

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX083023\
 Data File : VX037399.D
 Acq On : 30 Aug 2023 19:21
 Operator : JC/MD
 Sample : 04211-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TRE-1767

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\82X081723W.M

Title : SW846 8260

Signal : TIC: VX037399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.435	54	57	69	rBV	9056774	21583792	20.82%	7.758%
2	1.526	69	72	89	rVV	644638	1418863	1.37%	0.510%
3	2.093	155	165	185	rBV	423940	1330130	1.28%	0.478%
4	2.294	191	198	206	rBV	1298701	2478415	2.39%	0.891%
5	2.398	206	215	235	rVV	13021783	34797074	33.57%	12.507%
6	2.575	235	244	292	rVB	2658200	9183837	8.86%	3.301%
7	4.136	438	500	503	rBV	4541822	48207442	46.51%	17.327%
8	6.964	940	964	970	rBV2	19721065	103657682	100.00%	37.257%
9	7.245	998	1010	1017	rBV	11998028	30062303	29.00%	10.805%
10	7.830	1097	1106	1115	rBV	854527	1573357	1.52%	0.566%
11	8.683	1242	1246	1259	rVB	1740461	2838982	2.74%	1.020%
12	9.007	1291	1299	1318	rVB	8500162	13274273	12.81%	4.771%
13	9.165	1318	1325	1333	rBV	2593439	3568045	3.44%	1.282%
14	9.872	1435	1441	1448	rBV	988874	1300879	1.25%	0.468%
15	10.397	1522	1527	1540	rVB	831673	1051617	1.01%	0.378%
16	12.219	1820	1826	1837	rBV	1470590	1893407	1.83%	0.681%

