

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091422\
 Data File : VY010493.D
 Acq On : 14 Sep 2022 18:44
 Operator : KP/MD
 Sample : N4588-01
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 AUD-1647

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\82Y090922S.M

Title : SW846 8260

Signal : TIC: VY010493.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.936	335	347	381	rBV	13207988	35578093	40.59%	16.568%
2	6.680	785	797	808	rBV2	424763	1409583	1.61%	0.656%
3	7.521	927	935	949	rVB	368670	1056652	1.21%	0.492%
4	7.759	956	974	984	rBV	6655814	16027527	18.29%	7.464%
5	7.868	984	992	1001	rVV	2139380	5267035	6.01%	2.453%
6	7.996	1001	1013	1029	rVV	9100889	20281905	23.14%	9.445%
7	8.265	1046	1057	1063	rVV4	1064582	2869312	3.27%	1.336%
8	8.338	1063	1069	1075	rVV2	462109	1321241	1.51%	0.615%
9	8.411	1075	1081	1092	rVB2	509499	1247299	1.42%	0.581%
10	8.545	1092	1103	1114	rBV	5792317	10988077	12.54%	5.117%
11	9.179	1192	1207	1213	rBV2	1338074	3239723	3.70%	1.509%
12	9.240	1213	1217	1232	rVV2	477059	1015723	1.16%	0.473%
13	9.612	1270	1278	1291	rVB2	882670	1760511	2.01%	0.820%
14	9.953	1323	1334	1347	rVB4	353096	1079298	1.23%	0.503%
15	10.112	1355	1360	1365	rVB	524897	902294	1.03%	0.420%
16	10.173	1365	1370	1374	rVV2	747089	1307495	1.49%	0.609%
17	10.240	1374	1381	1394	rVV2	38862543	87650411	100.00%	40.818%
18	10.368	1394	1402	1409	rVB	1144208	2031749	2.32%	0.946%
19	10.801	1464	1473	1480	rBV4	390526	1256775	1.43%	0.585%
20	11.087	1515	1520	1525	rVV	583973	1092769	1.25%	0.509%
21	11.276	1542	1551	1562	rVB6	791058	2415933	2.76%	1.125%
22	11.380	1562	1568	1573	rBV2	820747	1507013	1.72%	0.702%
23	11.587	1595	1602	1611	rVB3	429854	981383	1.12%	0.457%
24	11.709	1611	1622	1625	rBV2	1592435	3398668	3.88%	1.583%
25	12.026	1662	1674	1679	rVB5	355060	996305	1.14%	0.464%
26	12.240	1705	1709	1719	rVB5	450498	954583	1.09%	0.445%
27	12.386	1727	1733	1740	rBV4	481398	1150938	1.31%	0.536%
28	12.733	1783	1790	1793	rBV	658178	1071023	1.22%	0.499%
29	12.800	1793	1801	1806	rBV5	739188	1767670	2.02%	0.823%
30	13.197	1858	1866	1872	rBV3	480269	1002249	1.14%	0.467%
31	13.587	1924	1930	1934	rBV	621826	1223301	1.40%	0.570%
32	13.751	1953	1957	1961	rBV	692906	881292	1.01%	0.410%

