

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030623\
 Data File : VY012833.D
 Acq On : 06 Mar 2023 18:52
 Operator : KP/MD
 Sample : 01742-01
 Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RBR251669

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\82Y030223S.M
 Title : SW846 8260

Signal : TIC: VY012833.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.716	462	475	487	rVB2	9996	31360	3.56%	0.482%
2	6.978	834	846	855	rBV2	2991	9282	1.05%	0.143%
3	7.716	957	967	973	rBV2	95842	230229	26.15%	3.540%
4	7.789	973	979	990	rVB	124828	278396	31.62%	4.280%
5	8.136	1028	1036	1049	rBV	94372	206510	23.45%	3.175%
6	8.545	1095	1103	1110	rBV3	5524	11236	1.28%	0.173%
7	8.691	1118	1127	1139	rBV	189446	375723	42.67%	5.777%
8	9.185	1193	1208	1214	rBV2	48638	110952	12.60%	1.706%
9	9.240	1214	1217	1224	rVB2	9584	17779	2.02%	0.273%
10	9.459	1243	1253	1261	rVB2	10217	26504	3.01%	0.407%
11	9.606	1269	1277	1284	rVB2	11416	22241	2.53%	0.342%
12	9.758	1295	1302	1306	rBV2	12477	23847	2.71%	0.367%
13	9.819	1306	1312	1325	rVB3	83588	196066	22.27%	3.014%
14	9.959	1325	1335	1346	rBV2	77106	172339	19.57%	2.650%
15	10.105	1355	1359	1364	rVV4	5608	11200	1.27%	0.172%
16	10.179	1364	1371	1386	rVB	453991	880519	100.00%	13.538%
17	10.307	1386	1392	1394	rBV2	11560	18952	2.15%	0.291%
18	10.368	1394	1402	1411	rVB	171950	305776	34.73%	4.701%
19	10.477	1411	1420	1422	rBV3	11502	20890	2.37%	0.321%
20	10.520	1422	1427	1434	rVB	57902	105927	12.03%	1.629%
21	10.618	1434	1443	1448	rBV	77218	149431	16.97%	2.297%
22	10.666	1448	1451	1454	rVV	13782	19794	2.25%	0.304%
23	10.709	1454	1458	1464	rVB2	24040	38093	4.33%	0.586%
24	10.800	1467	1473	1478	rBV2	45323	72449	8.23%	1.114%
25	10.904	1484	1490	1496	rBV	37610	76573	8.70%	1.177%
26	10.971	1496	1501	1504	rVV3	45902	87871	9.98%	1.351%
27	11.002	1504	1506	1508	rVV	36093	47422	5.39%	0.729%
28	11.038	1508	1512	1516	rVV	76912	125696	14.28%	1.933%
29	11.087	1516	1520	1526	rVV2	52192	97065	11.02%	1.492%
30	11.148	1526	1530	1533	rVB	9859	13894	1.58%	0.214%
31	11.203	1533	1539	1543	rBV2	28626	52587	5.97%	0.809%
32	11.282	1543	1552	1563	rVB4	121087	298829	33.94%	4.594%
33	11.380	1563	1568	1573	rBV	80926	124973	14.19%	1.921%
34	11.489	1580	1586	1596	rVV	256025	410375	46.61%	6.309%
35	11.593	1596	1603	1605	rVV2	15903	29685	3.37%	0.456%
36	11.624	1605	1608	1612	rVV2	19835	32122	3.65%	0.494%

