

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090523\
 Data File : VY015438.D
 Acq On : 05 Sep 2023 18:15
 Operator : SY/MD
 Sample : 04278-02
 Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 824-829

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_Y\methods\82Y082923S.M
 Title : SW846 8260

Signal : TIC: VY015438.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.710	952	966	970	rBV2	187573	465162	1.98%	0.631%
2	7.777	970	977	986	rVB2	365077	1014806	4.31%	1.377%
3	7.990	1003	1012	1024	rBV	186263	433602	1.84%	0.588%
4	8.137	1024	1036	1047	rVB2	209700	537436	2.28%	0.729%
5	8.539	1093	1102	1112	rBV	138469	273584	1.16%	0.371%
6	8.685	1116	1126	1144	rBV	512541	998526	4.24%	1.355%
7	10.173	1363	1370	1376	rBV	779149	1365735	5.81%	1.853%
8	10.240	1376	1381	1387	rVB	541471	903799	3.84%	1.226%
9	11.490	1578	1586	1591	rBV	687345	1147869	4.88%	1.557%
10	11.697	1611	1620	1631	rBV	341266	704752	3.00%	0.956%
11	12.026	1663	1674	1681	rBV	238861	439328	1.87%	0.596%
12	12.331	1717	1724	1734	rBV	266451	437169	1.86%	0.593%
13	12.477	1739	1748	1758	rVV2	560076	932563	3.96%	1.265%
14	12.800	1797	1801	1810	rVB3	346253	628286	2.67%	0.852%
15	13.337	1882	1889	1898	rBV	17124925	23523070	100.00%	31.913%
16	13.422	1898	1903	1908	rVV	595358	909513	3.87%	1.234%
17	13.483	1908	1913	1916	rVV	179481	307024	1.31%	0.417%
18	13.526	1916	1920	1926	rVB	643426	937838	3.99%	1.272%
19	13.751	1951	1957	1965	rBV2	312227	598641	2.54%	0.812%
20	13.873	1971	1977	1982	rBV	826192	1251595	5.32%	1.698%
21	14.178	2022	2027	2034	rBV3	196572	433016	1.84%	0.587%
22	14.288	2039	2045	2057	rVV3	431876	853677	3.63%	1.158%
23	14.392	2057	2062	2064	rVV	537276	815761	3.47%	1.107%
24	14.422	2064	2067	2079	rVV	2023325	3729355	15.85%	5.059%
25	14.544	2083	2087	2093	rVV	200453	315154	1.34%	0.428%
26	14.605	2093	2097	2101	rVB	310226	423963	1.80%	0.575%
27	14.660	2101	2106	2113	rBV	452522	694803	2.95%	0.943%
28	14.751	2113	2121	2129	rBV	2647959	4018489	17.08%	5.452%
29	14.861	2134	2139	2141	rBV2	171464	293142	1.25%	0.398%
30	14.891	2141	2144	2147	rVV	359233	621762	2.64%	0.844%
31	14.958	2151	2155	2163	rVB2	542813	1358030	5.77%	1.842%
32	15.038	2163	2168	2169	rBV	490260	676430	2.88%	0.918%
33	15.062	2169	2172	2174	rVV2	576279	915826	3.89%	1.242%
34	15.093	2174	2177	2182	rVB	916325	1308329	5.56%	1.775%
35	15.215	2194	2197	2200	rBV	579539	867825	3.69%	1.177%
36	15.257	2200	2204	2220	rVB	3246389	5814064	24.72%	7.888%

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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_Y\methods\82Y082923S.M
Title : SW846 8260

37	15.434	2229	2233	2241	rVB	231179	371600	1.58%	0.504%
38	15.532	2244	2249	2255	rVB	197454	338638	1.44%	0.459%
39	15.605	2255	2261	2277	rBV	5816196	8911505	37.88%	12.090%
40	15.910	2305	2311	2315	rBV	228791	390049	1.66%	0.529%
41	15.964	2315	2320	2326	rVB	248462	402793	1.71%	0.546%
42	16.166	2348	2353	2361	rVB	521928	976066	4.15%	1.324%
43	16.580	2415	2421	2439	rVB	671758	1369587	5.82%	1.858%