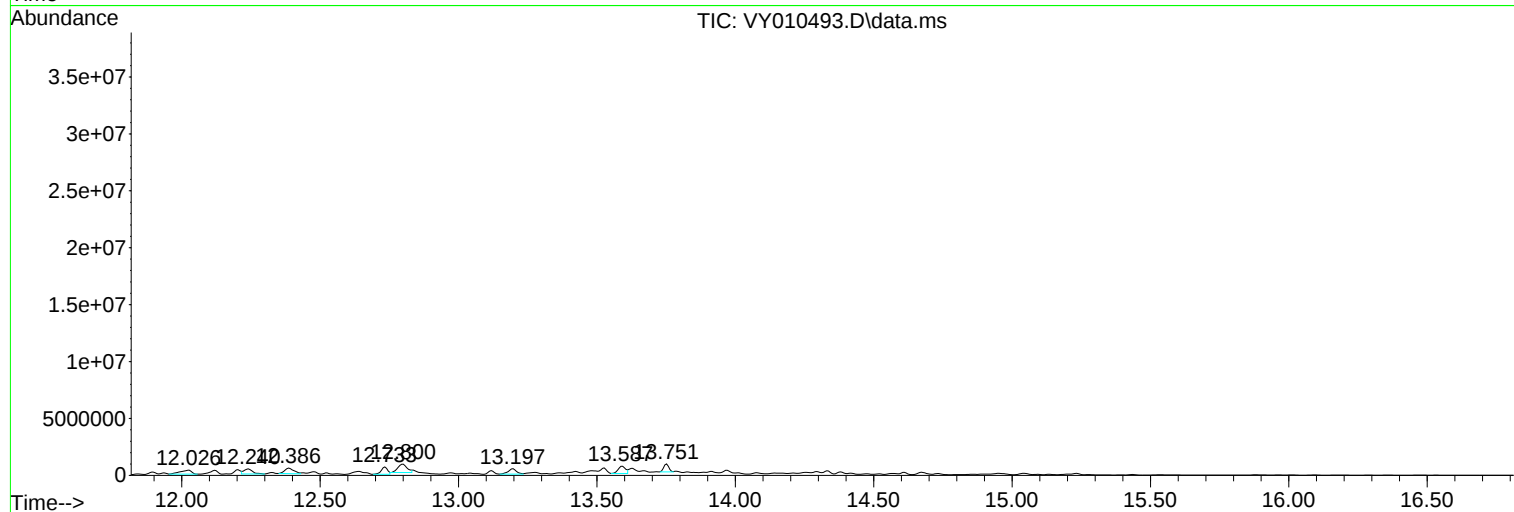
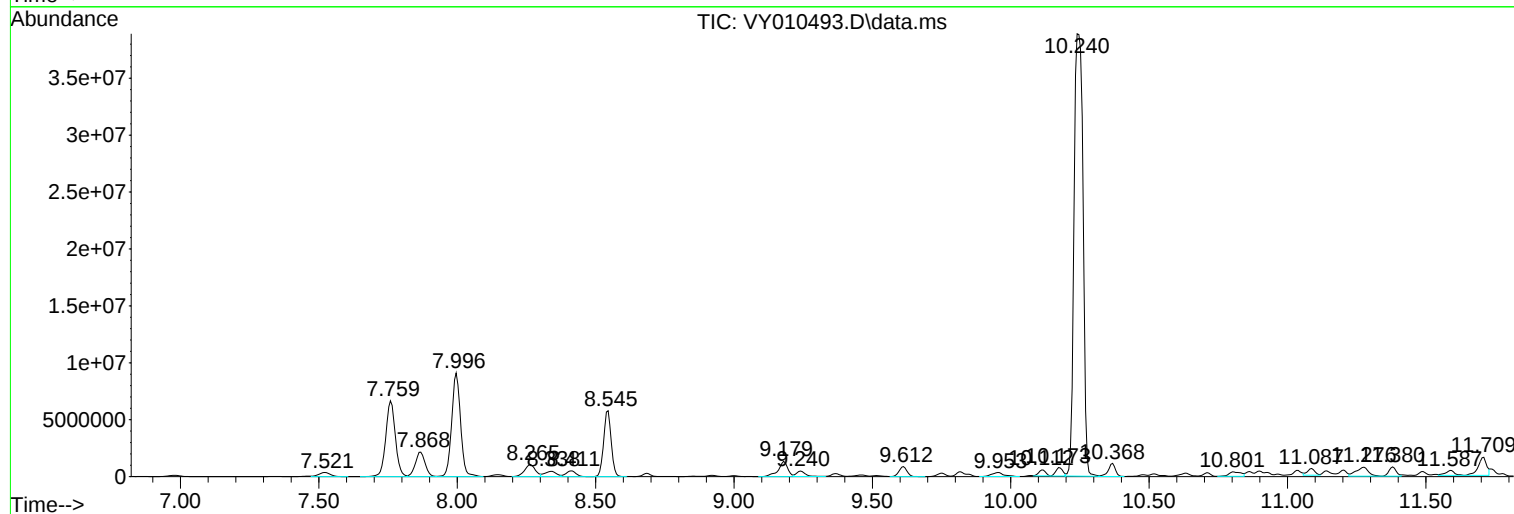
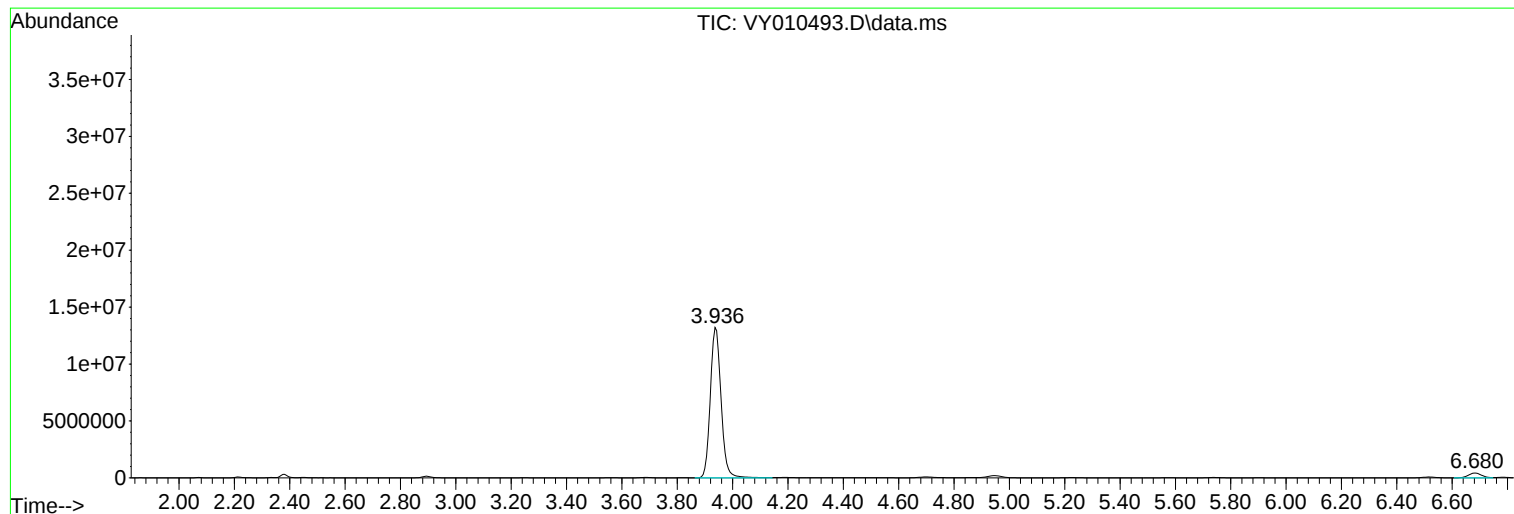
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090922S.M
Quant Title : SW846 8260

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



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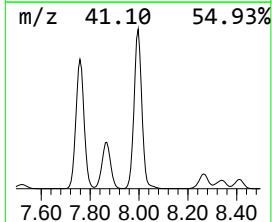
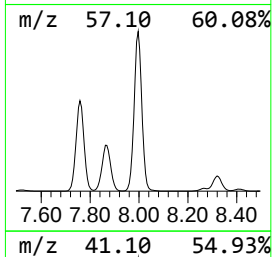
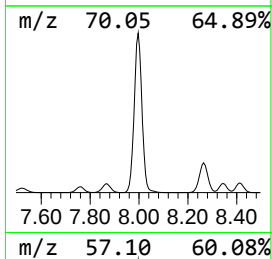
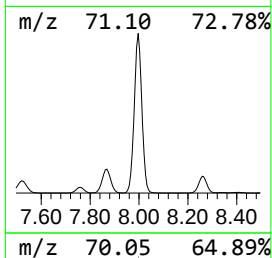
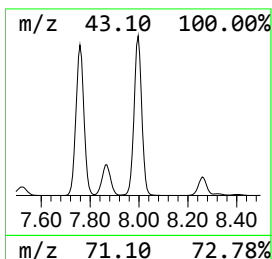
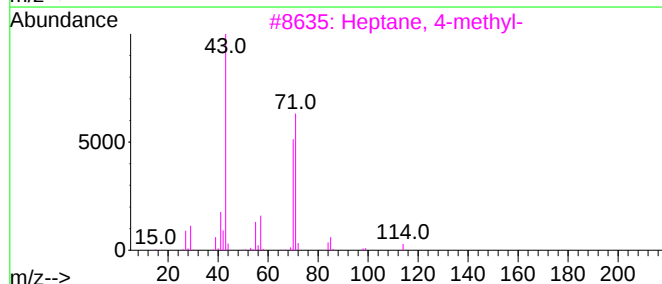
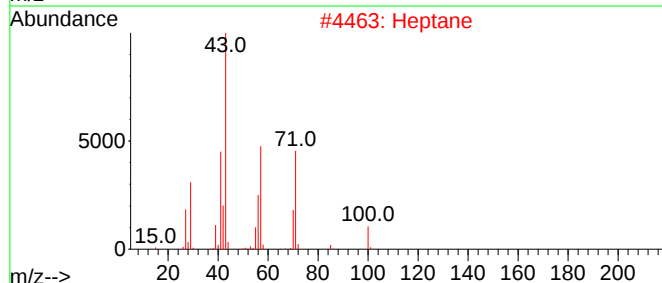
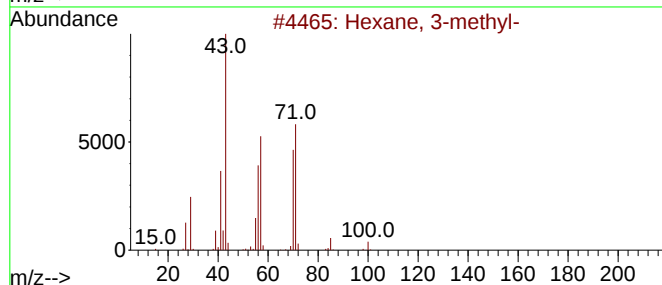
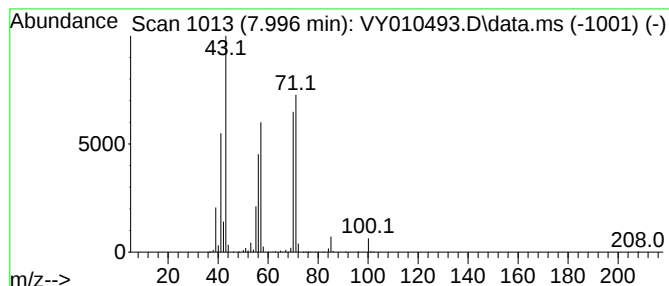
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090922S.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Hexane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.996	63.27 ug/l	20281900	Pentafluorobenzene	7.783