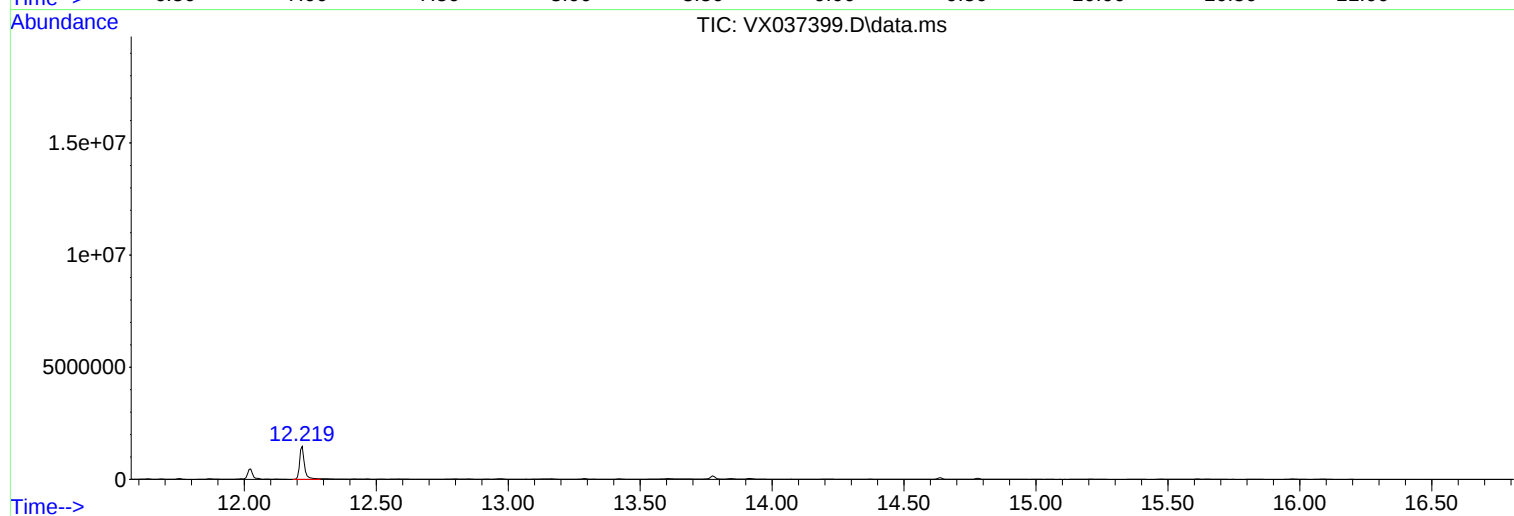
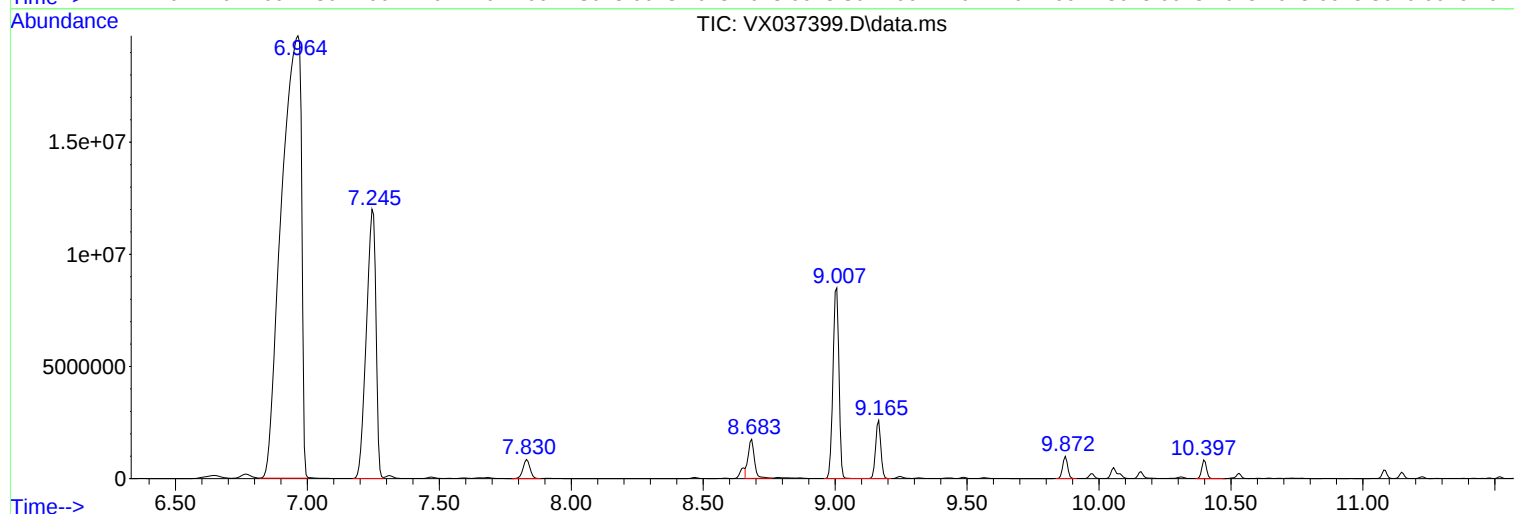
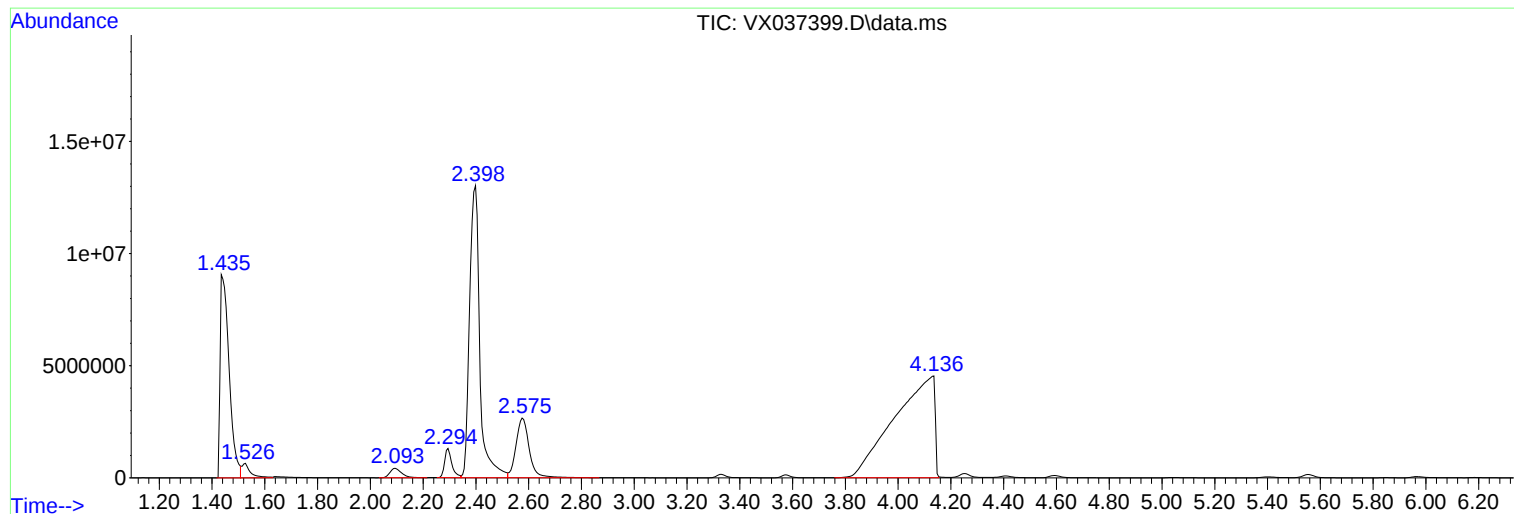
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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