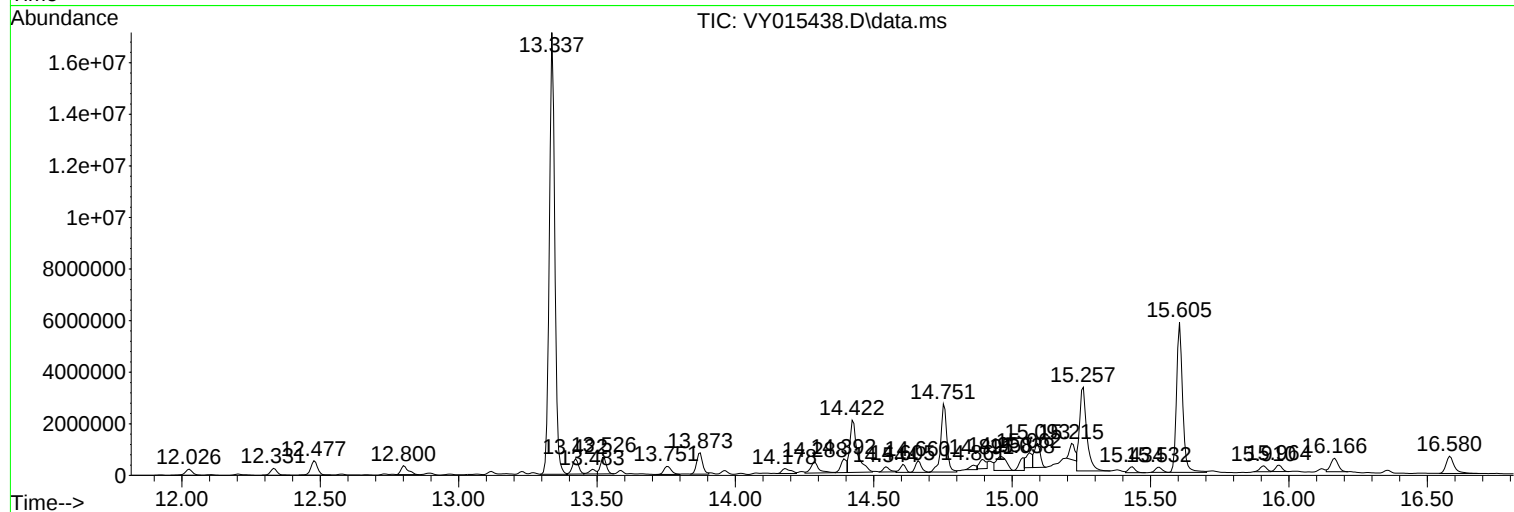
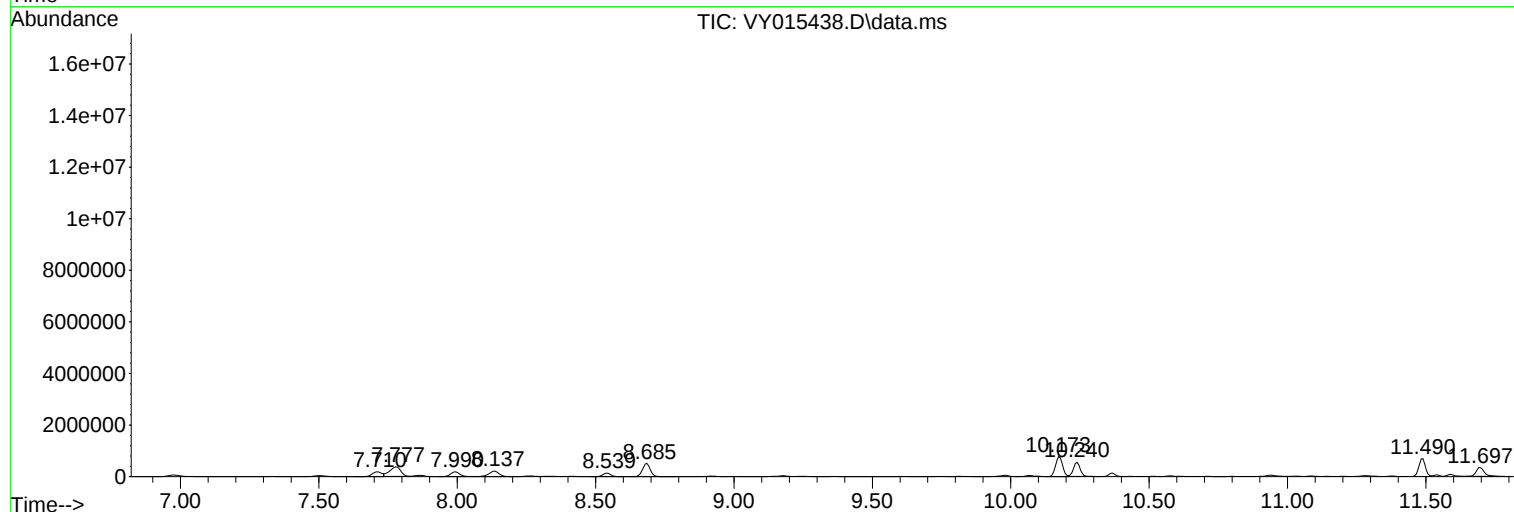
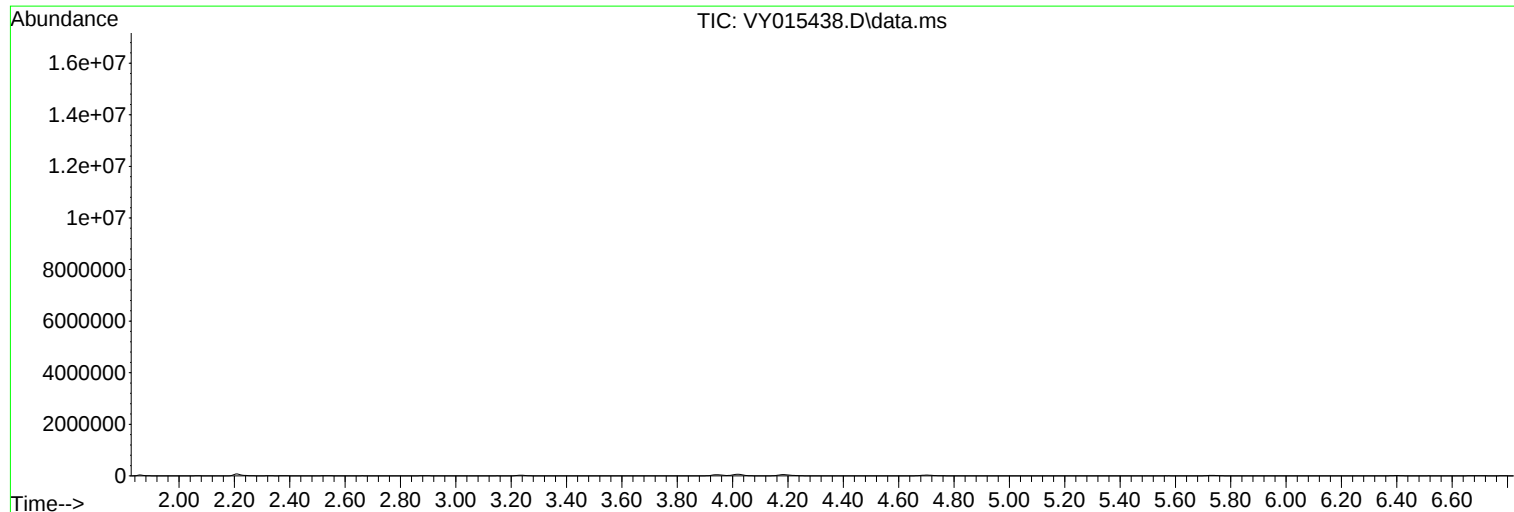
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082923S.M
Quant Title : SW846 8260

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



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
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824-829