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37	11.709	1612	1622	1631	rVV3	134577	337624	38.34%	5.191%
38	11.782	1631	1634	1639	rVB2	19528	29085	3.30%	0.447%
39	12.026	1663	1674	1682	rBV4	35055	106174	12.06%	1.632%
40	12.123	1686	1690	1694	rVB2	9656	12934	1.47%	0.199%
41	12.203	1699	1703	1706	rVV3	9619	16384	1.86%	0.252%
42	12.245	1706	1710	1719	rVB5	13216	30834	3.50%	0.474%
43	12.483	1744	1749	1755	rBV2	208993	320485	36.40%	4.927%
44	12.672	1772	1780	1784	rVB	8665	17277	1.96%	0.266%
45	12.733	1784	1790	1794	rVV	27374	46419	5.27%	0.714%
46	12.806	1798	1802	1808	rVV2	42987	74049	8.41%	1.138%
47	12.971	1821	1829	1834	rBV	15722	29534	3.35%	0.454%
48	13.038	1837	1840	1846	rVB3	9138	14575	1.66%	0.224%
49	13.123	1846	1854	1859	rBV	42716	66374	7.54%	1.020%
50	13.318	1879	1886	1890	rBV5	8536	15958	1.81%	0.245%
51	13.428	1897	1904	1913	rVB	219848	364228	41.37%	5.600%
52	13.623	1929	1936	1940	rBV	18301	32596	3.70%	0.501%
53	13.666	1940	1943	1952	rVB3	9739	21563	2.45%	0.332%
54	13.751	1952	1957	1962	rBV2	20272	31764	3.61%	0.488%
55	13.971	1987	1993	1998	rVB3	18823	32844	3.73%	0.505%
56	14.080	2006	2011	2016	rVB2	13286	21367	2.43%	0.329%
57	14.562	2086	2090	2095	rBV3	7192	12844	1.46%	0.197%
58	14.611	2095	2098	2103	rVB2	8707	12345	1.40%	0.190%
59	14.684	2103	2110	2115	rBV4	18112	35920	4.08%	0.552%
60	14.836	2129	2135	2141	rVB	14430	22537	2.56%	0.347%
61	15.056	2165	2171	2179	rVB4	5045	10771	1.22%	0.166%
62	15.294	2205	2210	2216	rVV5	4755	10066	1.14%	0.155%
63	15.391	2219	2226	2230	rVV3	7770	18946	2.15%	0.291%
64	15.726	2277	2281	2291	rVB2	9714	16951	1.93%	0.261%
65	16.037	2327	2332	2340	rBV6	4616	9078	1.03%	0.140%

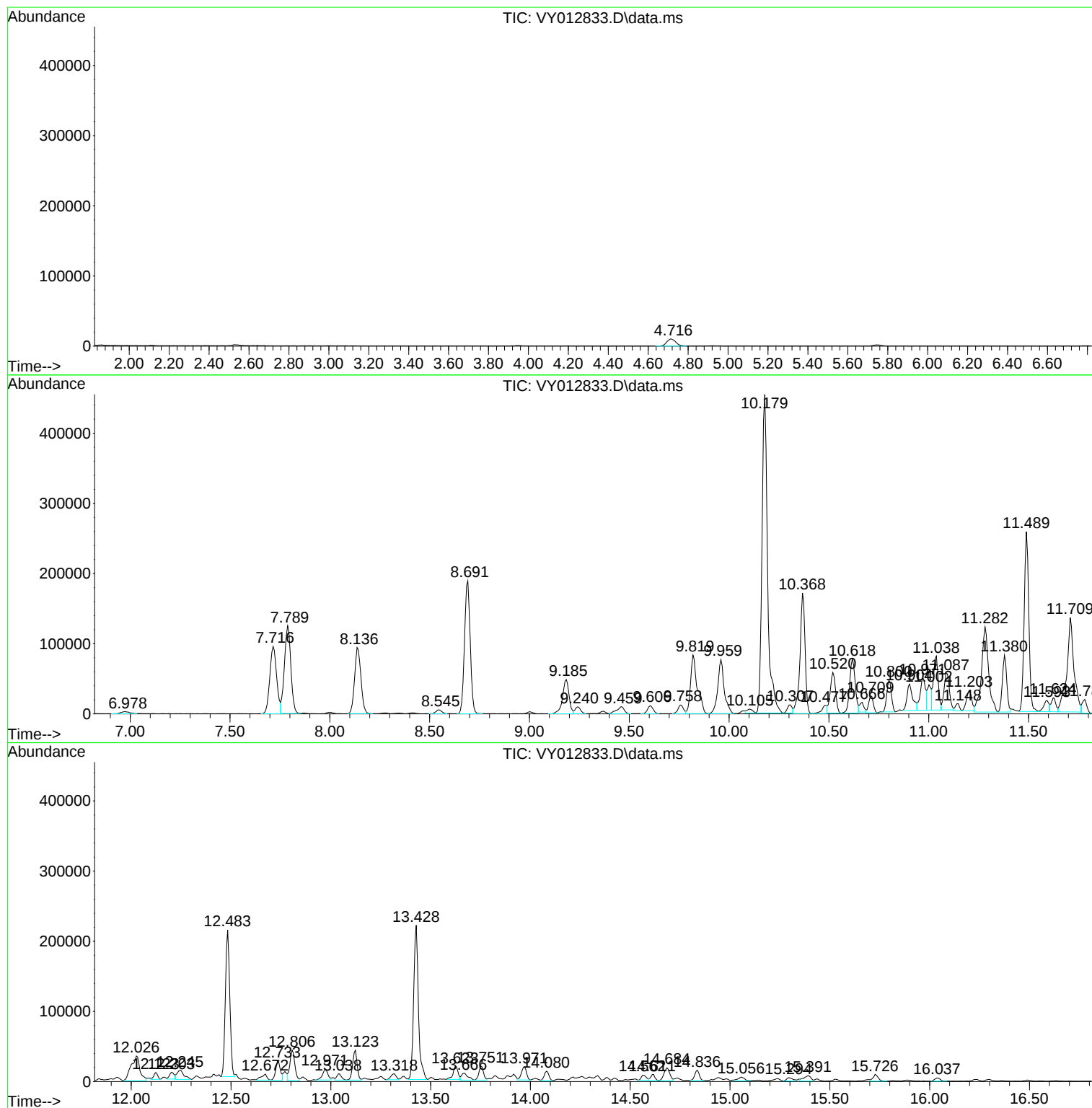
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ClientSampleId :
RBR251669