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2		Heptane	100	C7H16	000142-82-5	72
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	53
4		Pentane, 3-ethyl-	100	C7H16	000617-78-7	53
5		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



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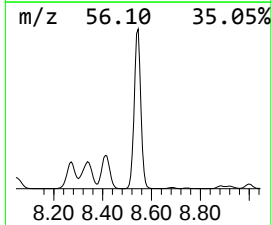
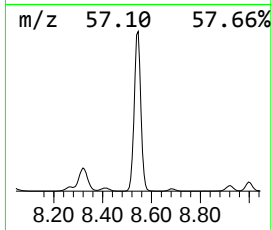
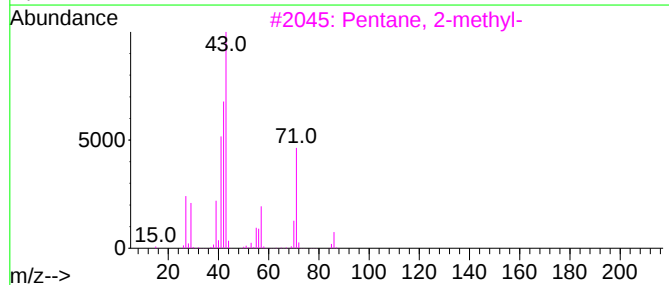
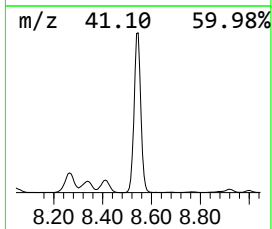
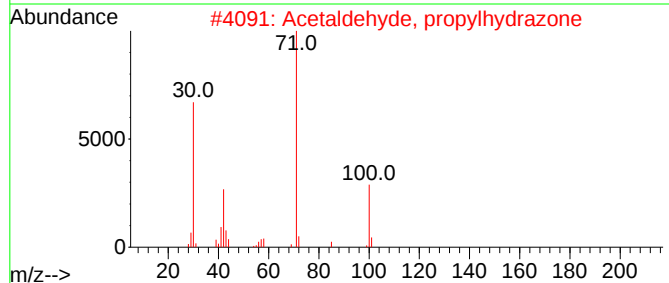
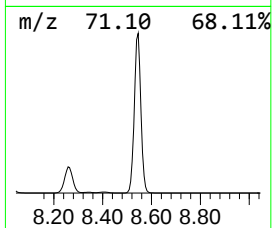
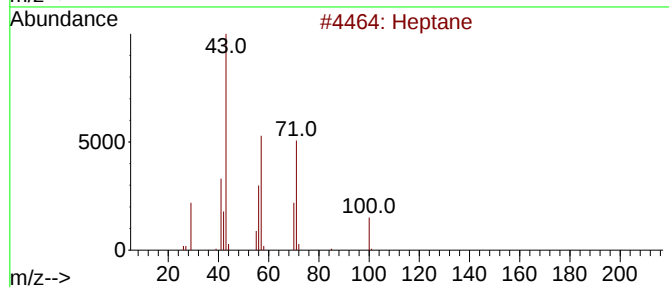
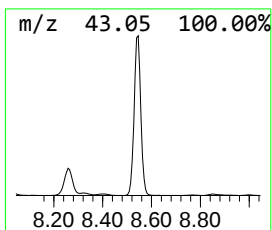
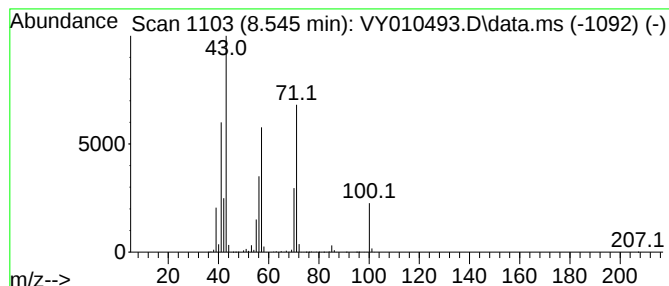
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Peak Number 2 Heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	50.00 ug/l	10988100	1,4-Difluorobenzene	8.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	49
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	43
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	37