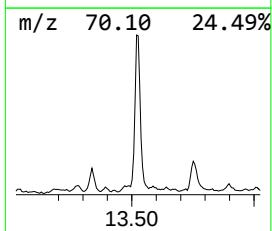
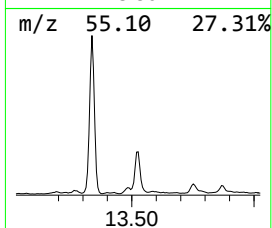
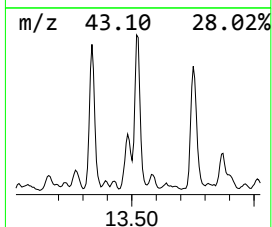
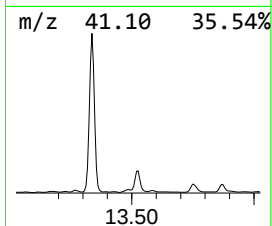
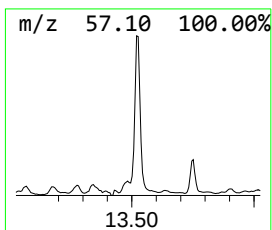
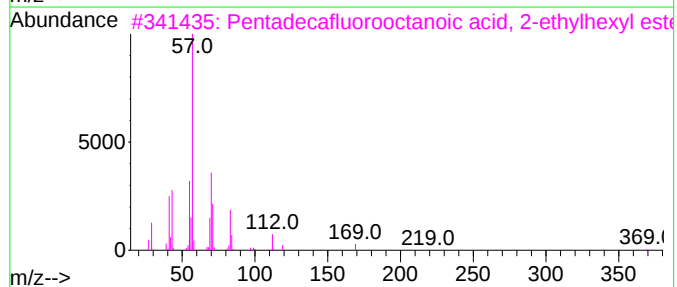
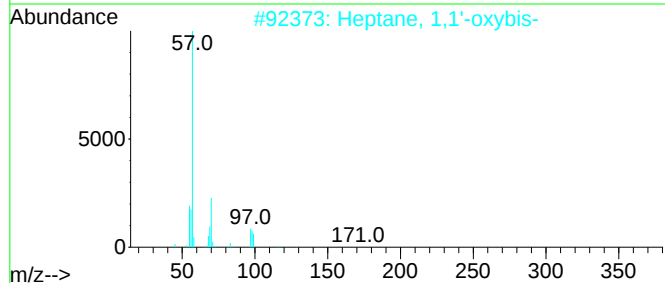
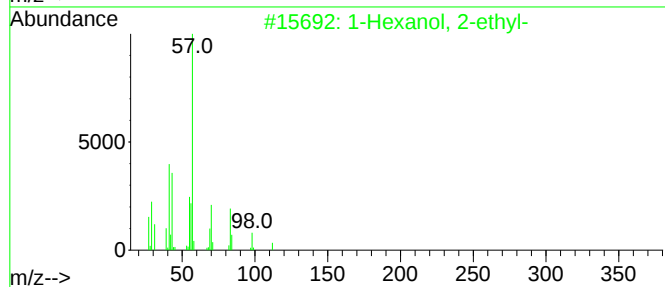
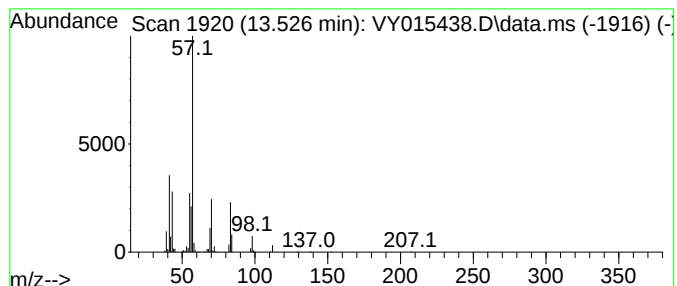
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082923S.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.526	51.56 ug/l	937838	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	45
5			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43



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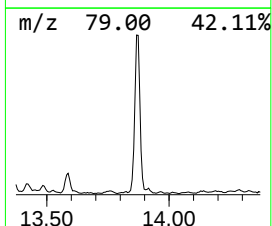
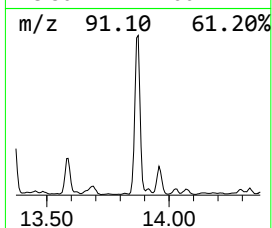
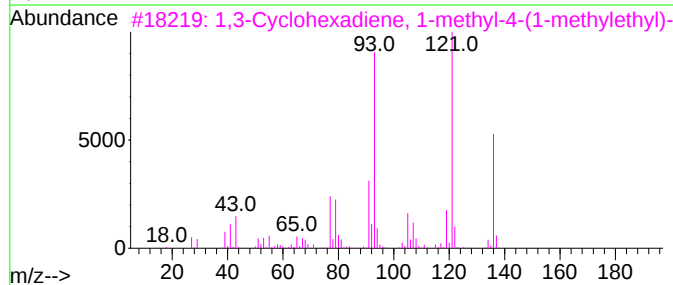
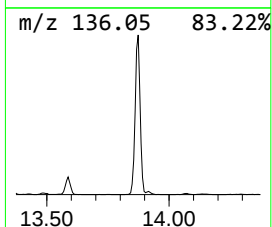
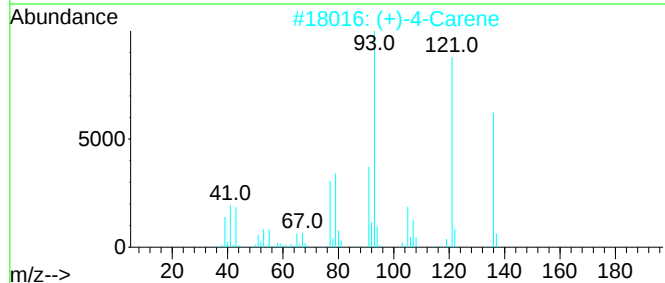
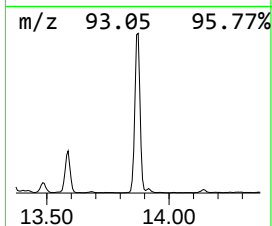
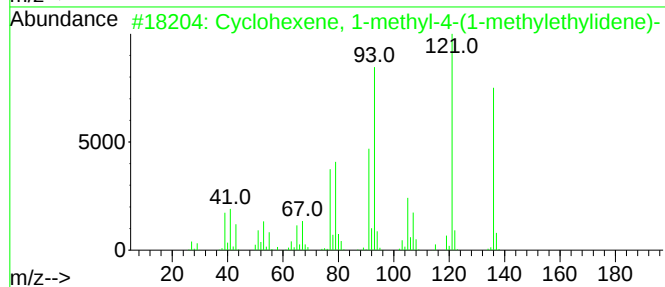
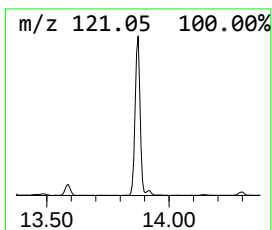
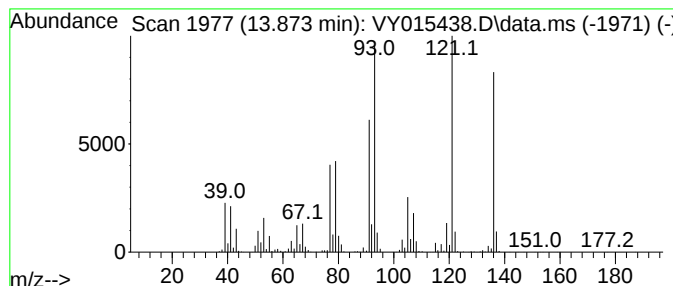
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082923S.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	68.81 ug/l	1251600	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	98
2			(+)-4-Carene	136	C10H16	029050-33-7	97
3			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	94
4			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
5			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	94



