

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112524\
 Data File : VY020440.D
 Acq On : 25 Nov 2024 19:17
 Operator : SY/MD
 Sample : P4946-02
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 BW-2

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\82Y111924S.M

Title : SW846 8260

Signal : TIC: VY020440.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.110	381	392	405	rBV	15350	44146	2.74%	0.732%
2	6.890	837	848	858	rBV	11914	36574	2.27%	0.607%
3	7.634	960	970	977	rBV2	90060	223310	13.86%	3.704%
4	7.713	977	983	995	rVB	151833	345218	21.42%	5.726%
5	8.067	1030	1041	1053	rVB	80848	183095	11.36%	3.037%
6	8.616	1123	1131	1145	rVB	259273	502698	31.19%	8.338%
7	9.999	1349	1358	1367	rBV2	9799	17899	1.11%	0.297%
8	10.109	1367	1376	1384	rBV	399916	680244	42.21%	11.283%
9	10.512	1436	1442	1449	rBV2	17558	32982	2.05%	0.547%
10	10.871	1495	1501	1510	rBV4	11906	23855	1.48%	0.396%
11	11.414	1583	1590	1601	rBV	369631	609314	37.80%	10.106%
12	11.950	1672	1678	1686	rBV	29983	44952	2.79%	0.746%
13	12.261	1723	1729	1734	rBV2	21783	35311	2.19%	0.586%
14	12.408	1746	1753	1762	rVB	288732	453730	28.15%	7.526%
15	12.536	1766	1774	1782	rVB4	7803	16714	1.04%	0.277%
16	12.688	1790	1799	1804	rBV	56191	93203	5.78%	1.546%
17	13.194	1878	1882	1888	rVB2	14050	20896	1.30%	0.347%
18	13.346	1901	1907	1917	rBV	312690	487135	30.22%	8.080%
19	13.450	1918	1924	1942	rBV	1094768	1611757	100.00%	26.733%
20	13.822	1980	1985	1989	rBV4	10730	19798	1.23%	0.328%
21	13.889	1992	1996	2001	rVB3	10162	17766	1.10%	0.295%
22	14.023	2013	2018	2022	rBV2	11270	17203	1.07%	0.285%
23	14.078	2022	2027	2030	rVV4	12077	23405	1.45%	0.388%
24	14.133	2030	2036	2043	rVB3	42714	72808	4.52%	1.208%
25	14.371	2068	2075	2088	rVV5	30513	89926	5.58%	1.492%
26	14.468	2088	2091	2097	rVV	18988	34096	2.12%	0.566%
27	14.523	2097	2100	2108	rVB5	8630	17809	1.10%	0.295%
28	14.651	2117	2121	2124	rBV3	9897	16187	1.00%	0.268%
29	14.785	2134	2143	2145	rBV5	13437	29051	1.80%	0.482%
30	14.816	2145	2148	2150	rBV3	14488	19234	1.19%	0.319%
31	14.883	2155	2159	2166	rVB4	30447	74248	4.61%	1.231%
32	14.956	2167	2171	2178	rBV2	24672	50027	3.10%	0.830%
33	15.102	2187	2195	2203	rVB2	18713	45510	2.82%	0.755%
34	15.194	2205	2210	2221	rVB5	16598	39091	2.43%	0.648%

