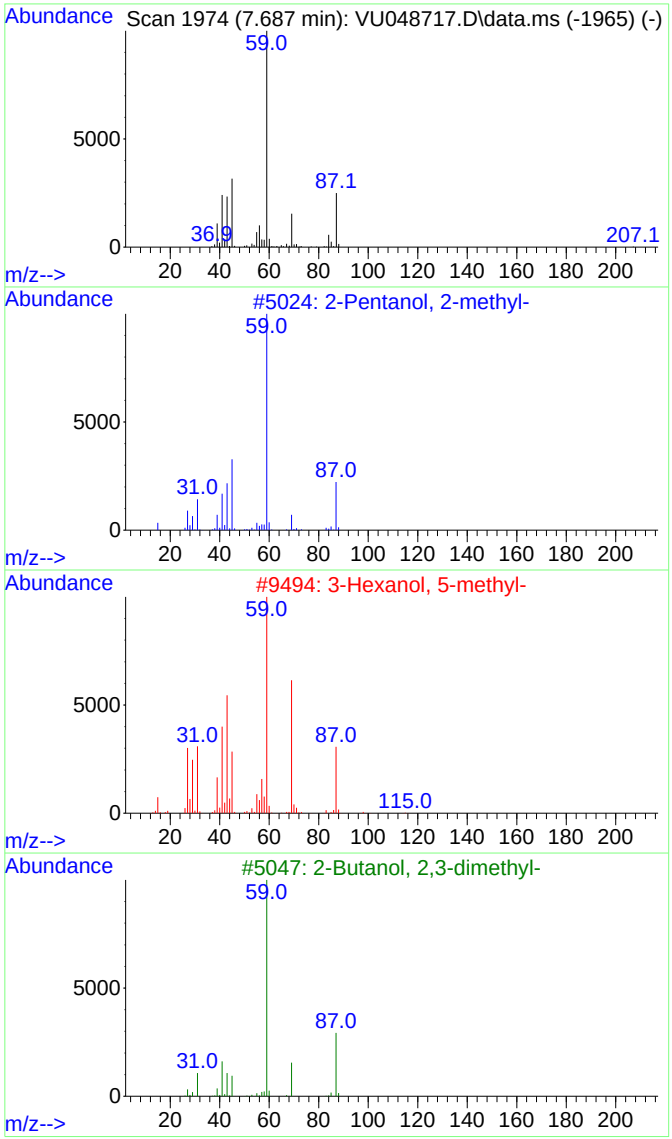
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

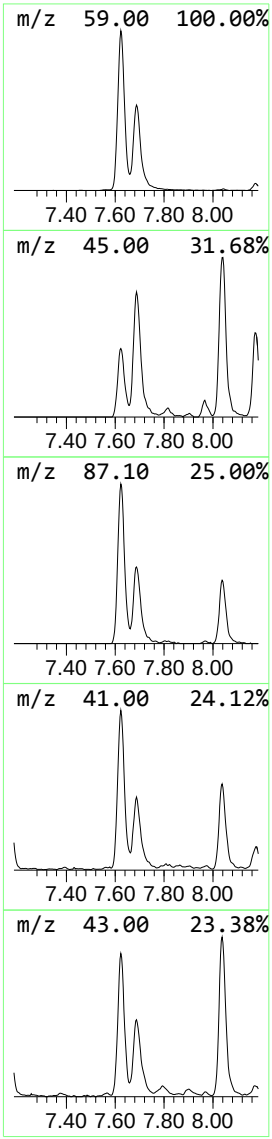
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.687	19.00 ug/l	348227	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
2	3-Hexanol, 5-methyl-	116	C7H16O	000623-55-2	72
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	59
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