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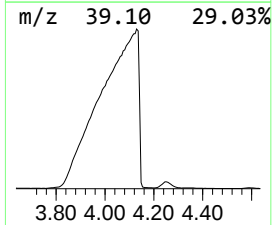
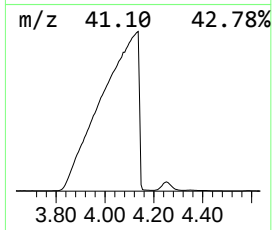
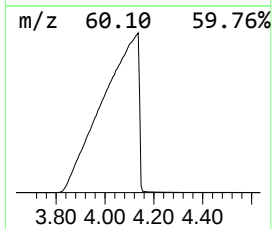
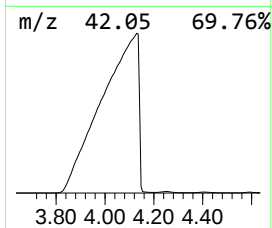
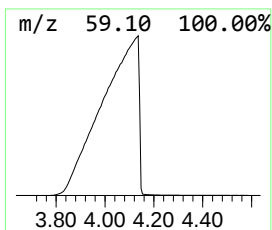
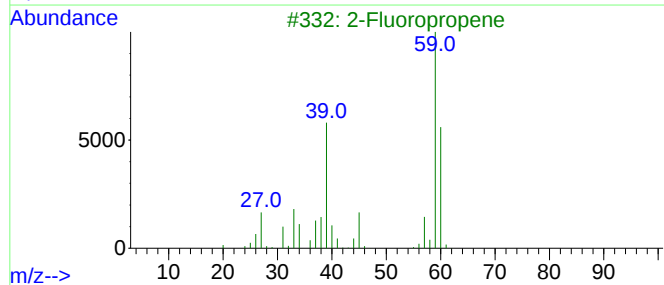
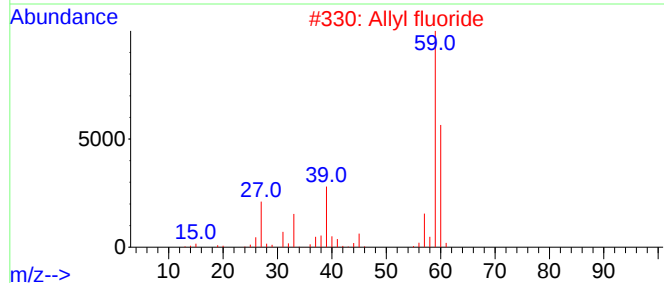
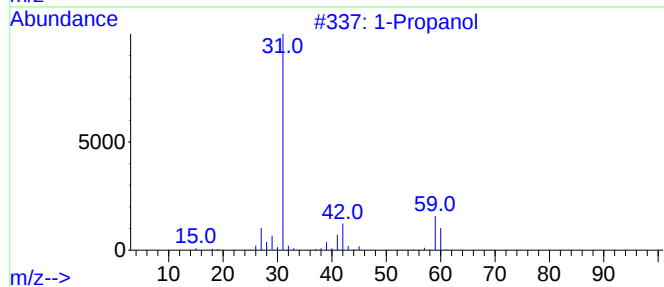
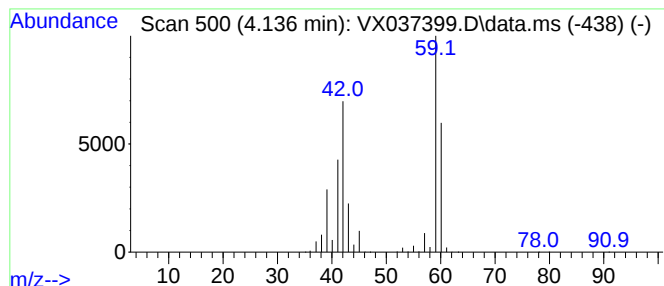
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.136	23.25 ug/l	48207400	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	72
2	Allyl fluoride			60	C3H5F	000818-92-8	42
3	2-Fluoropropene			60	C3H5F	001184-60-7	40
4	Methanamine, N-hydroxy-N-methyl-			61	C2H7NO	005725-96-2	9
5	Acetaldoxime			59	C2H5NO	000107-29-9	7



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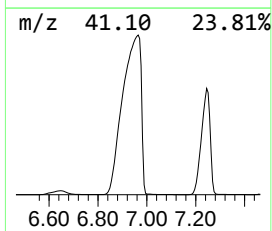
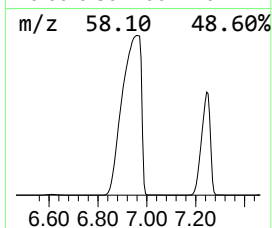
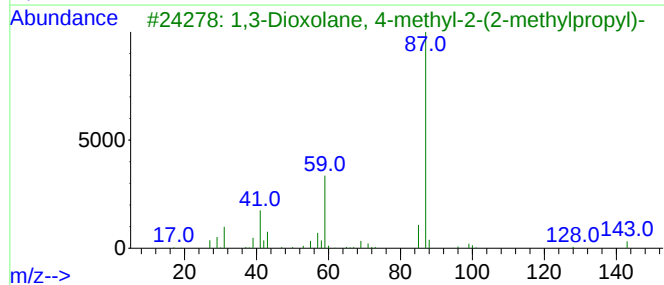
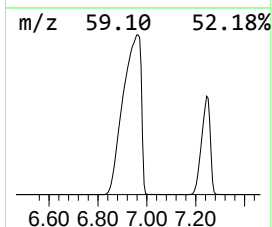
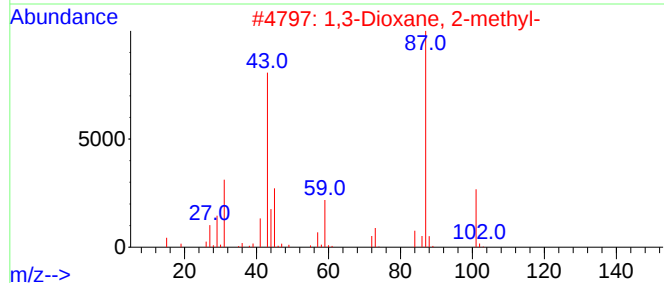
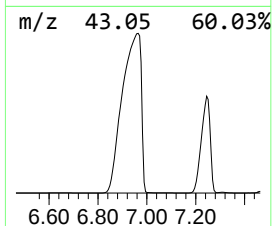
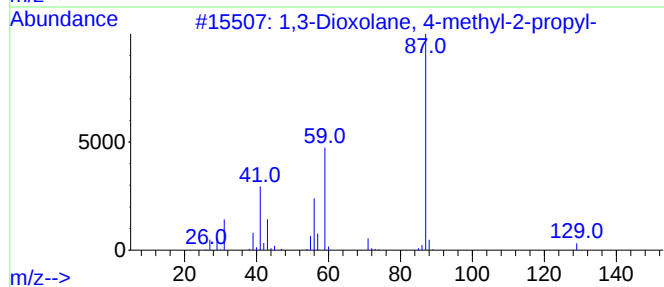
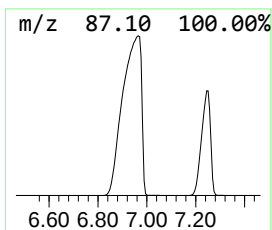
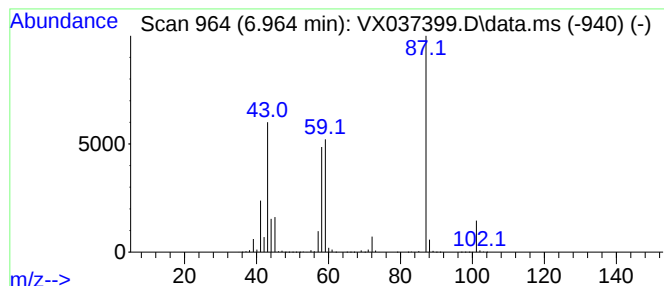
Instrument :
MSVOA_X
ClientSampleId :
TRE-1767