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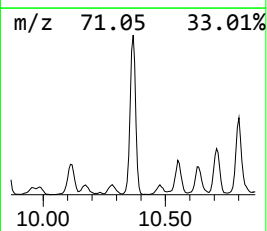
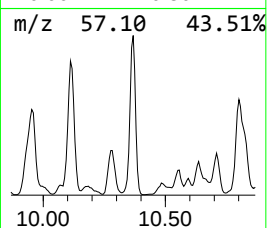
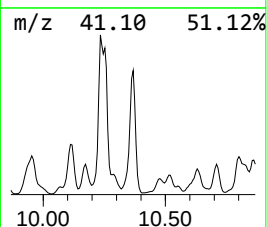
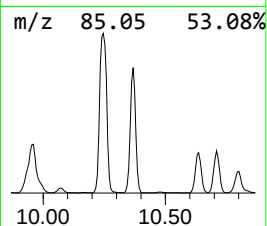
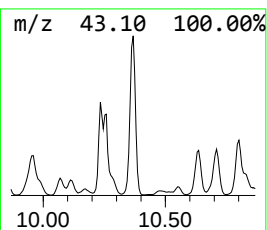
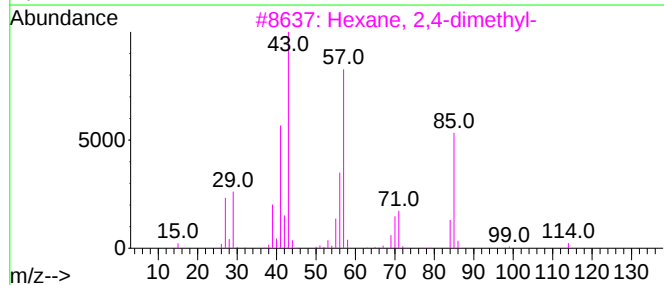
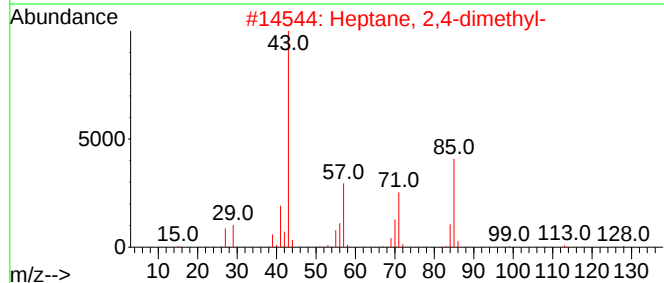
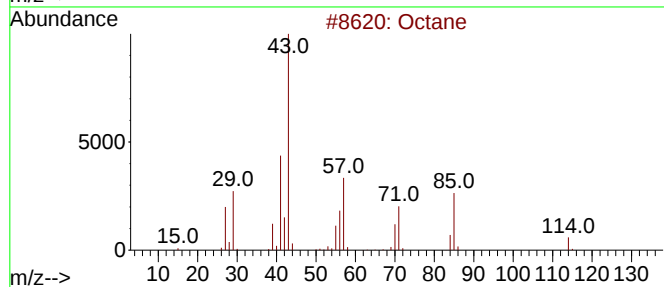
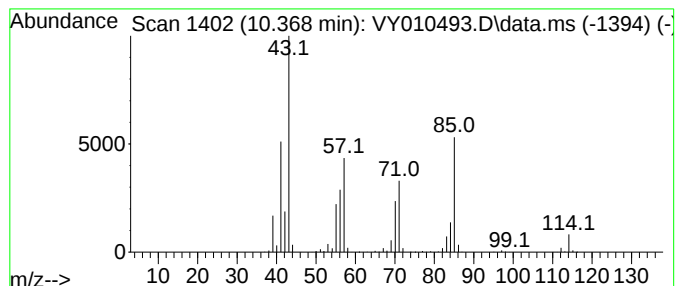
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.368	103.52 ug/l	2031750	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	91
2			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	80
3			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
4			Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	64
5			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	53



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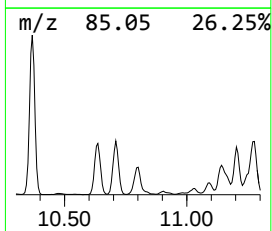
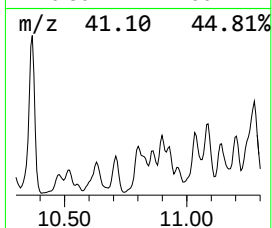
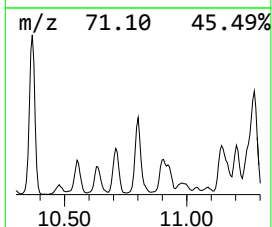
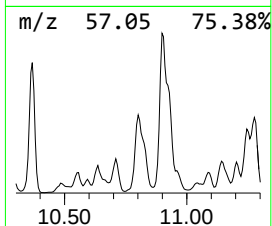
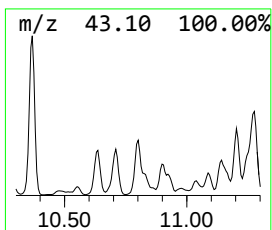
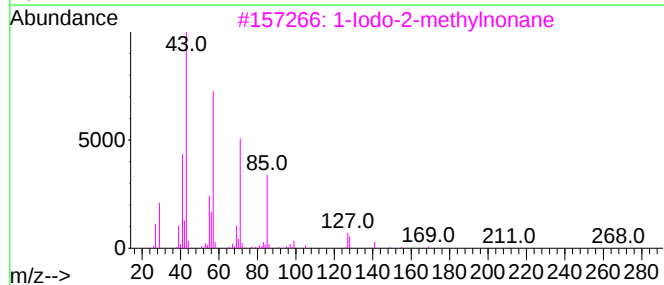
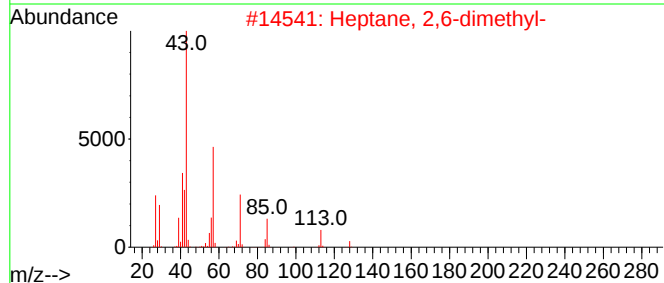
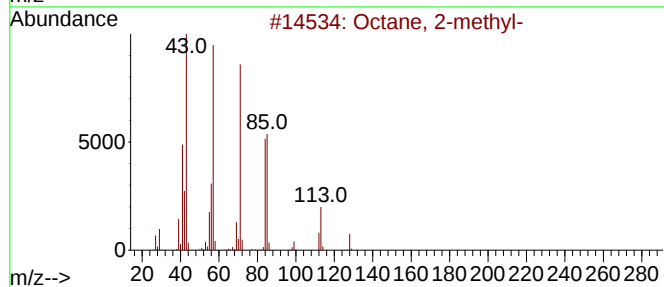
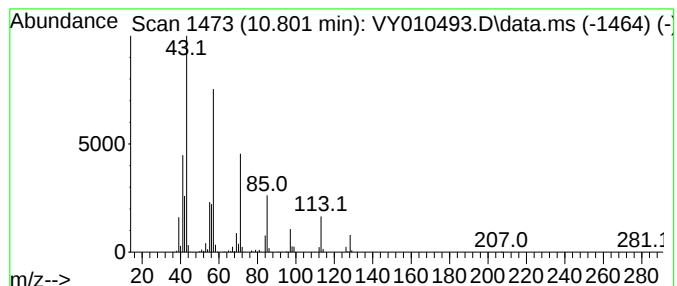
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.801	64.03 ug/l	1256780	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-methyl-	128	C9H20	003221-61-2	87
2			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	74
3			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	58
4			Nonane	128	C9H20	000111-84-2	52
5			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	50