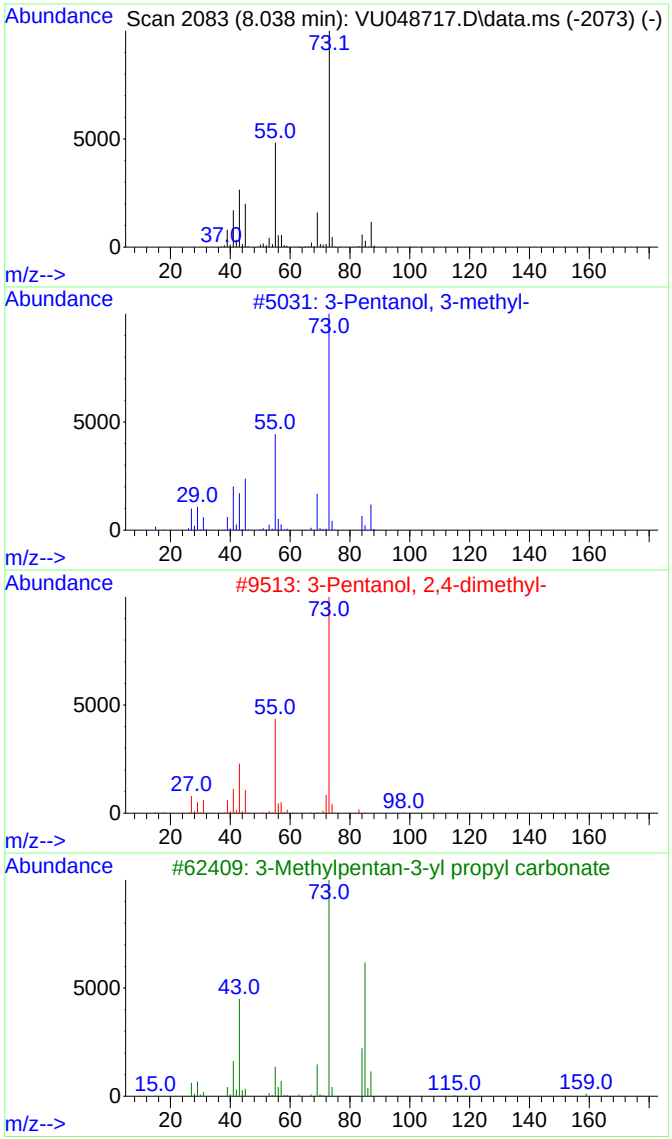
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

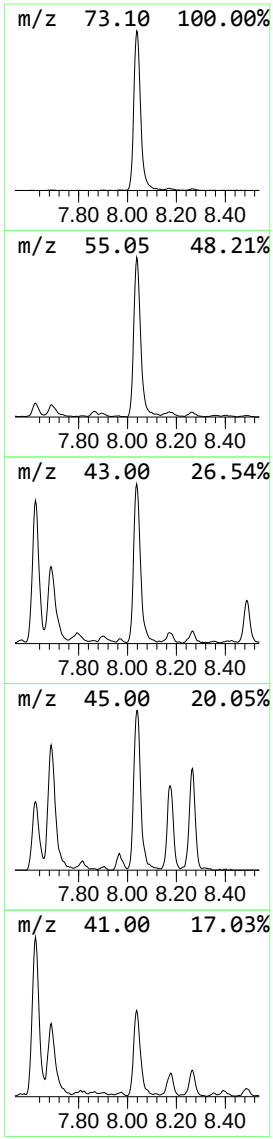
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanol, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.038	24.94 ug/l	599465	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	90
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	3-Methylpentan-3-yl propyl carbo...	188	C10H20O3	1000372-82-3	28
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