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 3 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.964	50.00 ug/l	103658000	1,4-Difluorobenzene	6.769	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	50
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	50
3	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	40
4	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	39
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1767

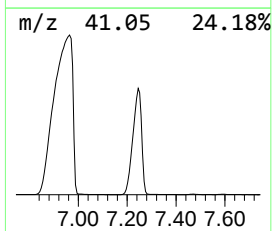
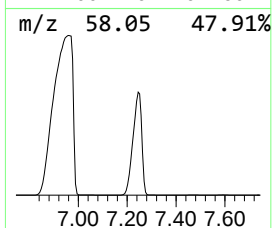
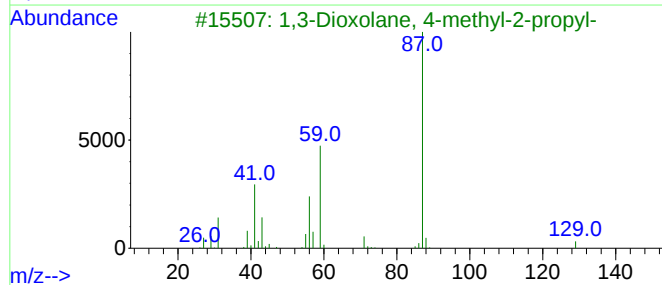
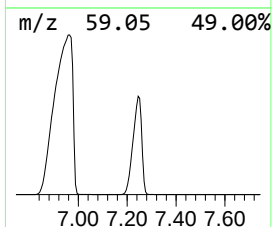
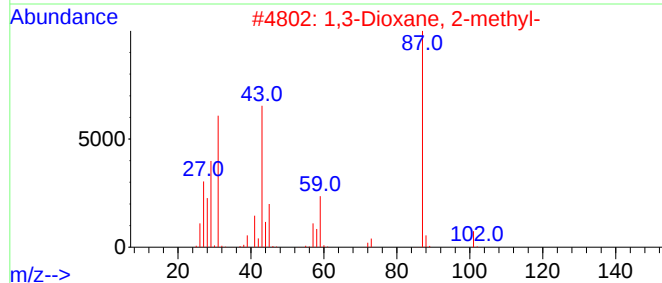
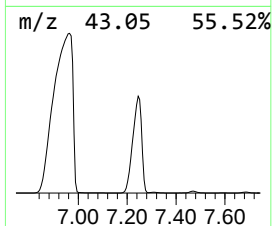
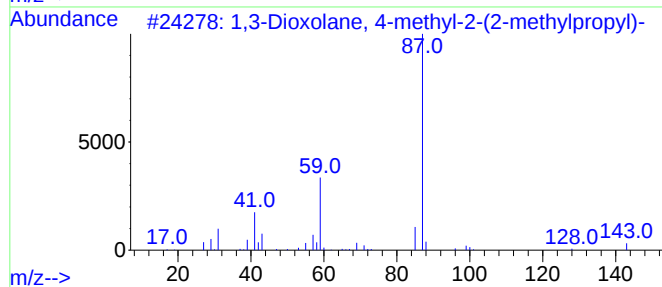
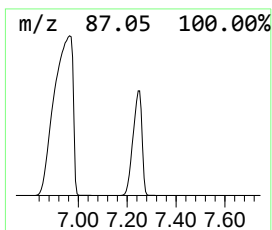
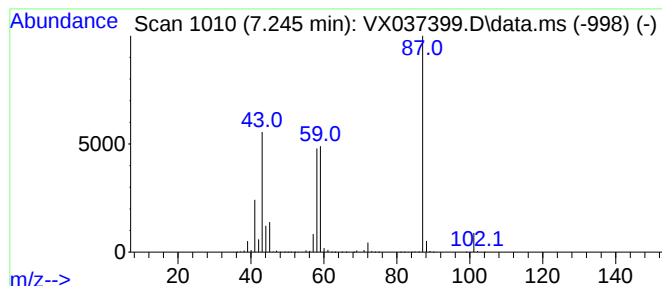
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Quant Title : SW846 8260

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

Peak Number 4 1,3-Dioxolane, 4-methyl-2-(... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.245	14.50 ug/l	30062300	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	50		
2	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	49		
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	40		
4	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40		
5	1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36		