Sum of corrected areas: 6029192

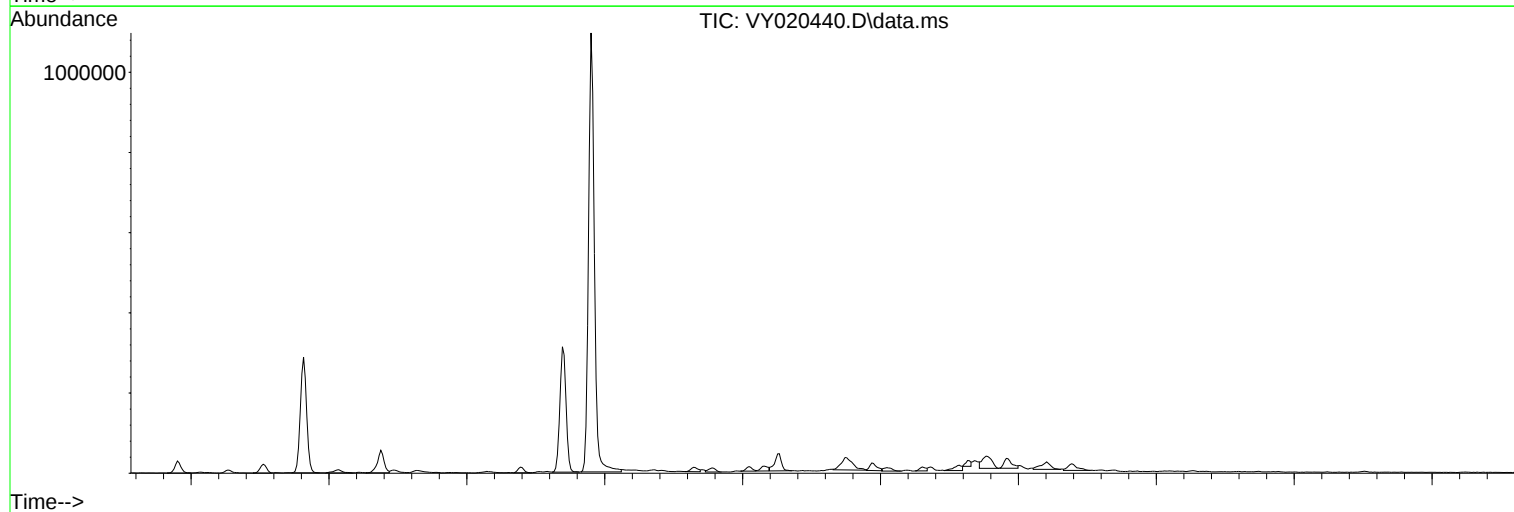
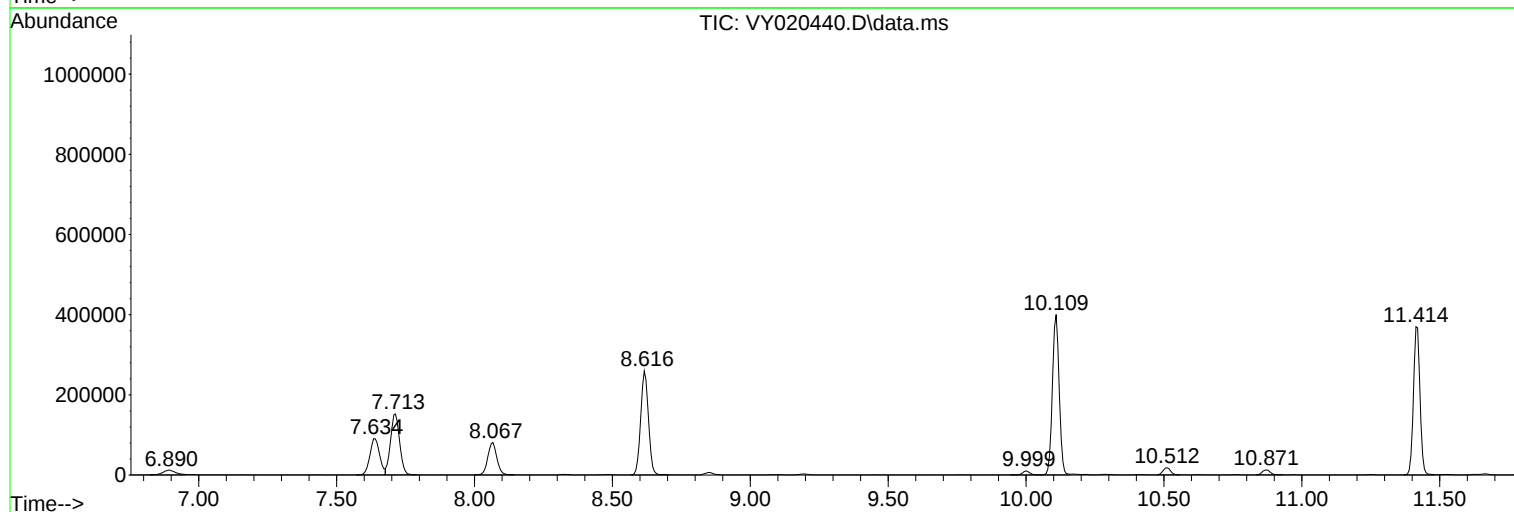
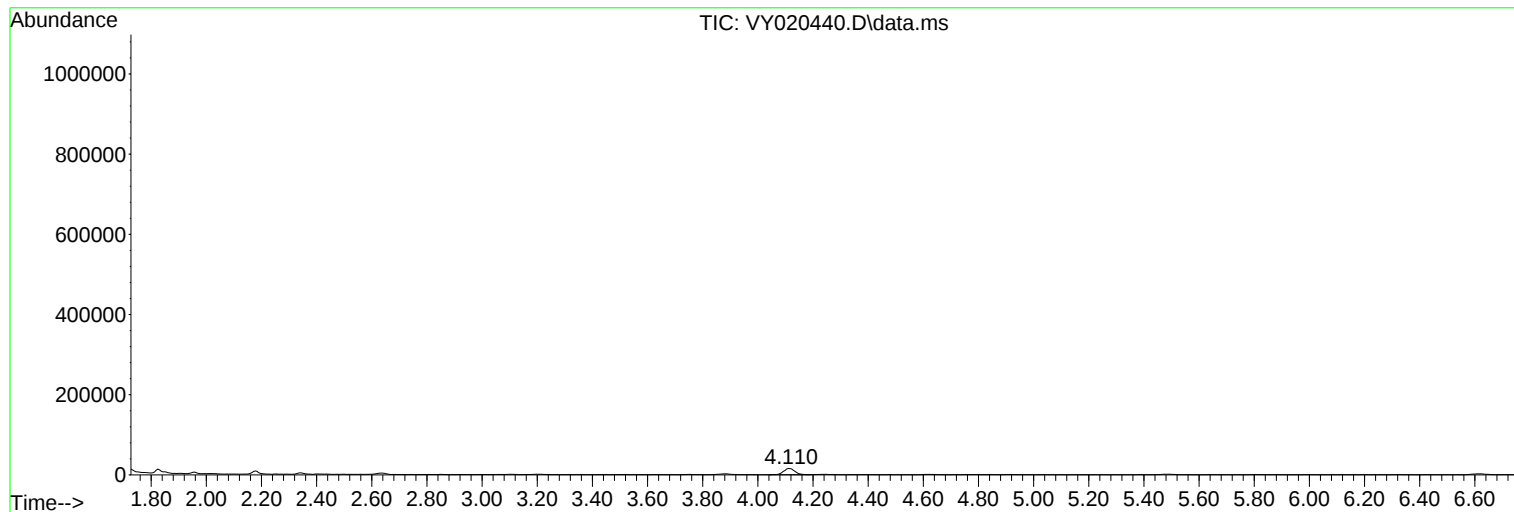
Instrument :
MSVOA_Y
ClientSampleId :
BW-2