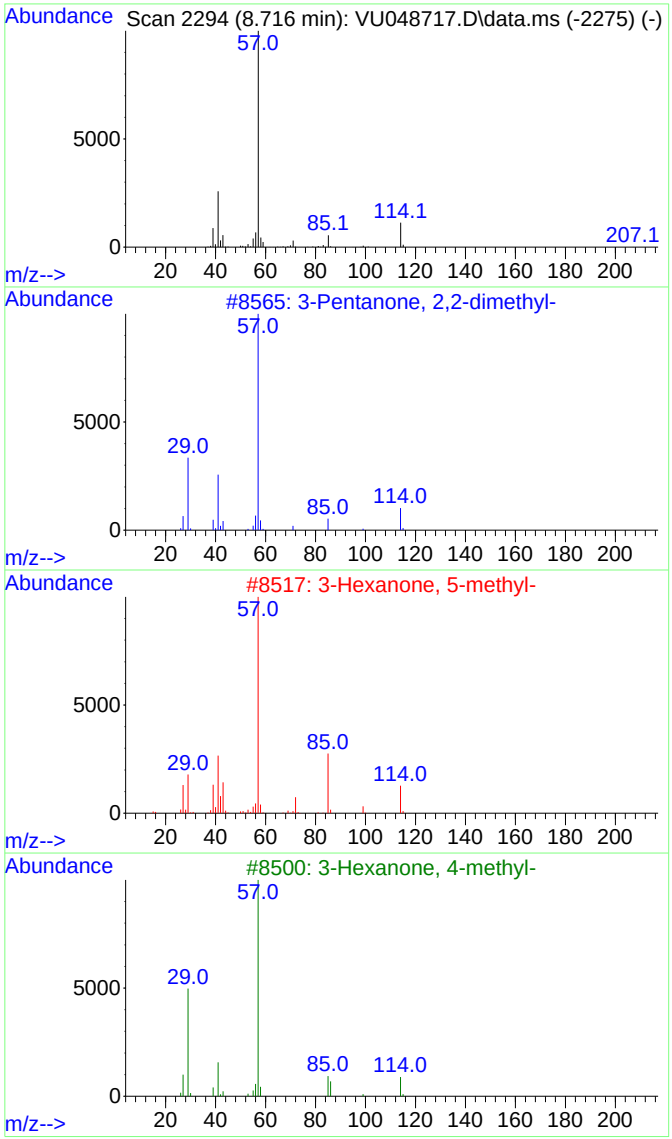
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

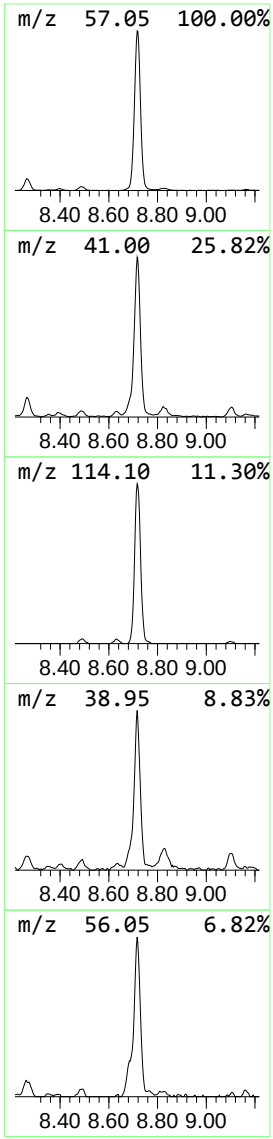
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Pentanone, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.716	26.13 ug/l	627988	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	83
2	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	59
3	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	59
4	3,4-Hexanedione	114	C6H10O2	004437-51-8	58
5	3-Heptanone	114	C7H14O	000106-35-4	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