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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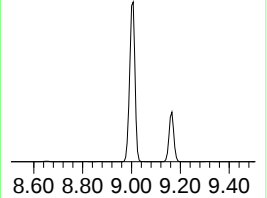
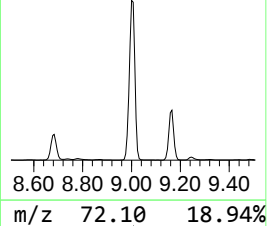
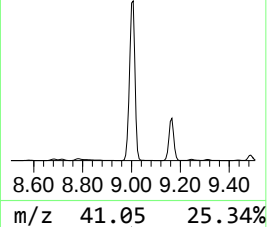
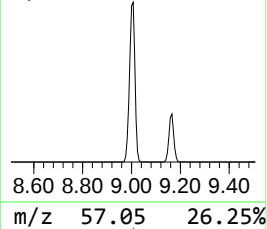
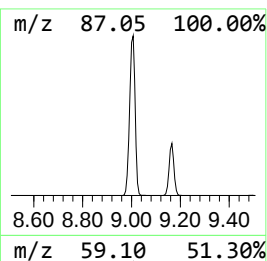
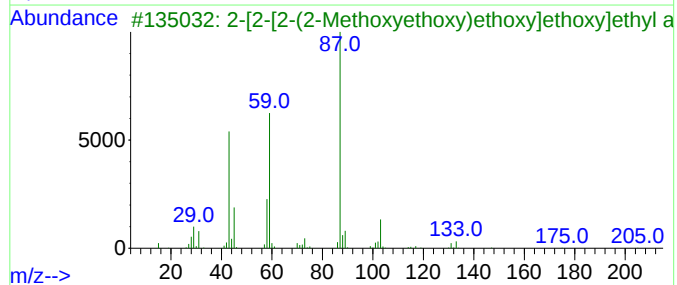
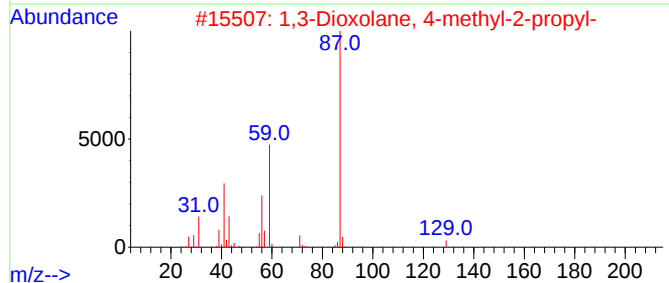
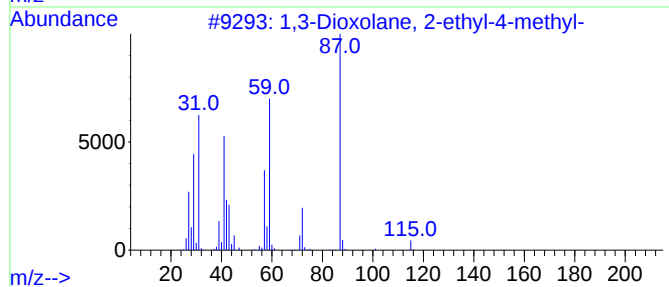
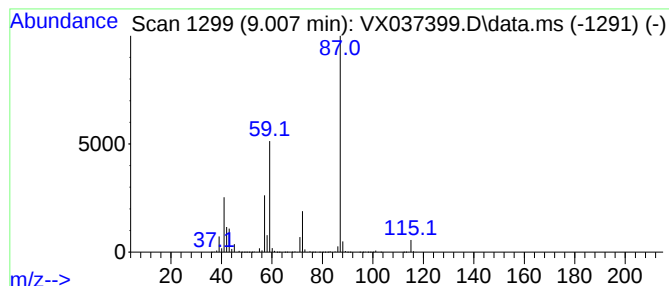
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.007	510.20 ug/l	13274300	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	91
2			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
3			2-[2-[2-(2-Methoxyethoxy)ethoxy]...	250	C11H22O6	1000351-91-4	64
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
5			2-Propanone, O-methylloxime	87	C4H9NO	003376-35-0	50