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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



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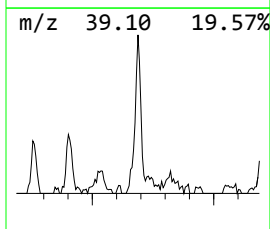
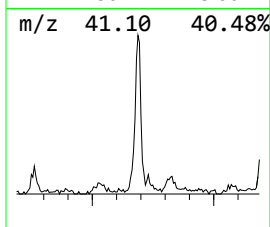
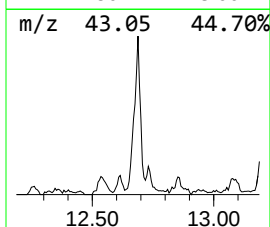
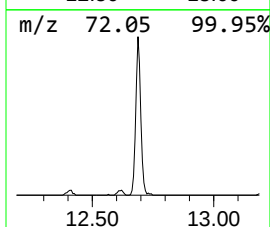
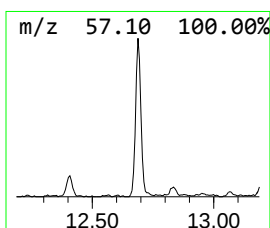
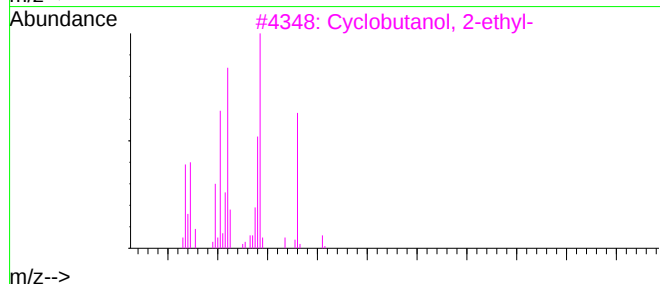
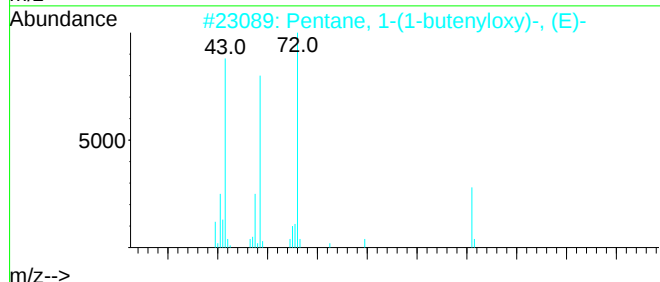
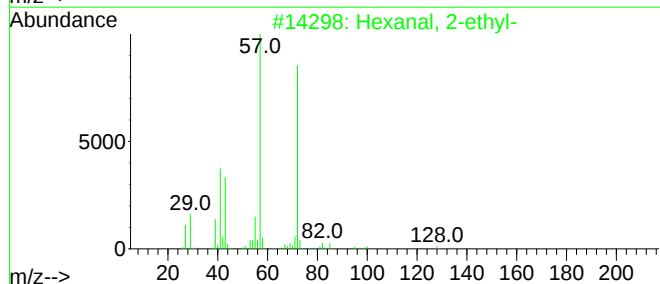
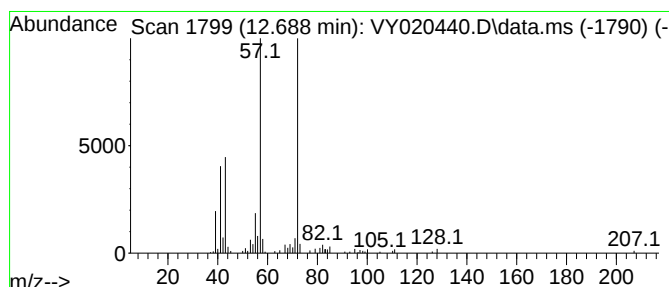
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 2 Hexanal, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.688	9.57 ug/l	93203	1,4-Dichlorobenzene-d4	13.352