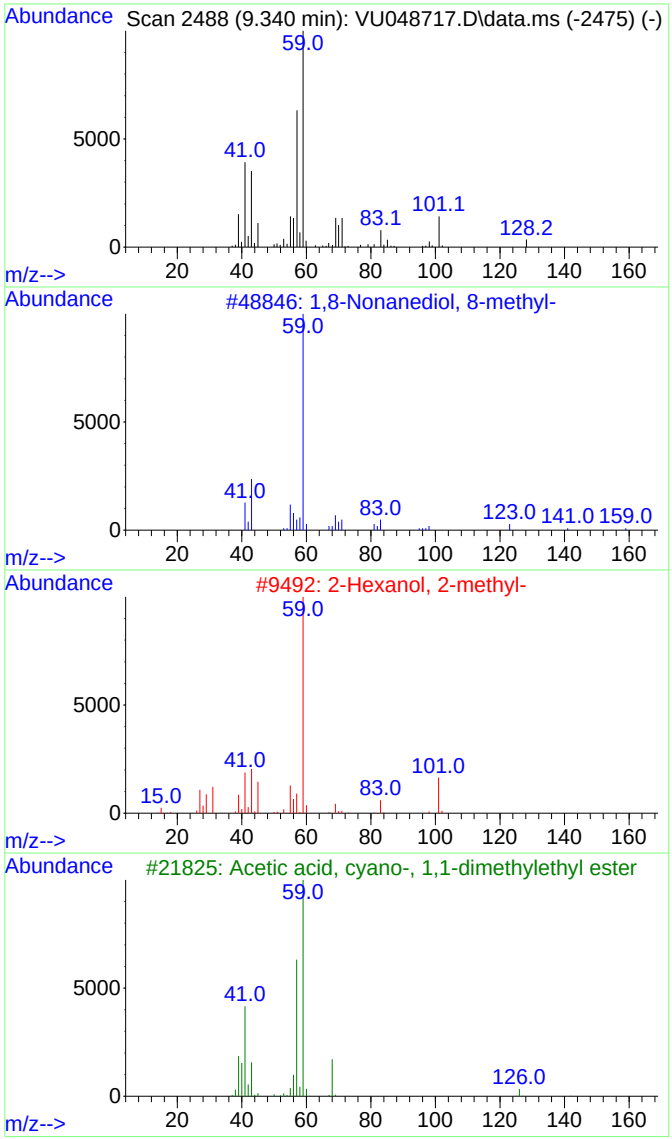
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

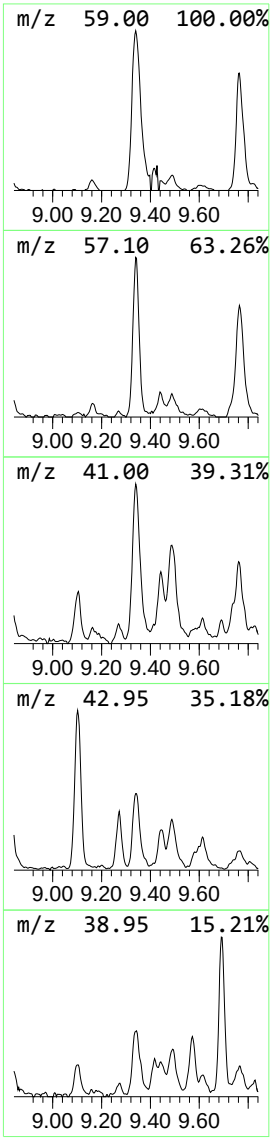
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,8-Nonanediol, 8-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.340	7.67 ug/l	184416	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	50
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	50
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