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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



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MSVOA_Y
ClientSampleId :
RBR251669

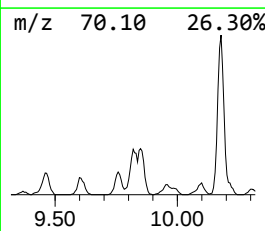
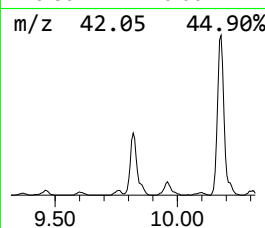
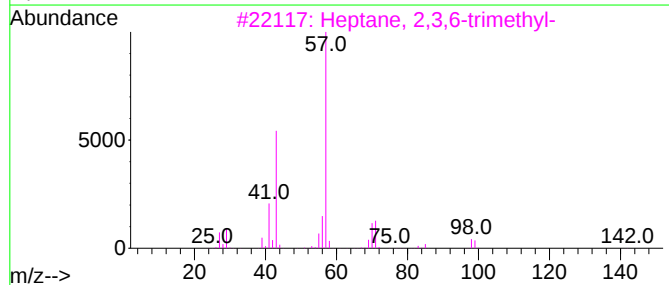
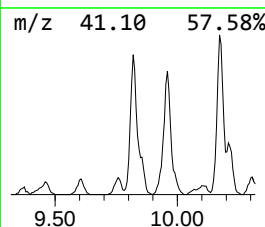
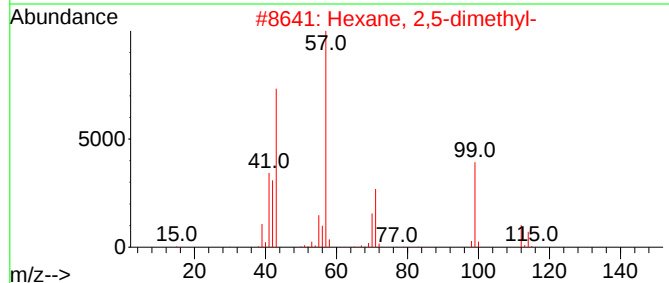
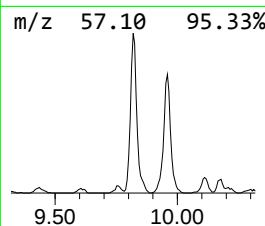
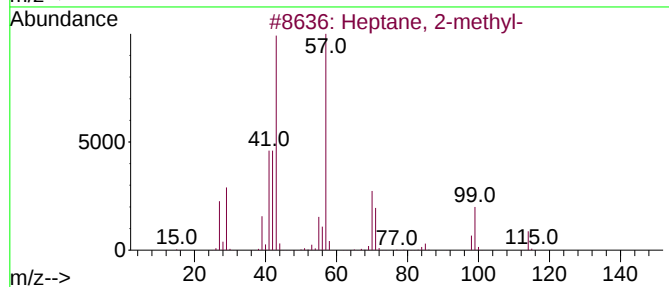
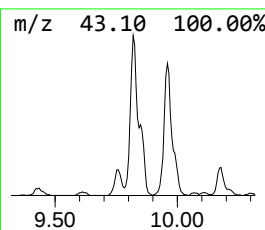
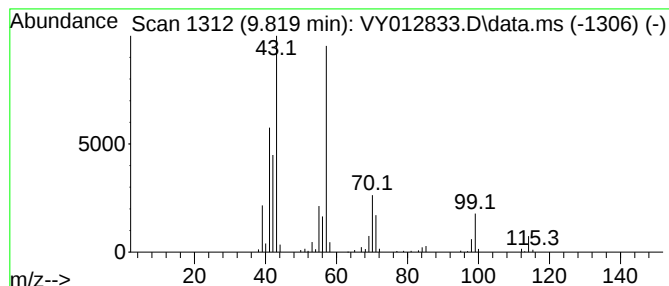
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.819	26.09 ug/l	196066	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	95
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	87
3			Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	47
4			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	38
5			Heptane, 3-ethyl-	128	C9H20	015869-80-4	32