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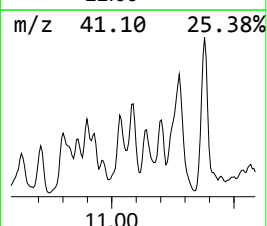
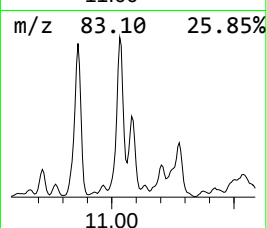
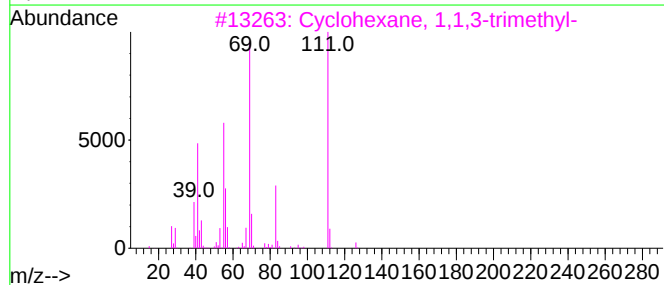
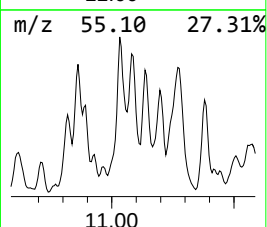
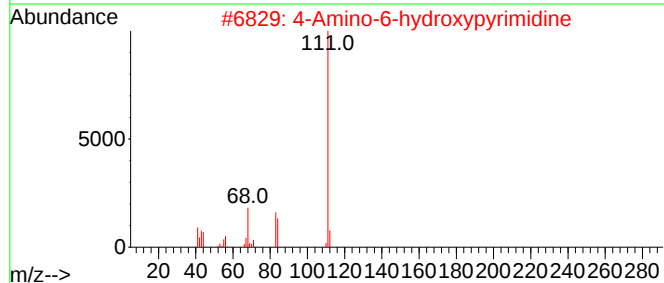
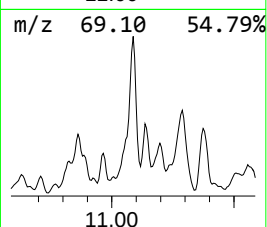
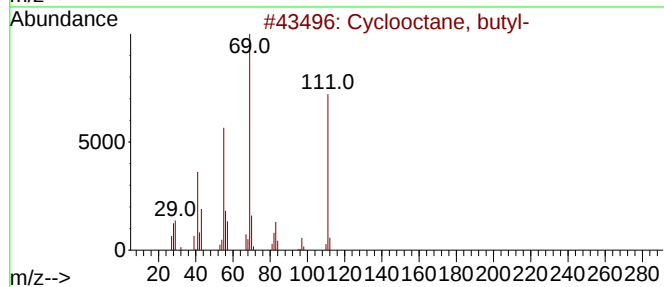
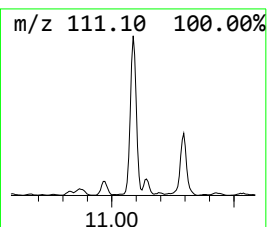
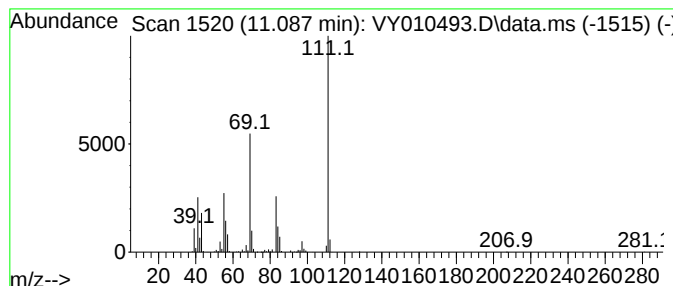
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Peak Number 5 Cyclooctane, butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.087	55.67 ug/l	1092770	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane, butyl-	168	C12H24	016538-93-5	64
2			4-Amino-6-hydroxypyrimidine	111	C4H5N3O	001193-22-2	59
3			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	56
4			Cyclohexane, 1,2,4-trimethyl-, (...)	126	C9H18	007667-60-9	50
5			Benzenamine, 3-fluoro-	111	C6H6FN	000372-19-0	42



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ClientSampleId :
AUD-1647

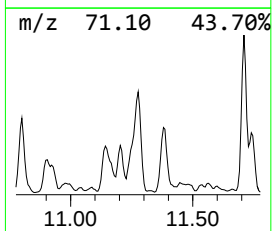
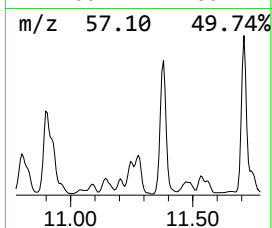
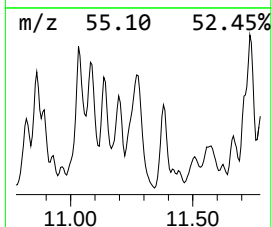
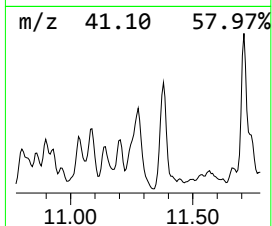
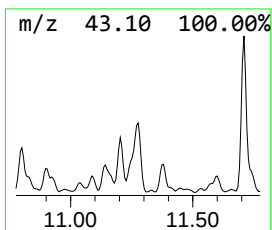
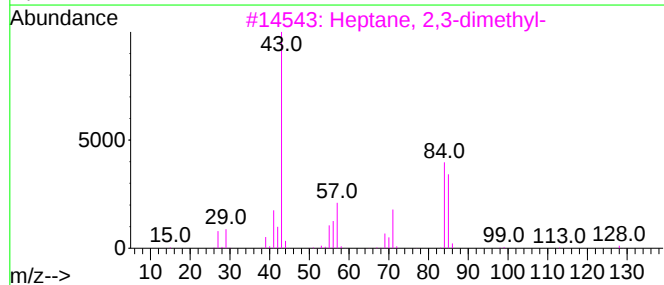
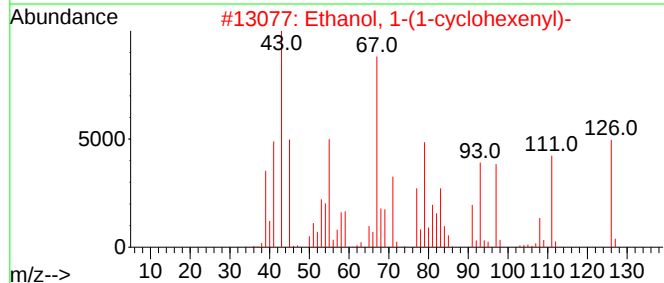
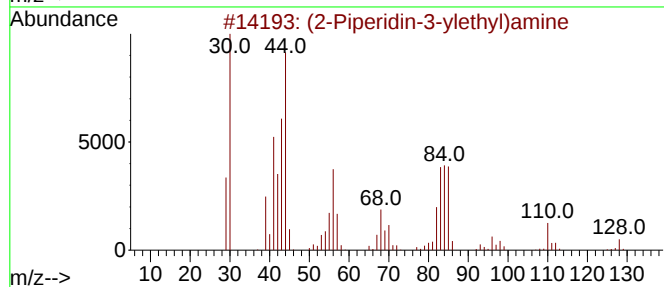
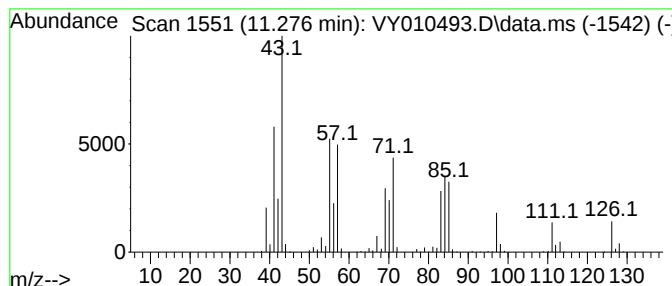
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Quant Title : SW846 8260