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Instrument :
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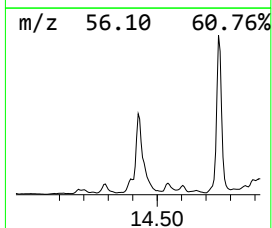
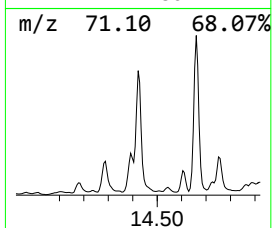
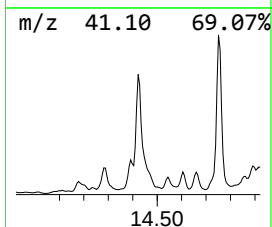
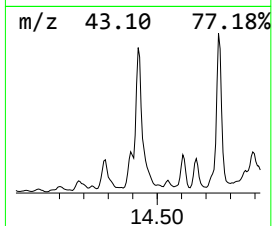
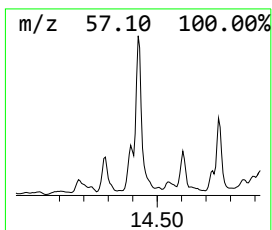
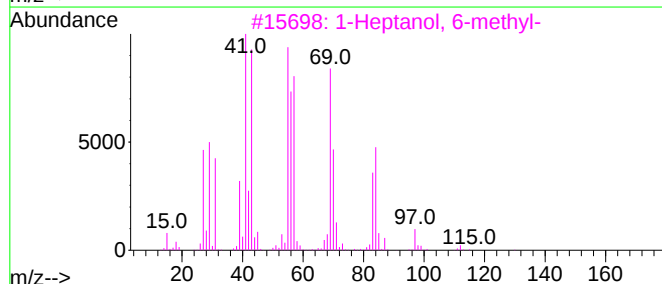
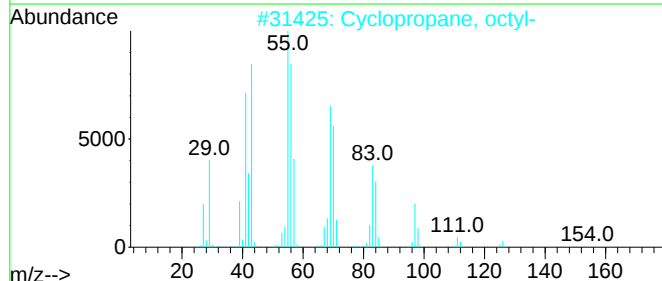
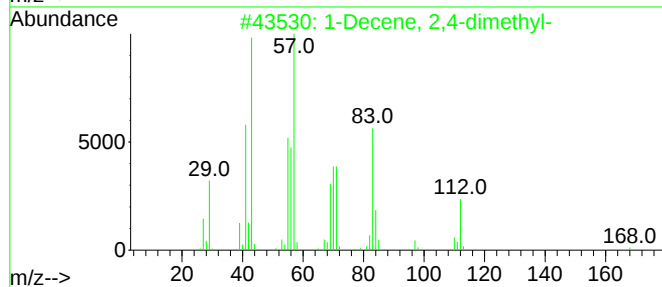
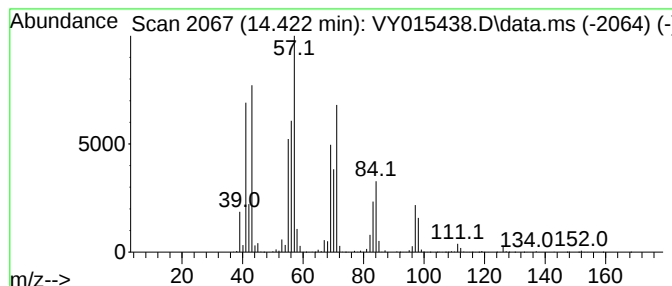
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082923S.M
Quant Title : SW846 8260

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

Peak Number 3 1-Decene, 2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	205.02 ug/l	3729360	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene, 2,4-dimethyl-			168	C12H24	055170-80-4	53
2	Cyclopropane, octyl-			154	C11H22	001472-09-9	50
3	1-Heptanol, 6-methyl-			130	C8H18O	001653-40-3	50
4	Cyclopropane, 1-methyl-2-octyl-			168	C12H24	037617-26-8	50
5	1-Nonene			126	C9H18	000124-11-8	38



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ClientSampleId :
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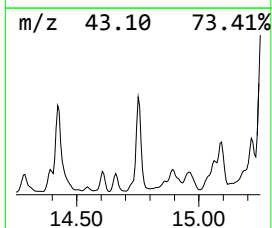
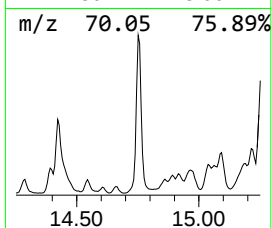
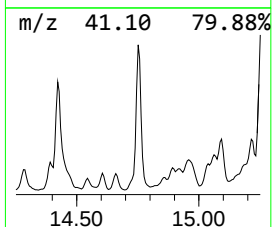
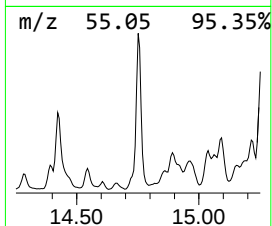
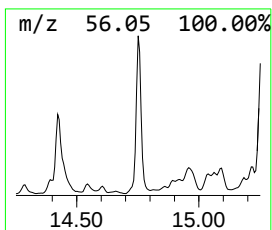
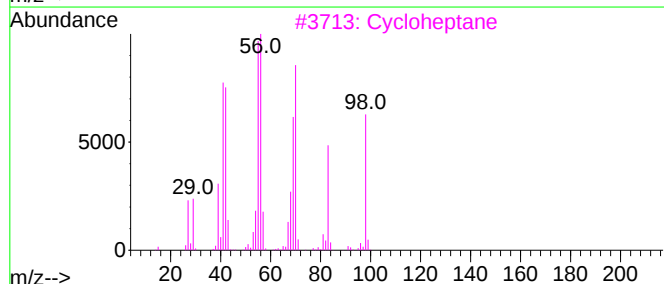
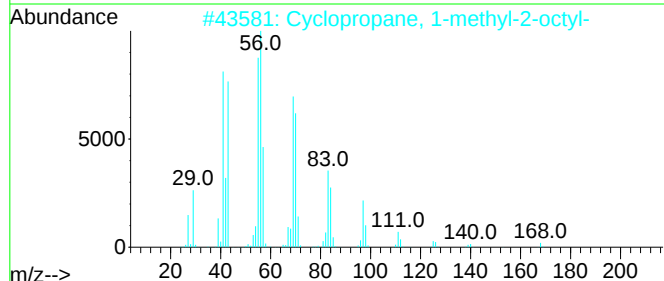
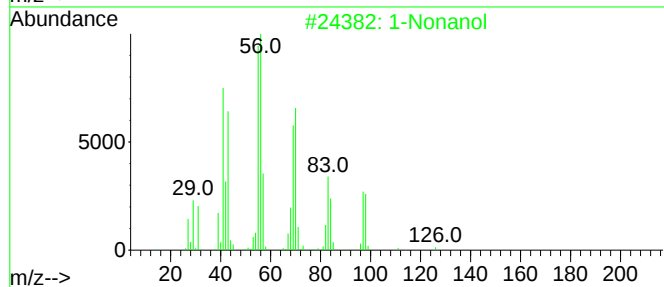
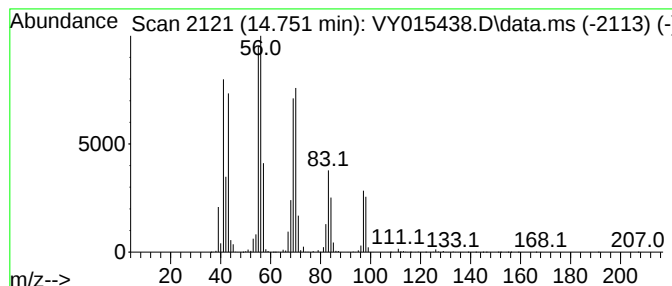
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082923S.M
Quant Title : SW846 8260