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	90
2	Pentane, 1-(1-butenyloxy)-, (E)-	142	C9H18O	054004-25-0	59
3	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	56
4	Butanamine, N-cyclohexylmethyl-1...	211	C14H29N	1000271-47-8	53
5	2-(dimethylamino)-1-(2-methoxyph...	207	C12H17NO2	1000456-74-3	53



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Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 19 Sample Multiplier: 1

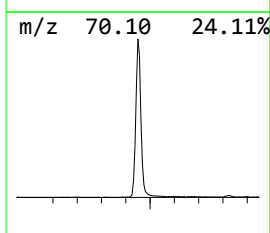
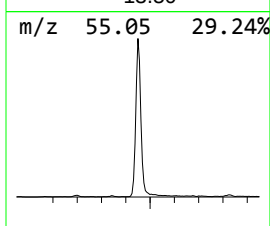
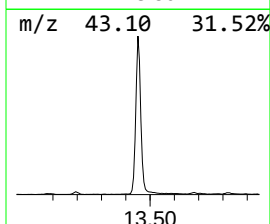
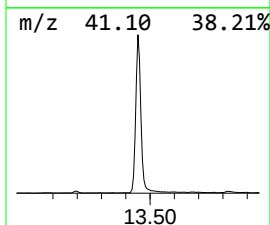
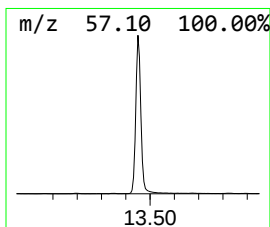
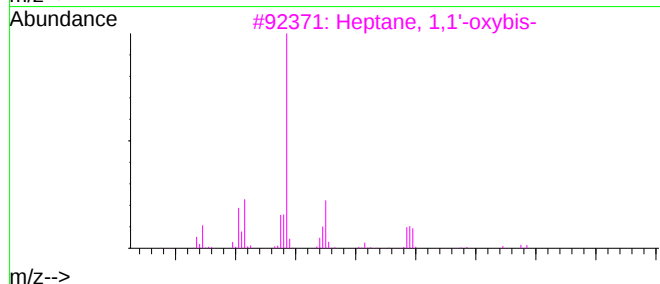
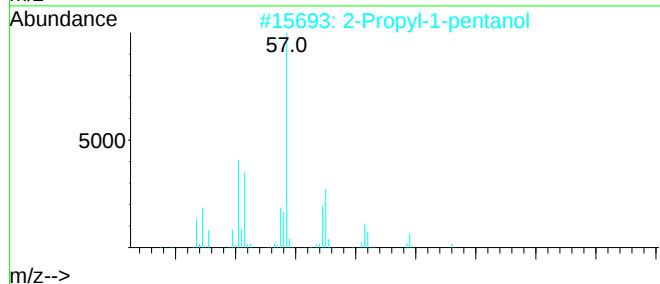
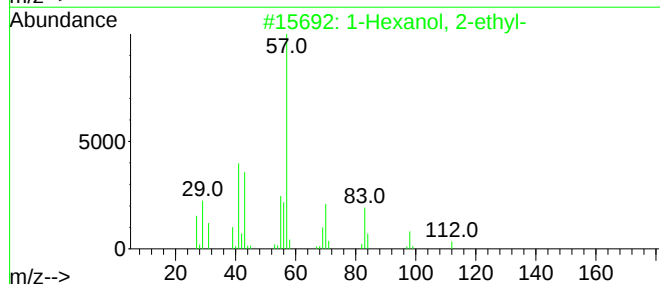
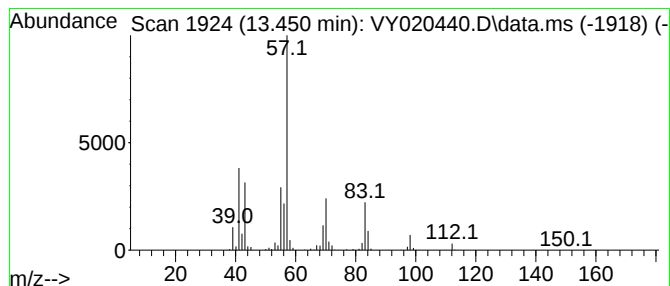
Instrument :
MSVOA_Y
ClientSampleId :