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

Peak Number 6 unknown11.276 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.276	123.09 ug/l	2415930	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2-Piperidin-3-ylethyl)amine	128	C7H16N2	089850-94-2	46
2			Ethanol, 1-(1-cyclohexenyl)-	126	C8H14O	003197-68-0	43
3			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	43
4			Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	007667-55-2	38
5			Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091422\
Data File : VY010493.D
Acq On : 14 Sep 2022 18:44
Operator : KP/MD
Sample : N4588-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1647

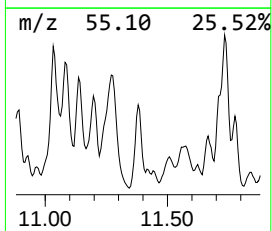
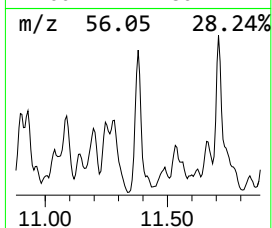
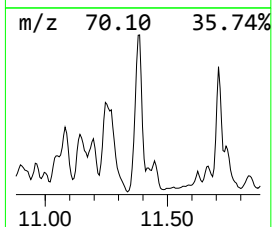
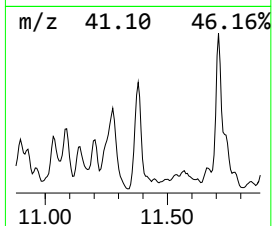
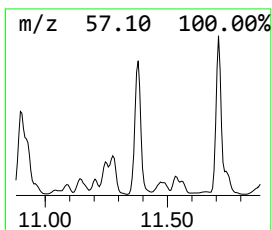
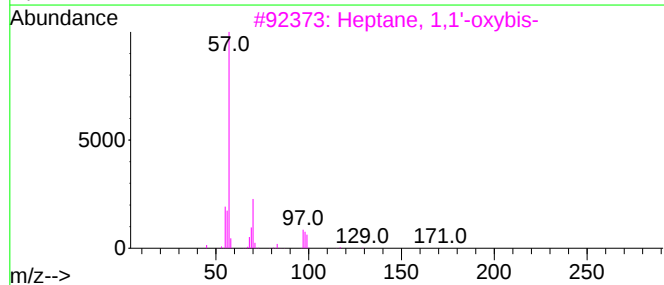
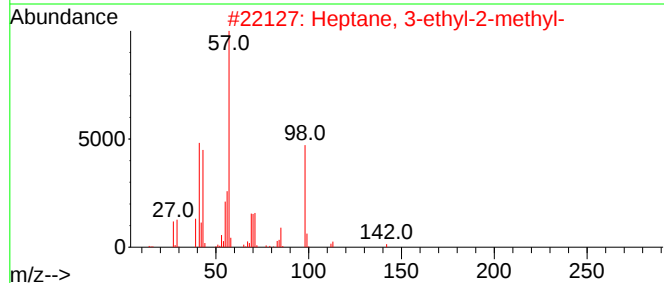
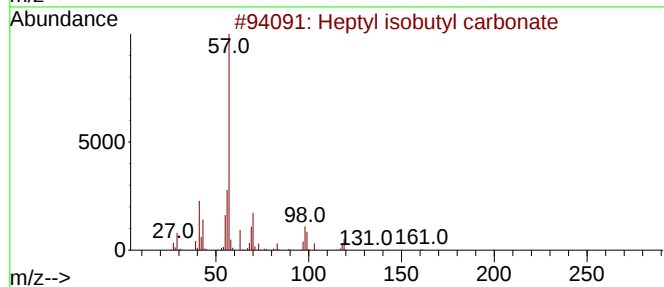
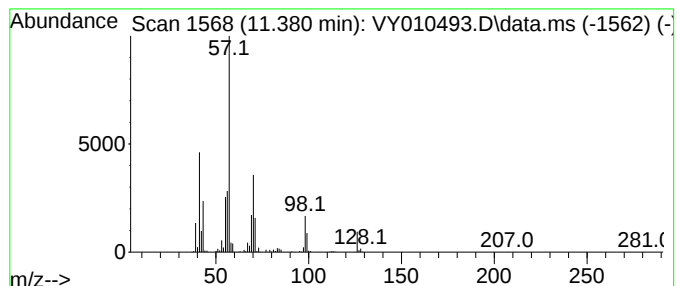
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Quant Title : SW846 8260