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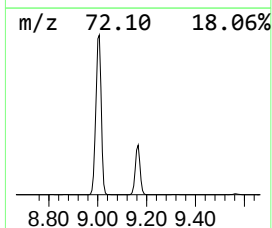
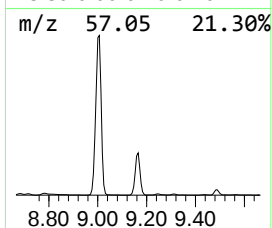
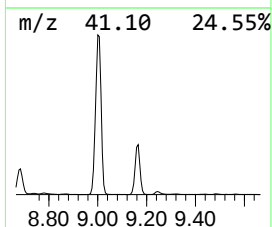
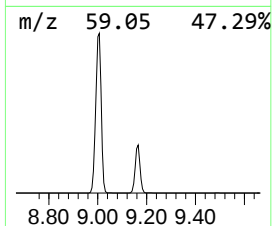
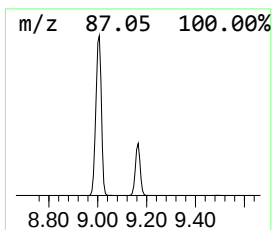
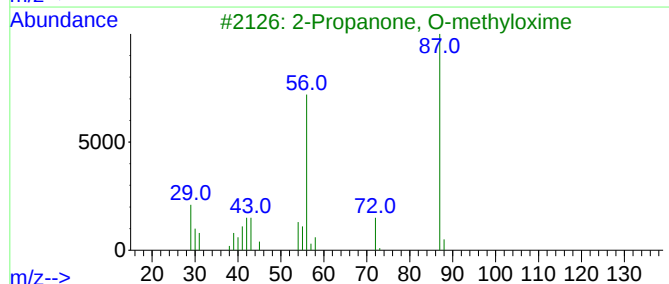
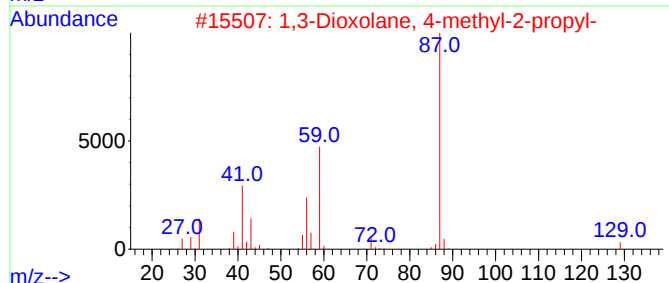
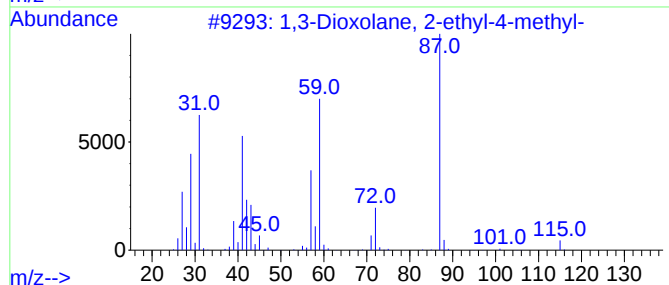
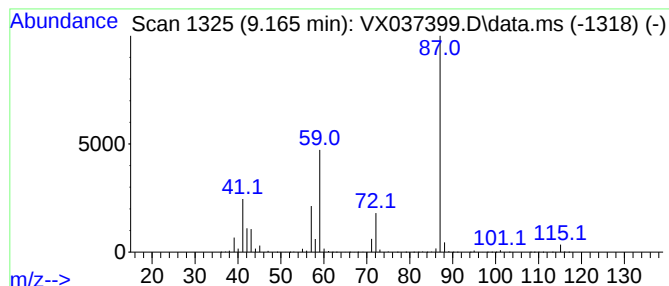
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TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Propanone, O-methyloxime Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.165	137.14 ug/l	3568050	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	91
2			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	64
3			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	50
4			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	50
5			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	50



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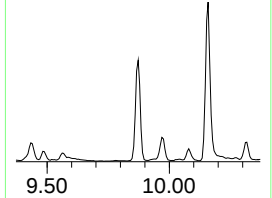
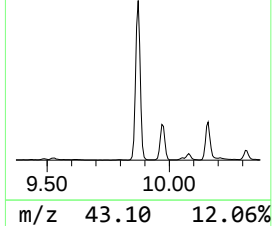
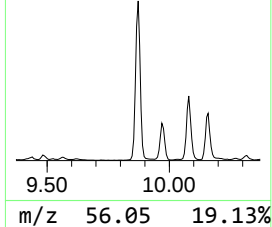
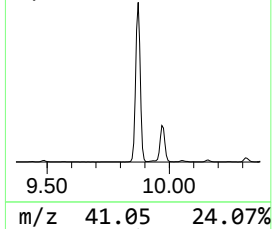
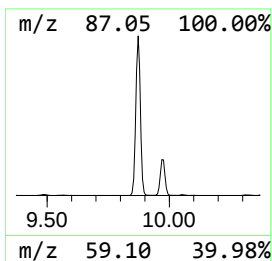
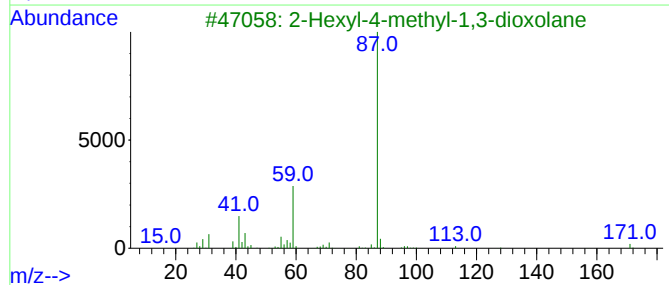
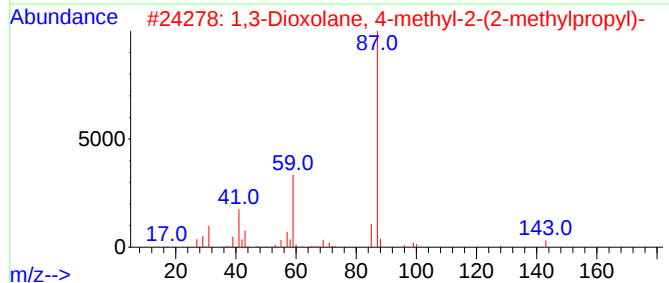
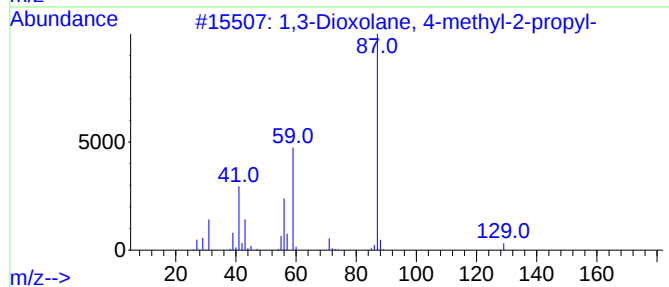
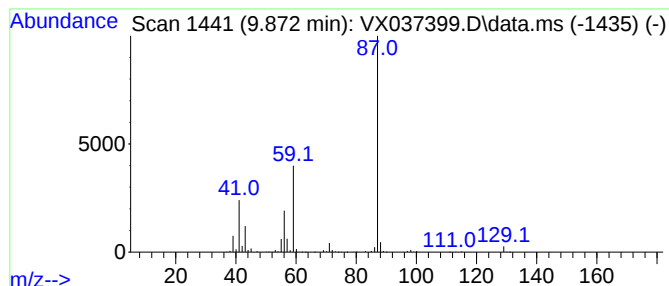
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Quant Title : SW846 8260