BW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.450	165.43 ug/l	1611760	1,4-Dichlorobenzene-d4	13.352	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	53
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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Instrument :
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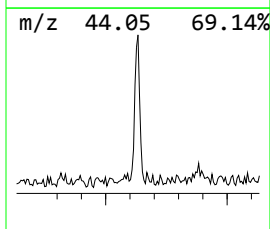
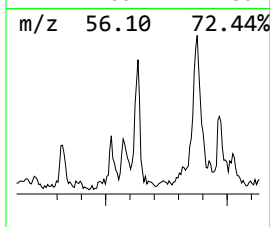
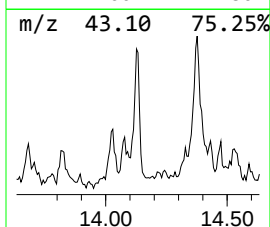
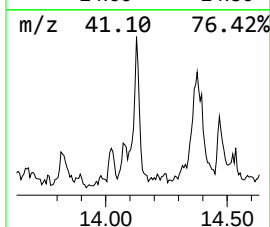
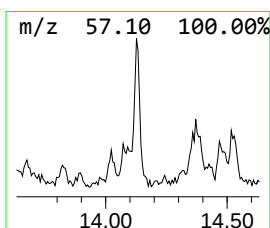
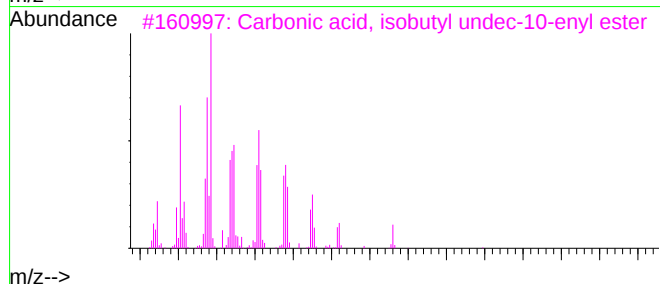
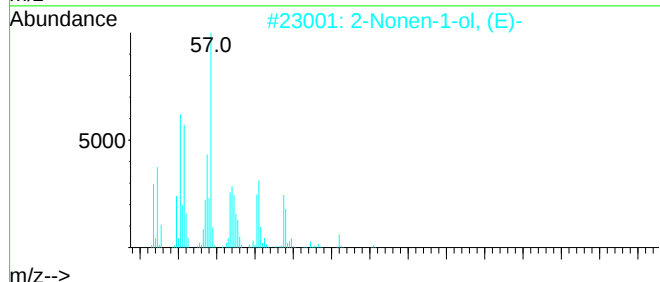
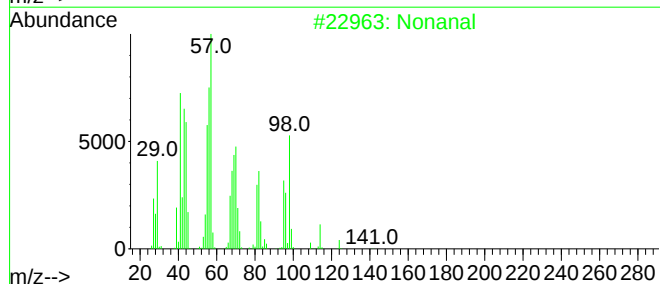
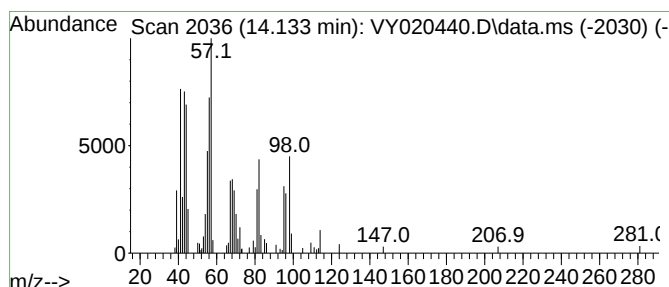
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 4 Nonanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.133	7.47 ug/l	72808	1,4-Dichlorobenzene-d4	13.352