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

Peak Number 4 1-Nonanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.751	220.91 ug/l	4018490	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol			144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-			168	C12H24	037617-26-8	86
3	Cycloheptane			98	C7H14	000291-64-5	72
4	Isopropylcyclobutane			98	C7H14	000872-56-0	68
5	1-Decanol			158	C10H22O	000112-30-1	64



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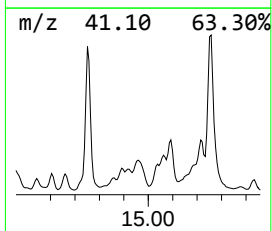
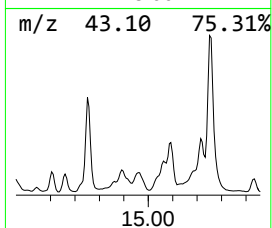
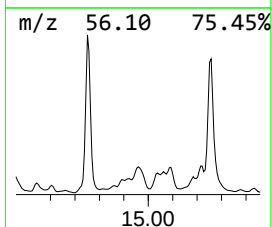
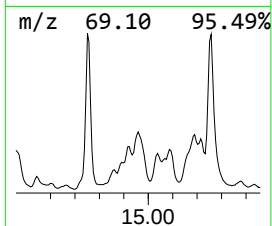
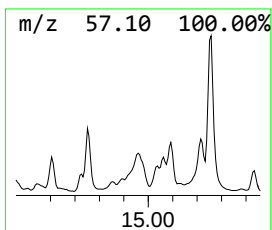
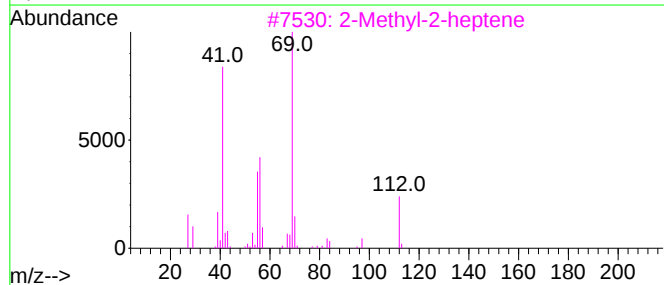
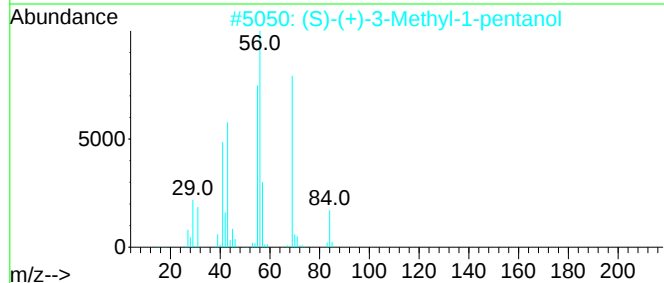
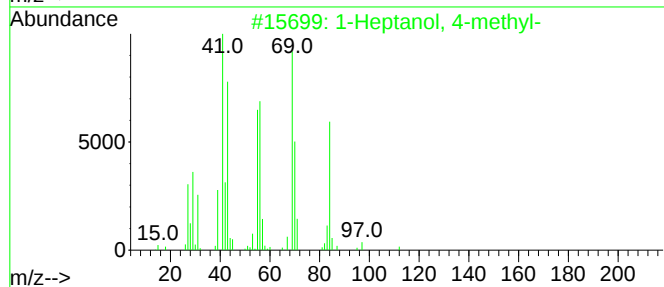
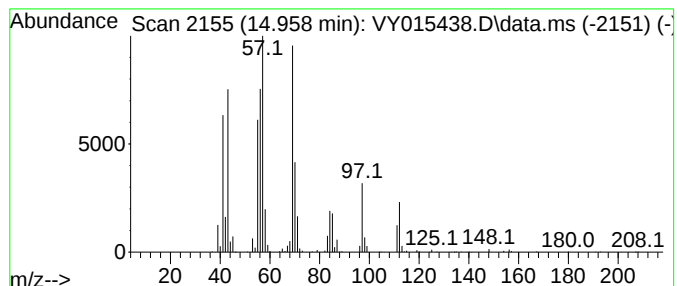
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Quant Title : SW846 8260

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

Peak Number 5 1-Heptanol, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	74.66 ug/l	1358030	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	58
2			(S)-(+)-3-Methyl-1-pentanol	102	C6H14O	042072-39-9	47
3			2-Methyl-2-heptene	112	C8H16	000627-97-4	38
4			3,3-Dimethyl-1,5-diazabicyclo[3....	112	C6H12N2	104518-71-0	38
5			2-Heptene, 4-methyl-, (E)-	112	C8H16	066225-17-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090523\
Data File : VY015438.D
Acq On : 05 Sep 2023 18:15
Operator : SY/MD
Sample : 04278-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
824-829