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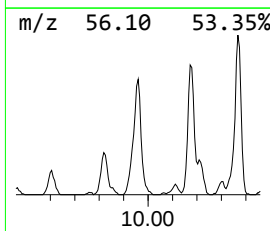
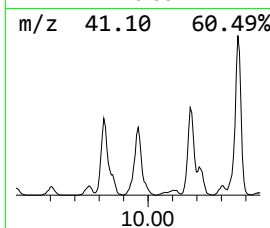
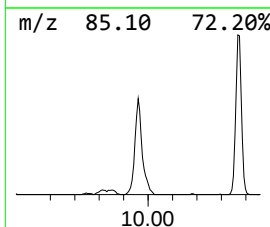
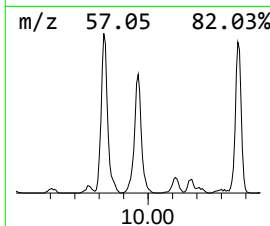
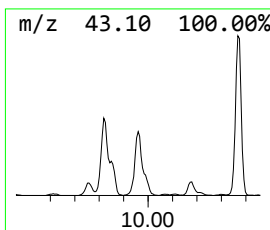
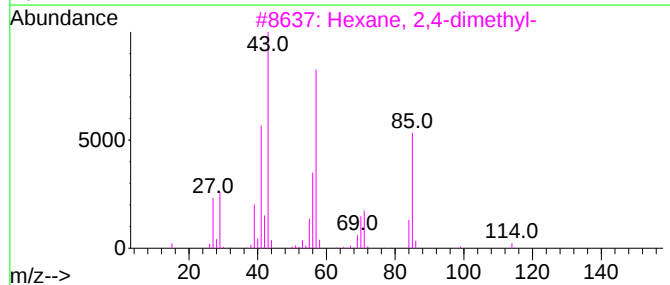
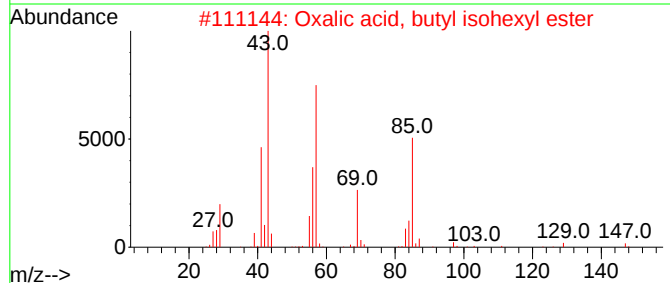
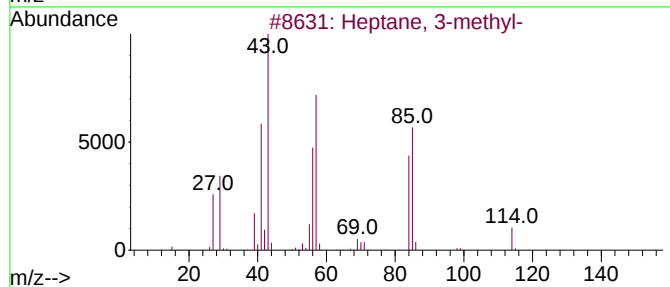
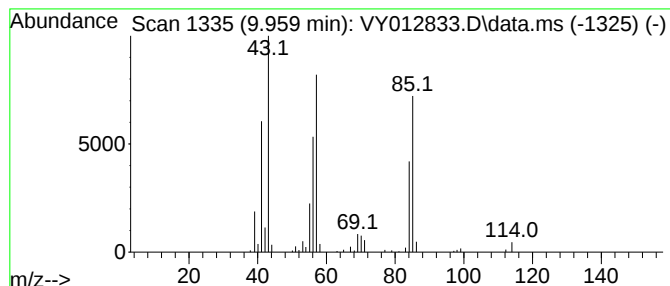
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.959	22.93 ug/l	172339	1,4-Difluorobenzene	8.691