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

Peak Number 7 Heptyl isobutyl carbonate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.380	76.78 ug/l	1507010	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	59
2			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	59
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	50
5			2-Hexene, 3,5,5-trimethyl-	126	C9H18	026456-76-8	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091422\
Data File : VY010493.D
Acq On : 14 Sep 2022 18:44
Operator : KP/MD
Sample : N4588-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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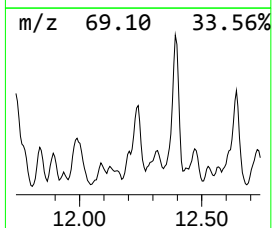
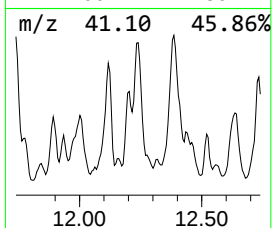
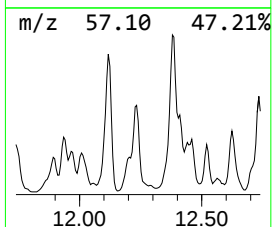
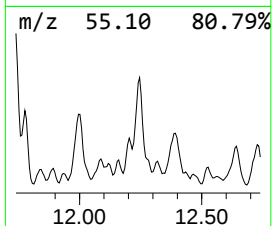
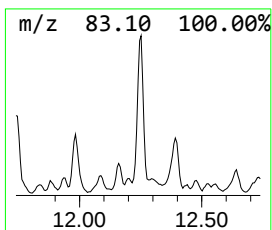
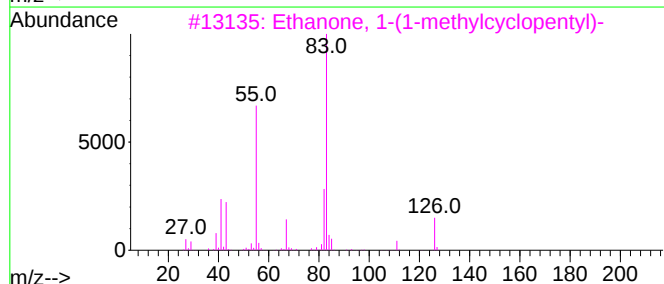
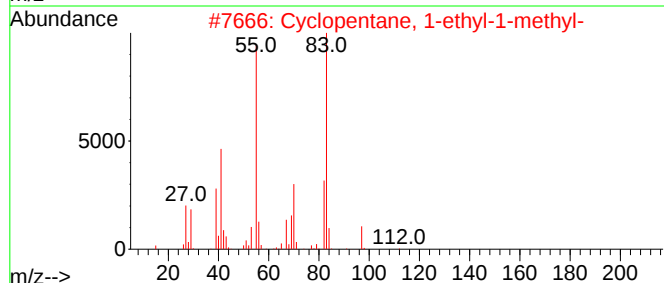
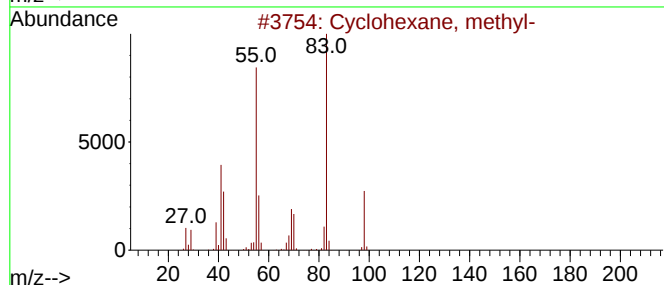
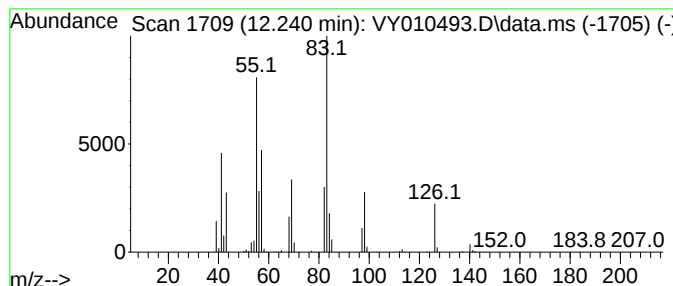
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Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.240	48.63 ug/l	954583	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, methyl-	98	C7H14	000108-87-2	59
2			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	58
3			Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	53
4			Cyclohexane, propyl-	126	C9H18	001678-92-8	50
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091422\
Data File : VY010493.D
Acq On : 14 Sep 2022 18:44
Operator : KP/MD
Sample : N4588-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

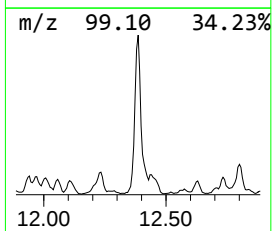
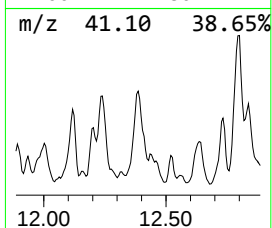
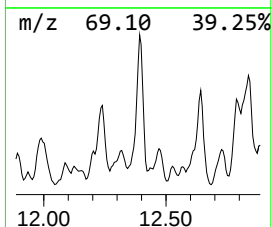
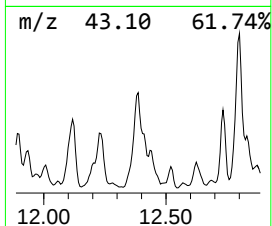
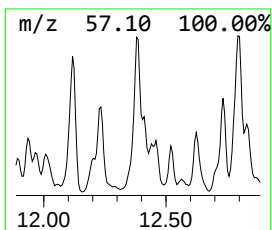
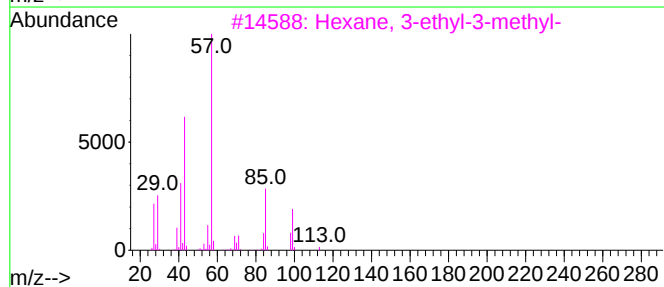
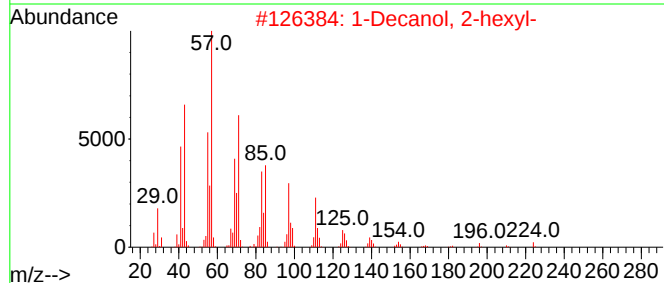
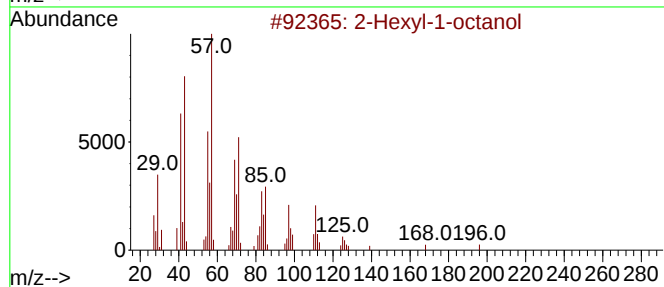
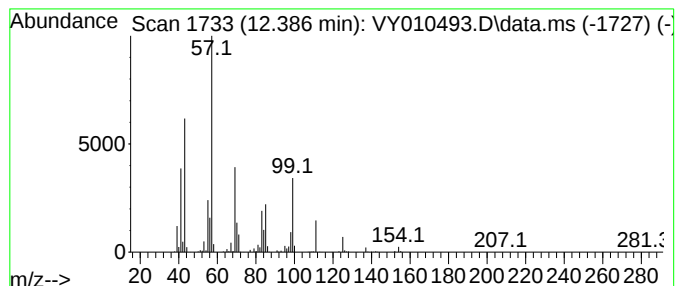
Instrument :
MSVOA_Y
ClientSampleId :
AUD-1647