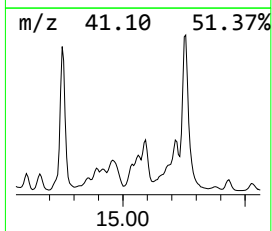
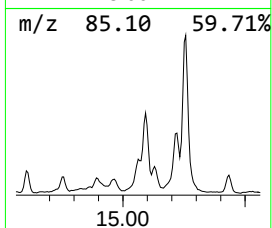
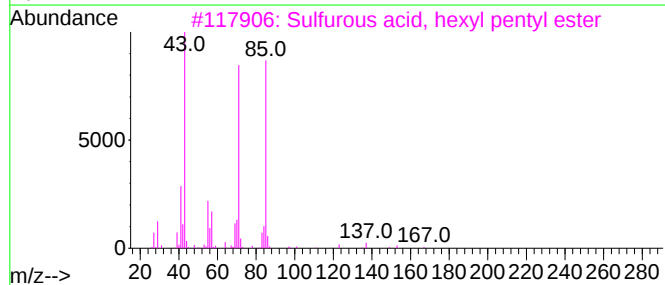
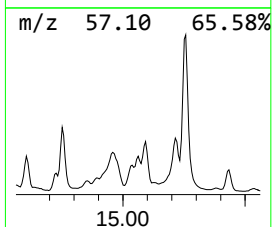
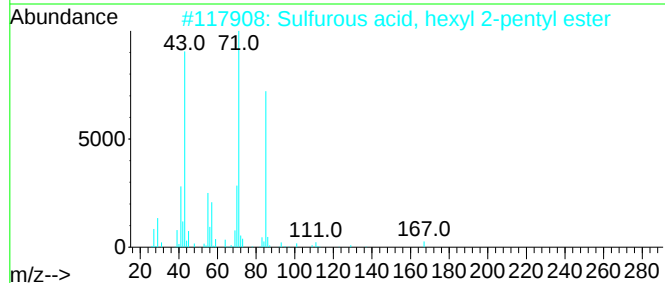
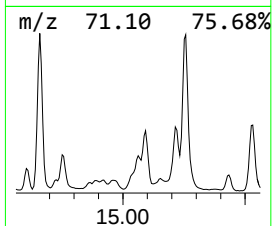
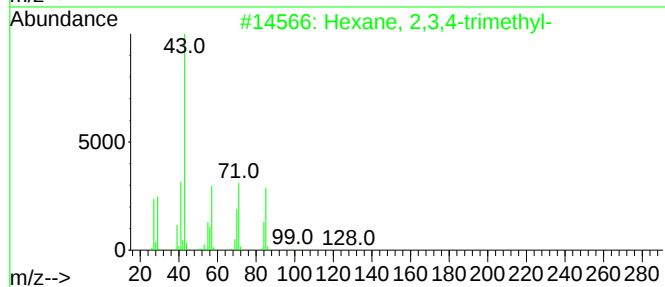
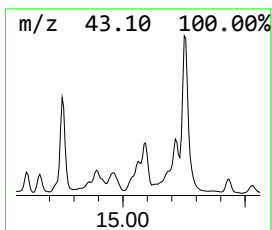
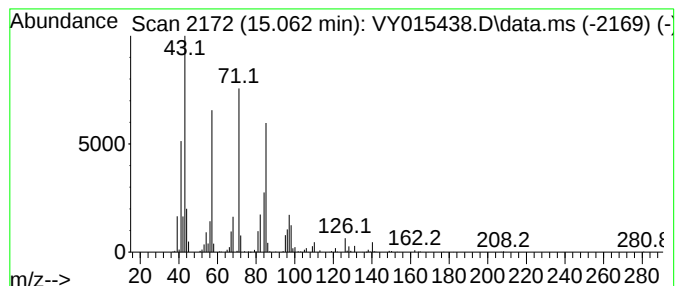
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Quant Title : SW846 8260

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

Peak Number 6 Hexane, 2,3,4-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.062	50.35 ug/l	915826	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50
2			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	47
3			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	47
4			2-Bromononane	206	C9H19Br	002216-35-5	47
5			Sulfurous acid, isohexyl pentyl ...	236	C11H24O3S	1000309-14-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090523\
Data File : VY015438.D
Acq On : 05 Sep 2023 18:15
Operator : SY/MD
Sample : 04278-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
824-829

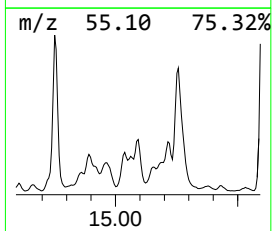
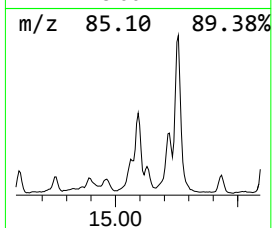
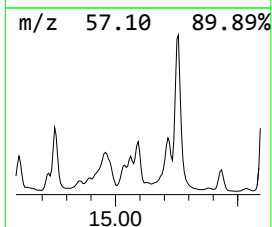
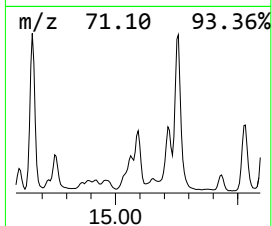
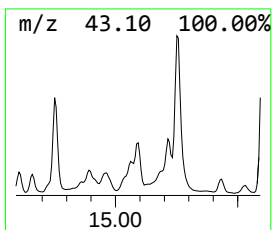
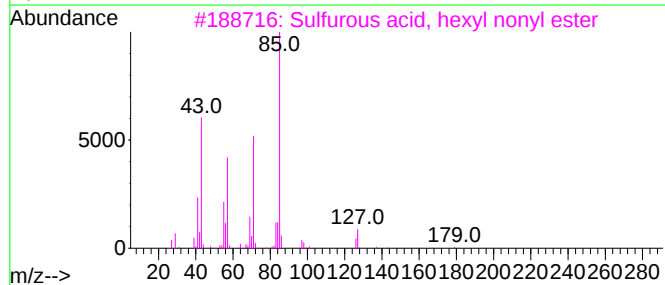
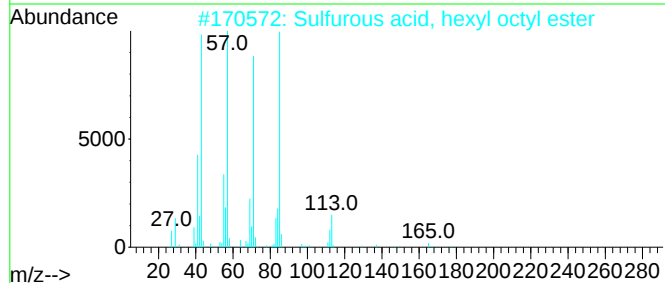
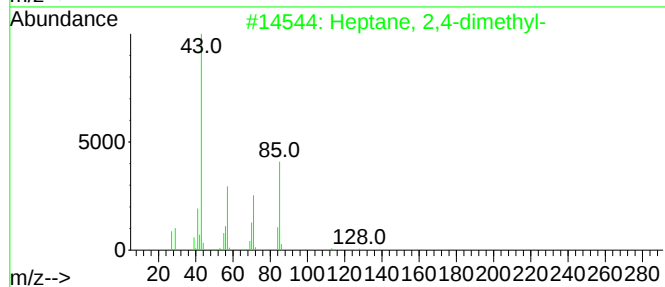
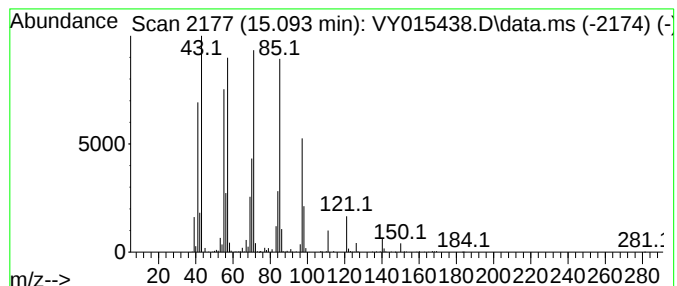
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Quant Title : SW846 8260

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

Peak Number 7 Heptane, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.093	71.92 ug/l	1308330	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
2			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	47
3			Sulfurous acid, hexyl nonyl ester	292	C15H32O3S	1000309-13-1	47
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	47
5			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090523\
Data File : VY015438.D
Acq On : 05 Sep 2023 18:15
Operator : SY/MD
Sample : 04278-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
824-829