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	91
2	2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	38
3	Carbonic acid, isobutyl undec-10...	270	C16H30O3	1000314-60-8	27
4	Cyclopentanol, 2-methyl-	100	C6H12O	024070-77-7	27
5	Cycloundecene (Z)	152	C11H20	013151-61-6	27



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Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
BW-2

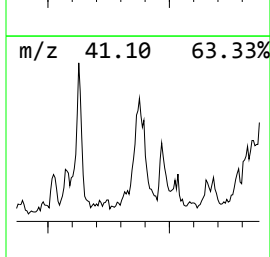
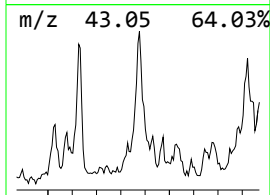
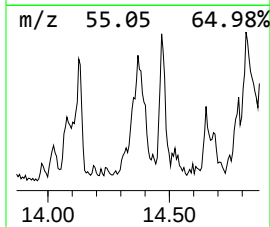
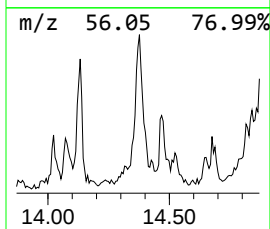
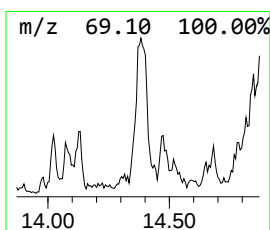
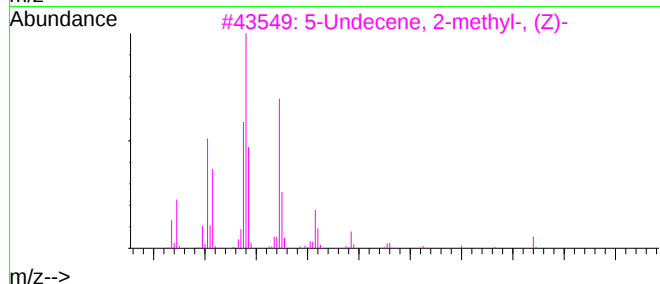
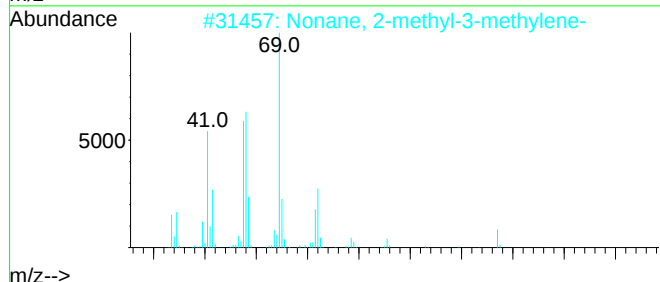
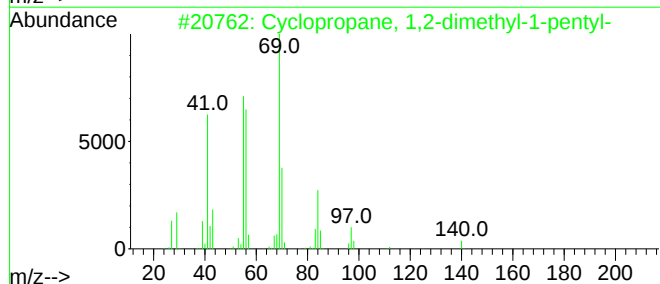
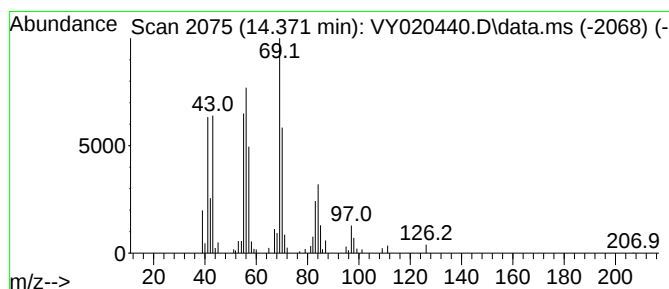
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.371	9.23 ug/l	89926	1,4-Dichlorobenzene-d4	13.352

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	64
2	Nonane, 2-methyl-3-methylene-	154	C11H22	055499-08-6	64
3	5-Undecene, 2-methyl-, (Z)-	168	C12H24	074630-63-0	64
4	2-Chloro-2-methylnonane	176	C10H21Cl	004325-50-2	59
5	1-Decene	140	C10H20	000872-05-9	50