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	59
3			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	58
4			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
5			Hexane, 3-ethyl-	114	C8H18	000619-99-8	49



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
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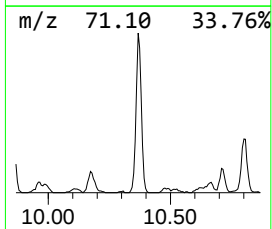
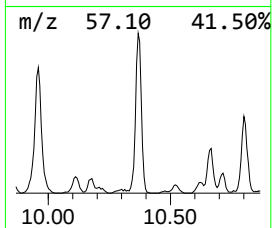
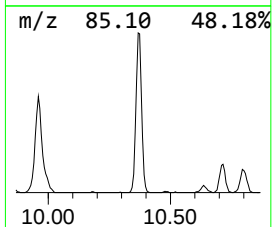
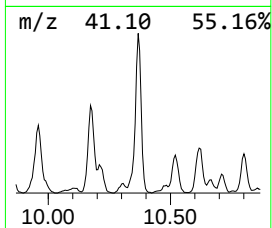
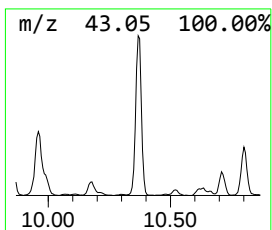
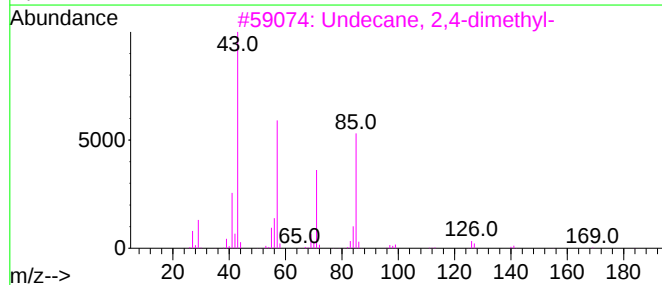
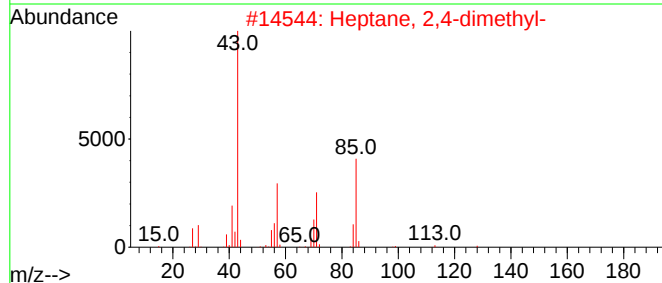
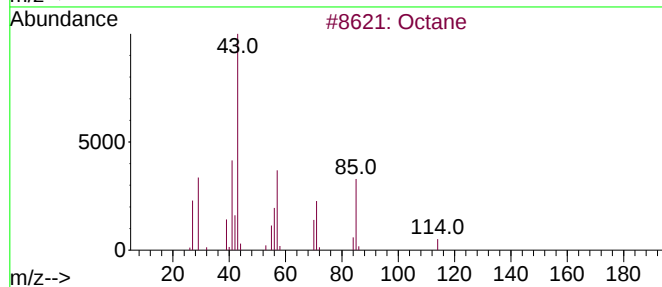
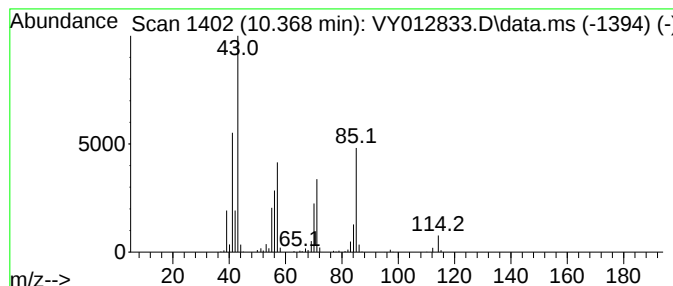
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Quant Title : SW846 8260