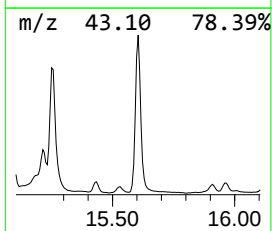
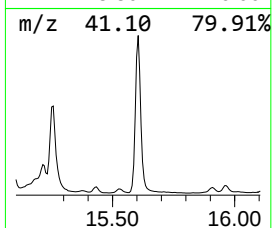
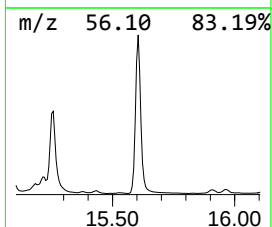
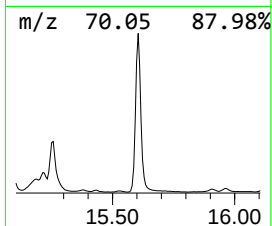
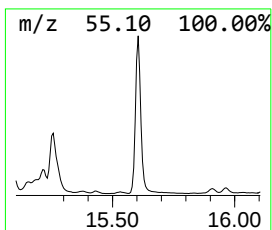
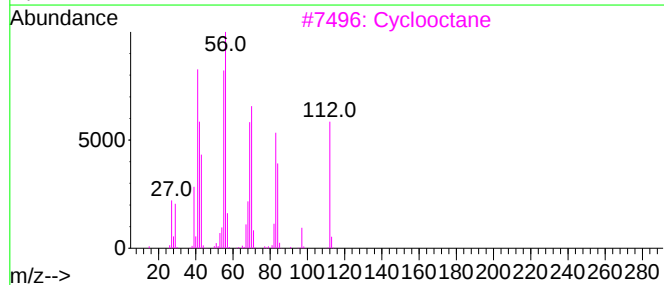
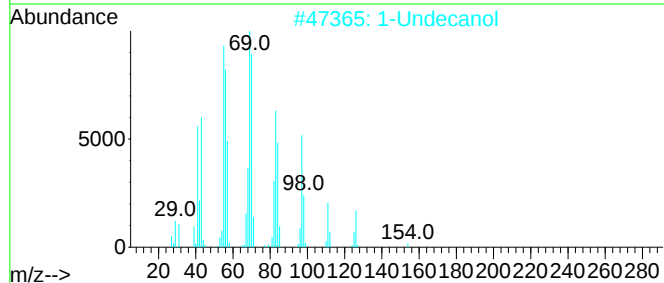
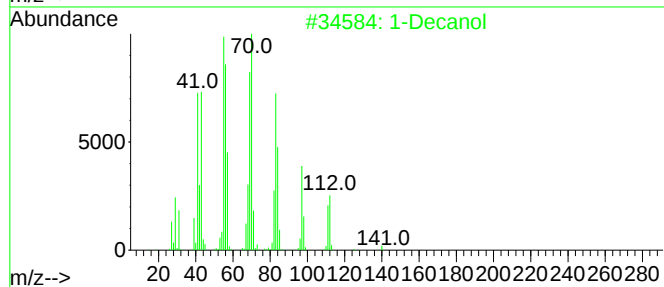
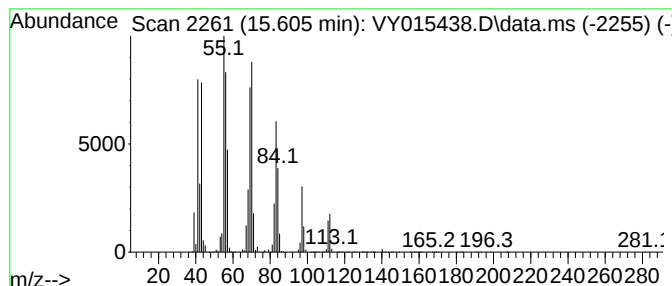
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Quant Title : SW846 8260

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

Peak Number 8 1-Decanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.605	489.90 ug/l	8911510	1,4-Dichlorobenzene-d4	13.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Decanol	158	C10H22O	000112-30-1	91
2		1-Undecanol	172	C11H24O	000112-42-5	90
3		Cyclooctane	112	C8H16	000292-64-8	87
4		Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	86
5		Octane, 3-chloro-	148	C8H17Cl	001117-79-9	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090523\
Data File : VY015438.D
Acq On : 05 Sep 2023 18:15
Operator : SY/MD
Sample : 04278-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
824-829

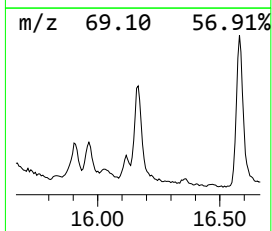
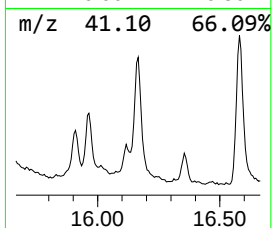
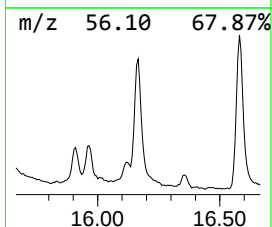
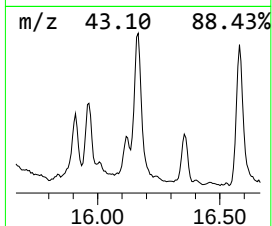
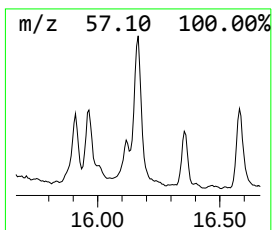
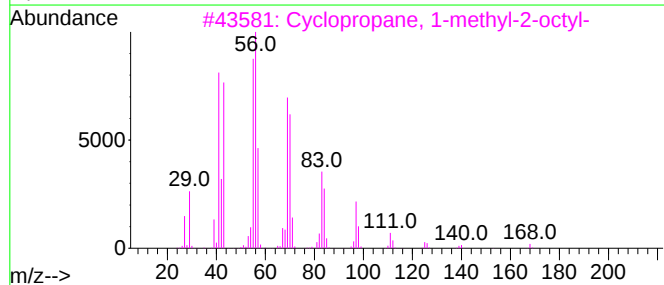
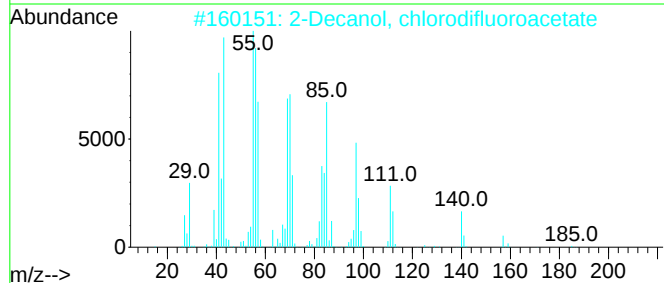
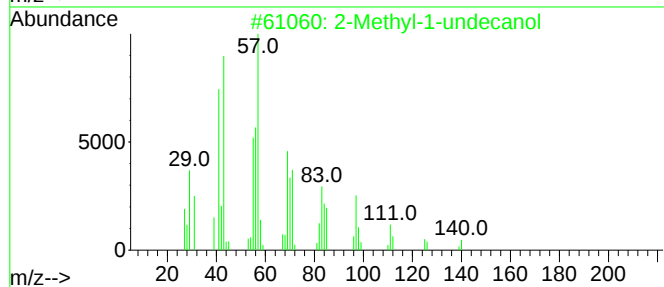
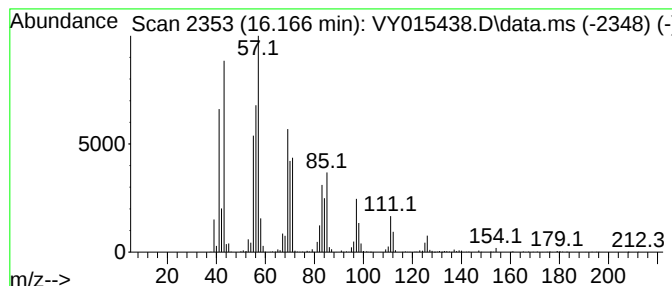
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Quant Title : SW846 8260