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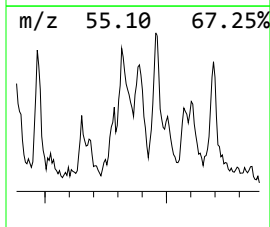
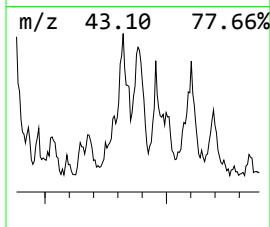
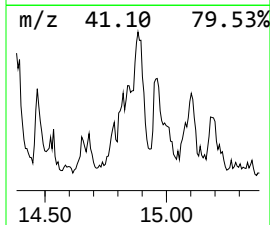
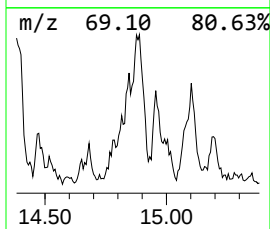
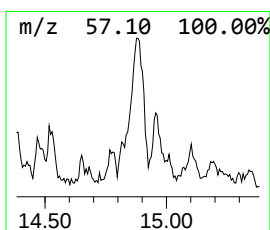
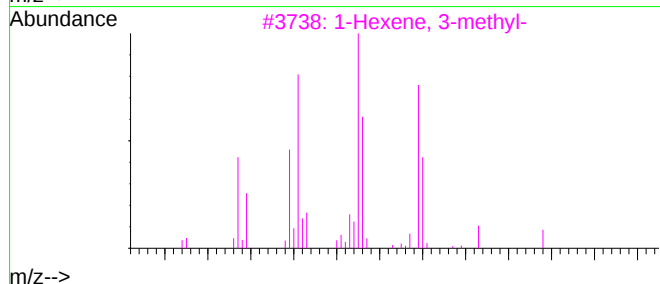
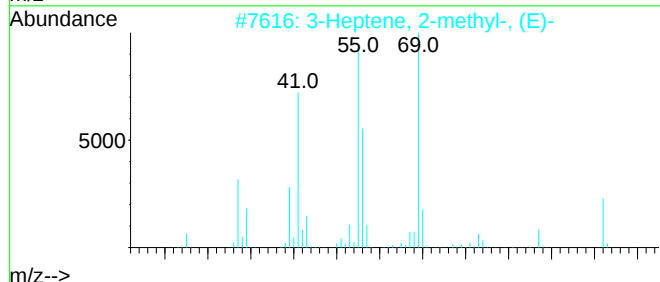
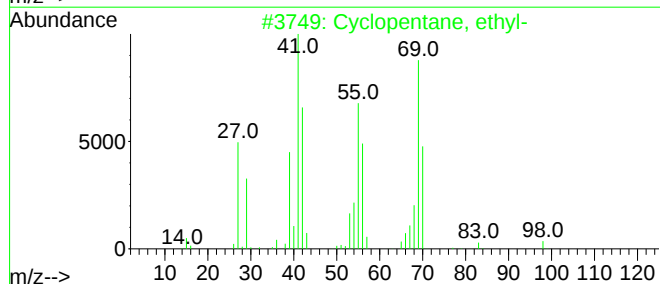
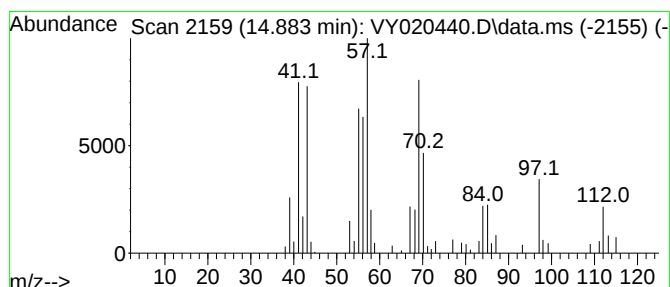
Instrument :
MSVOA_Y
ClientSampleId :
BW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown14.883 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.883	7.62 ug/l	74248	1,4-Dichlorobenzene-d4		13.352	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclopentane, ethyl-		98	C7H14	001640-89-7	49
2	3-Heptene, 2-methyl-, (E)-		112	C8H16	000692-96-6	43
3	1-Hexene, 3-methyl-		98	C7H14	003404-61-3	43
4	3-Heptene, 2-methyl-		112	C8H16	017618-76-7	43
5	Ethanone, 1-cyclopentyl-		112	C7H12O	006004-60-0	38



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Data File : VY020440.D
Acq On : 25 Nov 2024 19:17
Operator : SY/MD
Sample : P4946-02
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 19 Sample Multiplier: 1