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090922S.M
Quant Title : SW846 8260

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

Peak Number 9 2-Hexyl-1-octanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.386	58.64 ug/l	1150940	Chlorobenzene-d5	11.490	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	59
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	59
3	Hexane, 3-ethyl-3-methyl-	128	C9H20	003074-76-8	43
4	Decane	142	C10H22	000124-18-5	43
5	2,2,4,4-Tetramethyloctane	170	C12H26	062183-79-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091422\
Data File : VY010493.D
Acq On : 14 Sep 2022 18:44
Operator : KP/MD
Sample : N4588-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1647

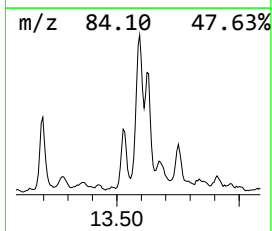
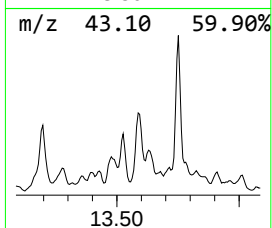
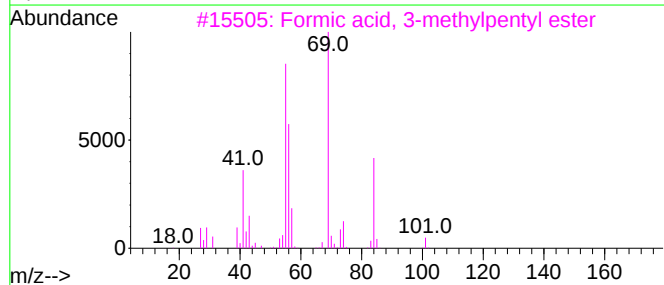
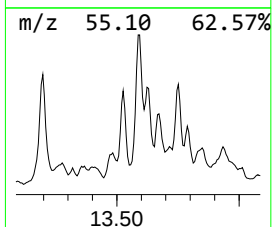
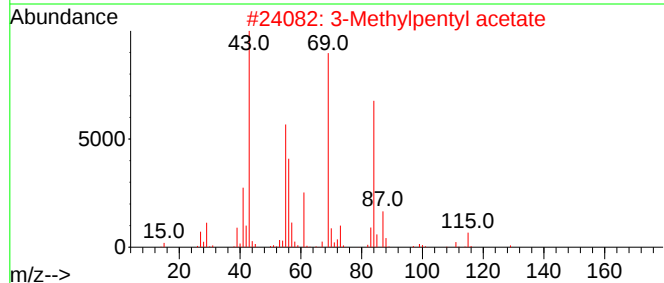
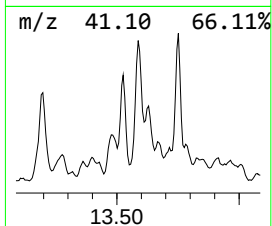
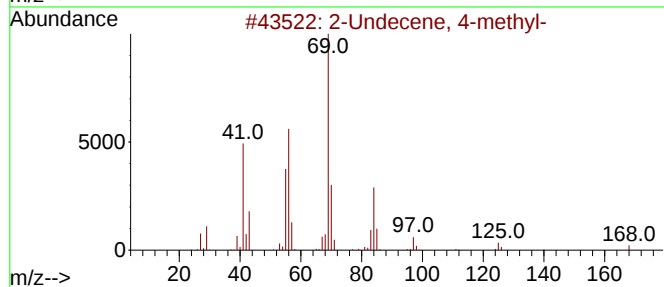
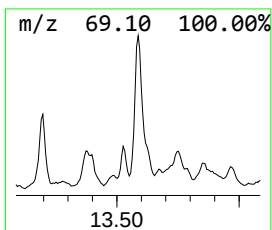
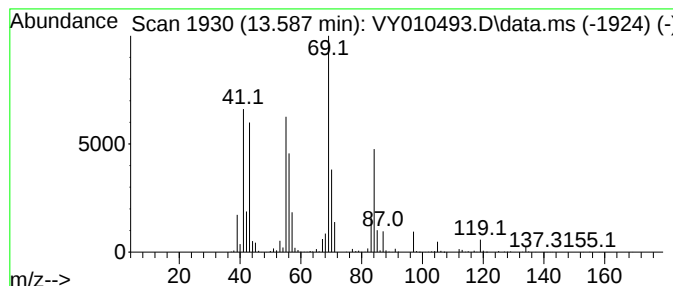
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Quant Title : SW846 8260

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

Peak Number 10 2-Undecene, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.587	50.00 ug/l	1223300	1,4-Dichlorobenzene-d4	13.422

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Undecene, 4-methyl-	168	C12H24	091695-32-8	59
2		3-Methylpentyl acetate	144	C8H16O2	035897-13-3	53
3		Formic acid, 3-methylpentyl ester	130	C7H14O2	1000368-21-3	50
4		(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	50
5		1-Hexene, 3,3,5-trimethyl-	126	C9H18	013427-43-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091422\
Data File : VY010493.D
Acq On : 14 Sep 2022 18:44
Operator : KP/MD
Sample : N4588-01
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
AUD-1647

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090922S.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
Hexane, 3-methyl-	7.996	63.3	ug/l	20281900	1	7.783	16027500	50.0
Heptane	8.545	50.0	ug/l	10988100	2	8.685	10988100	50.0
Octane	10.368	103.5	ug/l	2031750	3	11.490	981383	50.0
Octane, 2-methyl-	10.801	64.0	ug/l	1256780	3	11.490	981383	50.0
Cyclooctane, bu...	11.087	55.7	ug/l	1092770	3	11.490	981383	50.0
unknown11.276	11.276	123.1	ug/l	2415930	3	11.490	981383	50.0
Heptyl isobutyl...	11.380	76.8	ug/l	1507010	3	11.490	981383	50.0
Cyclohexane, me...	12.240	48.6	ug/l	954583	3	11.490	981383	50.0
2-Hexyl-1-octanol	12.386	58.6	ug/l	1150940	3	11.490	981383	50.0
2-Undecene, 4-m...	13.587	50.0	ug/l	1223300	4	13.422	1223300	50.0