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

Peak Number 9 2-Methyl-1-undecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.166	53.66 ug/l	976066	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-1-undecanol	186	C12H26O	010522-26-6	90
2			2-Decanol, chlorodifluoroacetate	270	C12H21ClF2O2	1000447-45-4	87
3			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	72
4			Pentadecafluorooctanoic acid, un...	568	C19H23F15O2	1010406-04-1	64
5			Cyclopropane, 1-methyl-2-pentyl-	126	C9H18	041977-37-1	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090523\
Data File : VY015438.D
Acq On : 05 Sep 2023 18:15
Operator : SY/MD
Sample : 04278-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
824-829

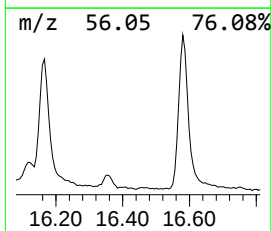
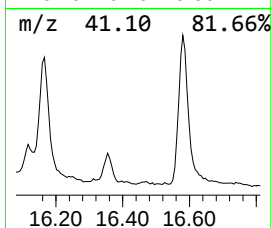
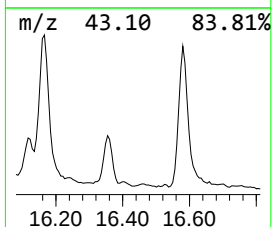
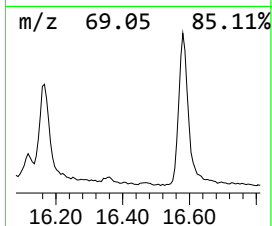
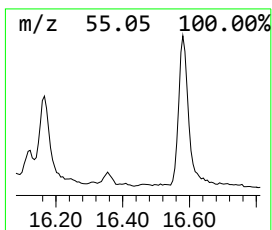
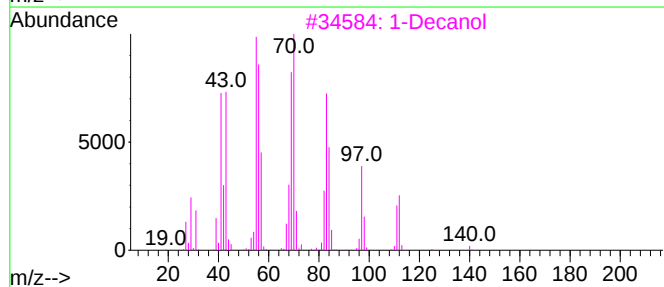
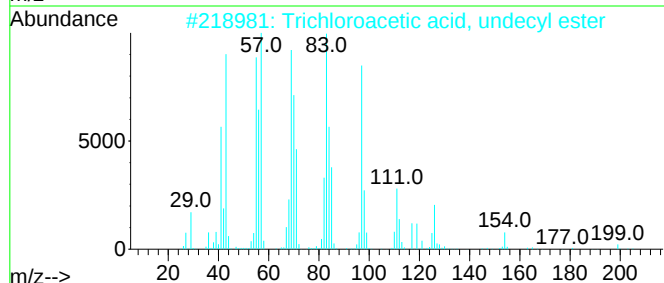
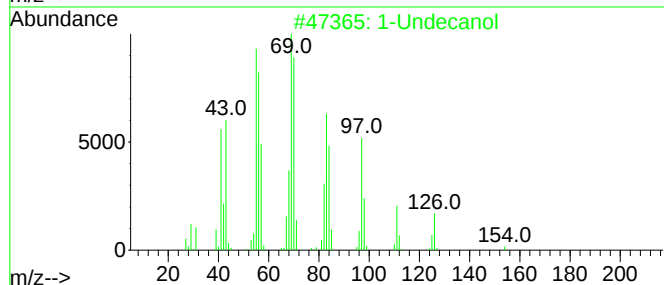
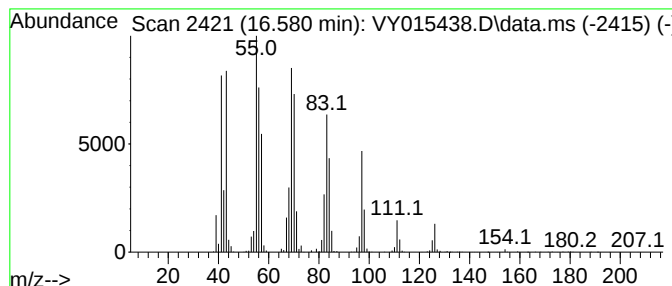
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Quant Title : SW846 8260

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

Peak Number 10 1-Undecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.580	75.29 ug/l	1369590	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Undecanol	172	C11H24O	000112-42-5	91
2			Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	90
3			1-Decanol	158	C10H22O	000112-30-1	87
4			n-Tridecan-1-ol	200	C13H28O	000112-70-9	87
5			Cyclodecane, methyl-	154	C11H22	013151-43-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY090523\
Data File : VY015438.D
Acq On : 05 Sep 2023 18:15
Operator : SY/MD
Sample : 04278-02
Misc : 5.01g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
824-829

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y082923S.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
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Cyclohexene, 1-...	13.873	68.8	ug/l	1251600	4	13.422	909513	50.0
1-Decene, 2,4-d...	14.422	205.0	ug/l	3729360	4	13.422	909513	50.0
1-Nonanol	14.751	220.9	ug/l	4018490	4	13.422	909513	50.0
1-Heptanol, 4-m...	14.959	74.7	ug/l	1358030	4	13.422	909513	50.0
Hexane, 2,3,4-t...	15.062	50.4	ug/l	915826	4	13.422	909513	50.0
Heptane, 2,4-di...	15.093	71.9	ug/l	1308330	4	13.422	909513	50.0
1-Decanol	15.605	489.9	ug/l	8911510	4	13.422	909513	50.0
2-Methyl-1-unde...	16.166	53.7	ug/l	976066	4	13.422	909513	50.0
1-Undecanol	16.580	75.3	ug/l	1369590	4	13.422	909513	50.0