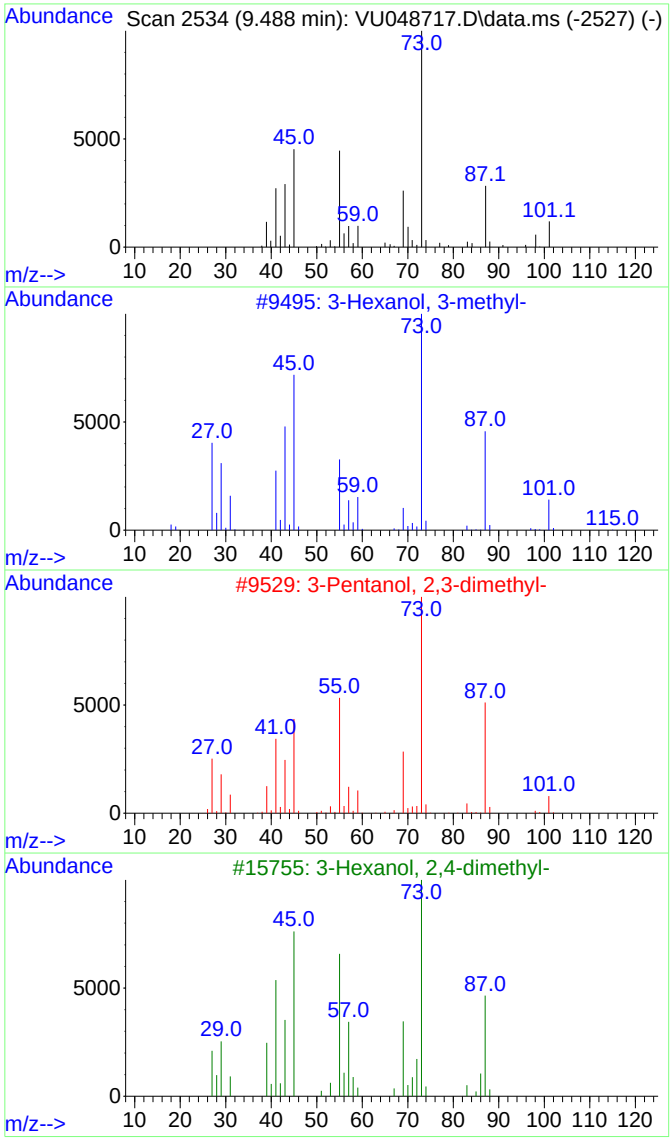
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

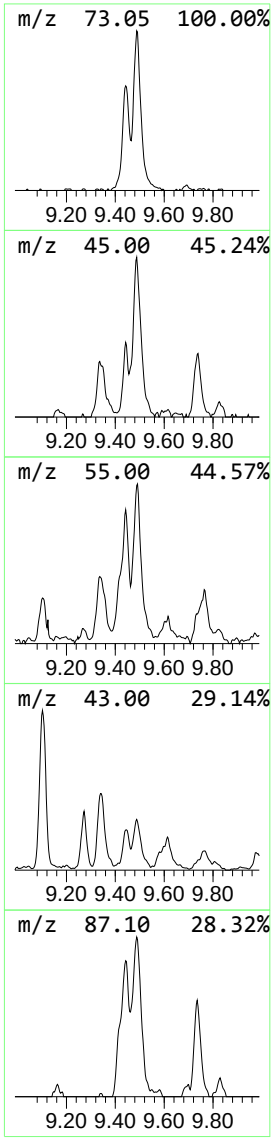
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 3-Hexanol, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	5.89 ug/l	141557	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	59
2	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	50
3	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	28
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	17
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