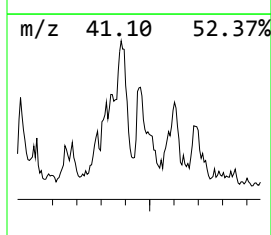
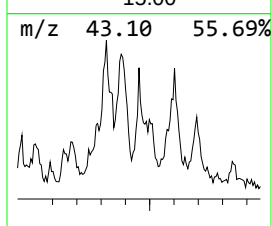
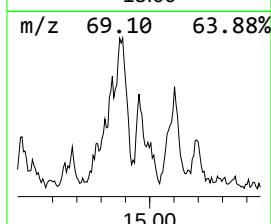
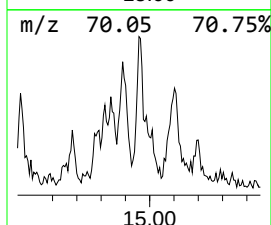
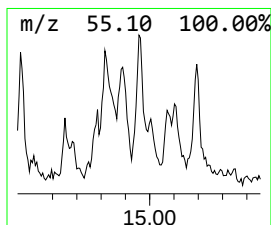
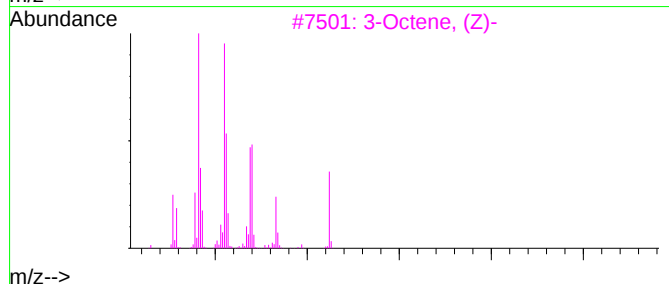
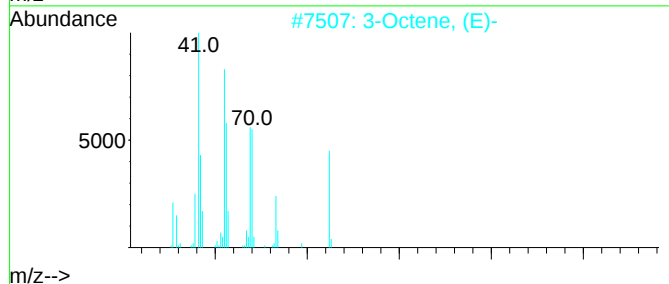
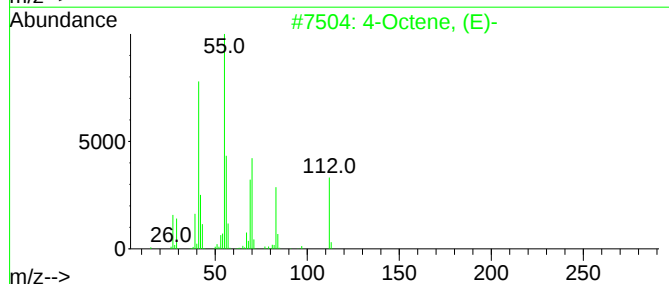
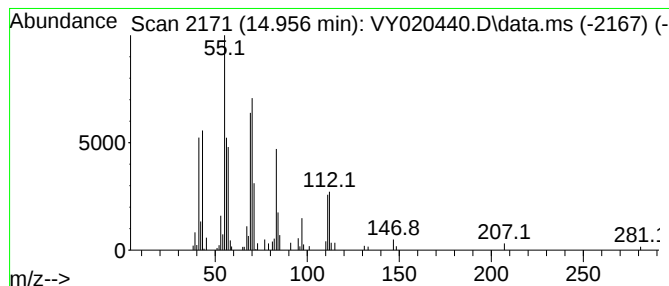
Instrument :
MSVOA_Y
ClientSampleId :
BW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

Peak Number 7 4-Octene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.956	5.13 ug/l	50027	1,4-Dichlorobenzene-d4	13.352	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Octene, (E)-	112	C8H16	014850-23-8	72
2	3-Octene, (E)-	112	C8H16	014919-01-8	62
3	3-Octene, (Z)-	112	C8H16	014850-22-7	58
4	Diphosphoric acid, diisooctyl ester	402	C16H36O7P2	072101-07-6	58
5	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY112524\
Data File : VY020440.D
Acq On : 25 Nov 2024 19:17
Operator : SY/MD
Sample : P4946-02
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
BW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111924S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal, 2-ethyl-	12.688	9.6	ug/l	93203	4	13.352	487135	50.0
1-Hexanol, 2-et...	13.450	165.4	ug/l	1611760	4	13.352	487135	50.0
Nonanal	14.133	7.5	ug/l	72808	4	13.352	487135	50.0
Cyclopropane, 1...	14.371	9.2	ug/l	89926	4	13.352	487135	50.0
unknown14.883	14.883	7.6	ug/l	74248	4	13.352	487135	50.0
4-Octene, (E)-	14.956	5.1	ug/l	50027	4	13.352	487135	50.0