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

Peak Number 7 2-Hexyl-4-methyl-1,3-dioxolane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.872	50.00 ug/l	1300880	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	90
2			1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	64
3			2-Hexyl-4-methyl-1,3-dioxolane	172	C10H20O2	004351-10-4	64
4			Arachidamide, N-ethyl-	339	C22H45NO	1000420-44-1	28
5			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX083023\
Data File : VX037399.D
Acq On : 30 Aug 2023 19:21
Operator : JC/MD
Sample : 04211-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1767

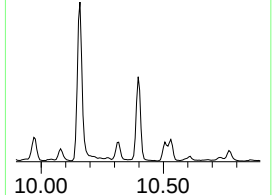
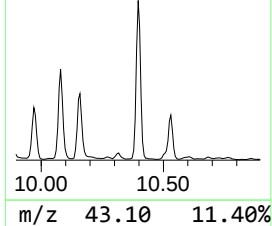
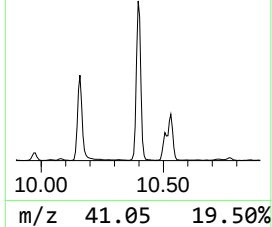
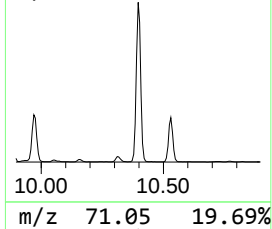
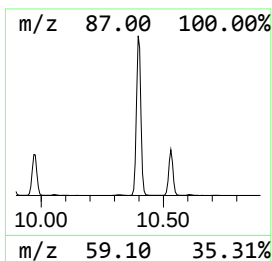
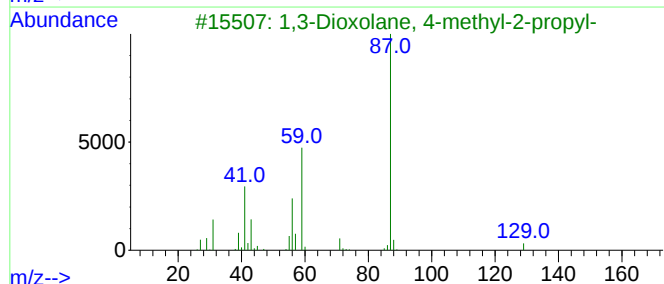
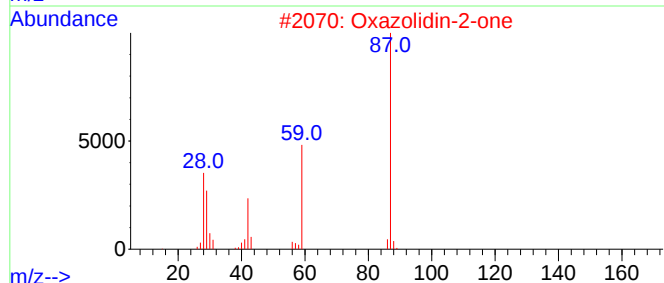
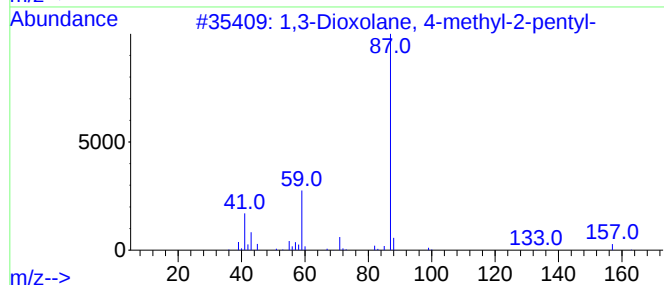
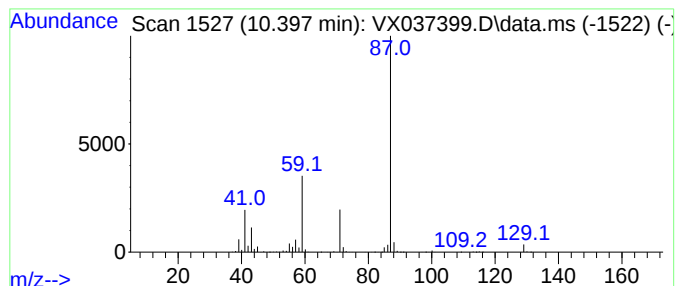
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 8 1,3-Dioxolane, 4-methyl-2-p... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.397	40.42 ug/l	1051620	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 4-methyl-2-pentyl-	158	C9H18O2	001599-49-1	64
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
3			1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	56
4			2-Hexyl-4-methyl-1,3-dioxolane	172	C10H20O2	004351-10-4	50
5			1,3-Dioxolane, 2-heptyl-4-methyl-	186	C11H22O2	074094-61-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX083023\
Data File : VX037399.D
Acq On : 30 Aug 2023 19:21
Operator : JC/MD
Sample : 04211-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1767