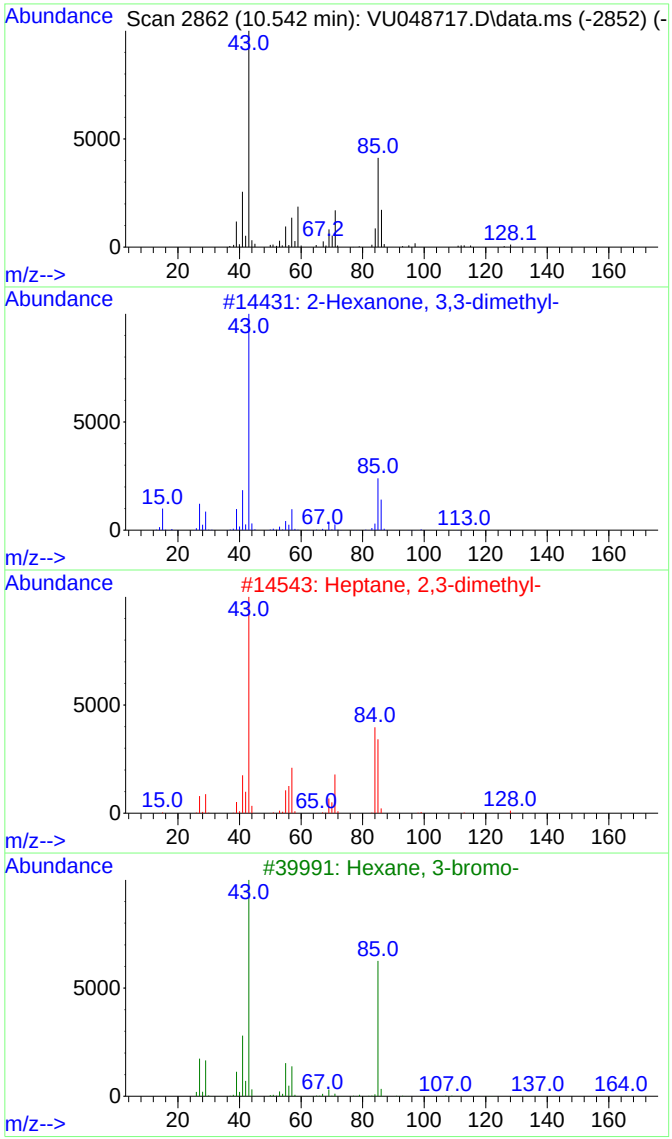
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

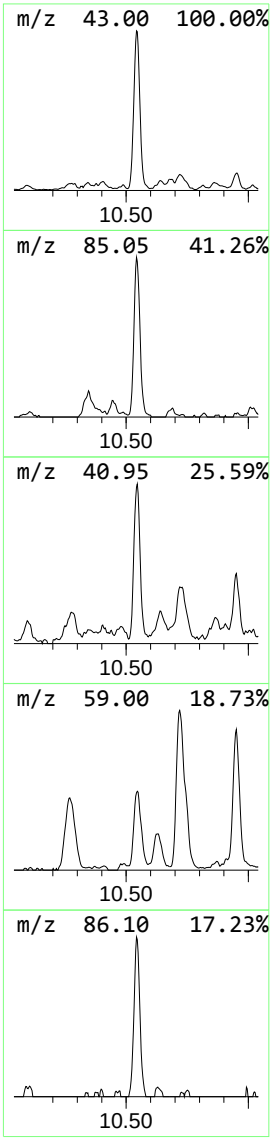
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Hexanone, 3,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.542	6.36 ug/l	152874	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 3,3-dimethyl-	128	C8H16O	026118-38-7	59
2	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	50
3	Hexane, 3-bromo-	164	C6H13Br	003377-87-5	50
4	Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	47
5	2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048717.D
Acq On : 28 May 2022 01:37
Operator : SY/MD
Sample : N3033-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-17

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.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
Butane	1.601	6.7	ug/l	92967	1	5.375	699175	50.0
Butane, 2-methyl-	1.996	9.9	ug/l	138691	1	5.375	699175	50.0
2-Butanone, 3,3...	7.163	11.9	ug/l	218463	2	6.250	916456	50.0
2-Butanol, 2,3-...	7.623	31.0	ug/l	567884	2	6.250	916456	50.0
2-Pentanol, 2-m...	7.687	19.0	ug/l	348227	2	6.250	916456	50.0
3-Pentanol, 3-m...	8.038	24.9	ug/l	599465	3	9.417	1201810	50.0
3-Pentanone, 2,...	8.716	26.1	ug/l	627988	3	9.417	1201810	50.0
1,8-Nonanediol,...	9.340	7.7	ug/l	184416	3	9.417	1201810	50.0
3-Hexanol, 3-me...	9.488	5.9	ug/l	141557	3	9.417	1201810	50.0
2-Hexanone, 3,3...	10.542	6.4	ug/l	152874	3	9.417	1201810	50.0