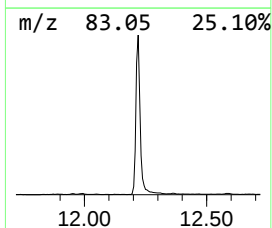
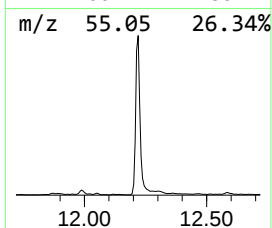
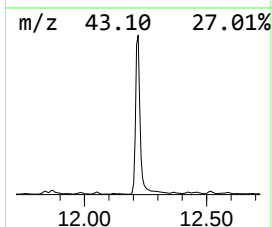
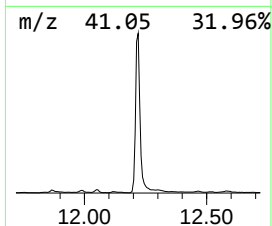
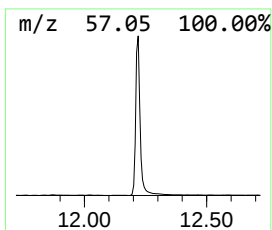
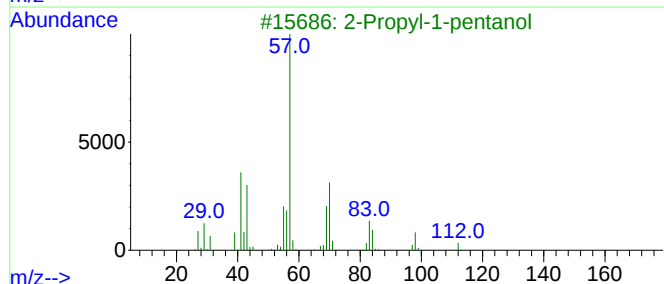
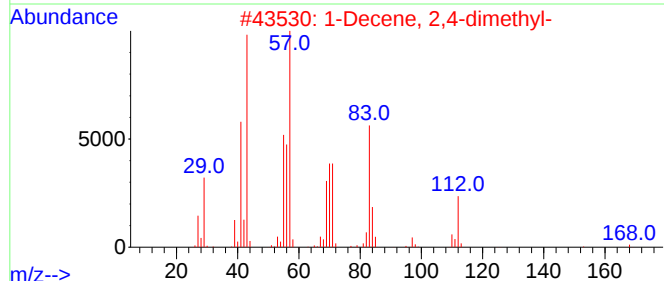
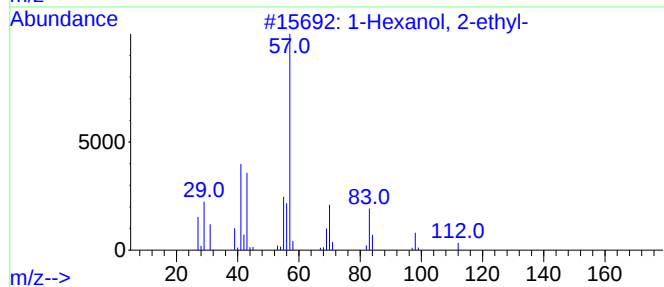
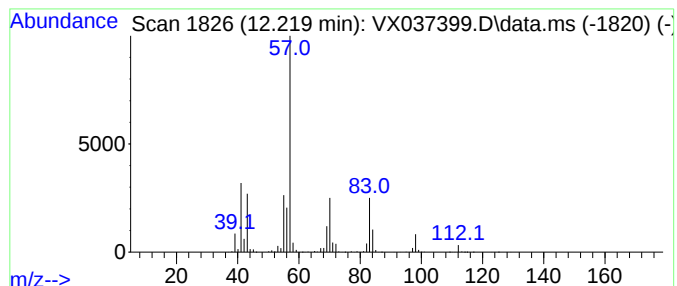
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	50.00 ug/l	1893410	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			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	50
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX083023\
Data File : VX037399.D
Acq On : 30 Aug 2023 19:21
Operator : JC/MD
Sample : 04211-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TRE-1767

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanol	4.136	23.3	ug/l	48207400	1	5.550	103658000	50.0
1,3-Dioxolane, ...	6.964	50.0	ug/l	103658000	2	6.769	103658000	50.0
1,3-Dioxolane, ...	7.245	14.5	ug/l	30062300	2	6.769	103658000	50.0
1,3-Dioxolane, ...	9.007	510.2	ug/l	13274300	3	10.055	1300880	50.0
2-Propanone, O-...	9.165	137.1	ug/l	3568050	3	10.055	1300880	50.0
2-Hexyl-4-methy...	9.872	50.0	ug/l	1300880	3	10.055	1300880	50.0
1,3-Dioxolane, ...	10.397	40.4	ug/l	1051620	3	10.055	1300880	50.0
1-Hexanol, 2-et...	12.219	50.0	ug/l	1893410	4	12.024	1893410	50.0