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

Peak Number 3 Octane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.368	37.26 ug/l	305776	Chlorobenzene-d5	11.489

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	72
3			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	53
4			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	50
5			Hexane, 1,1'-oxybis-	186	C12H26O	000112-58-3	50



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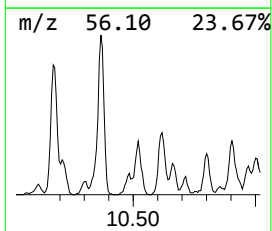
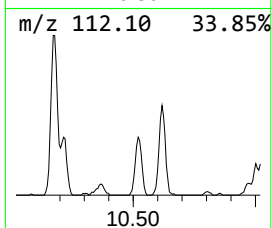
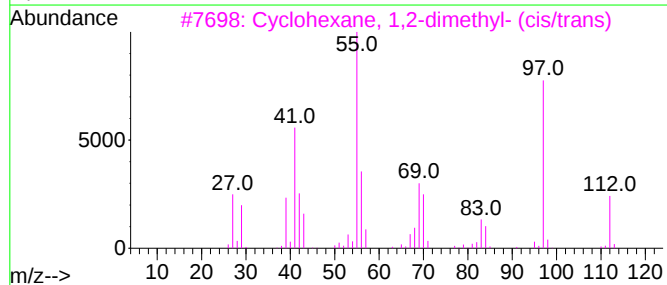
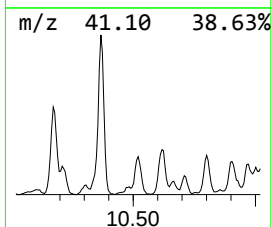
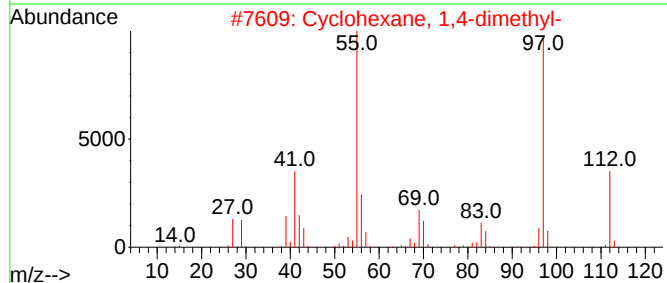
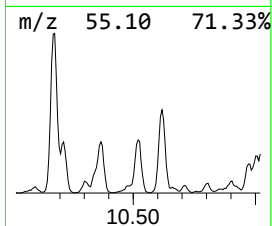
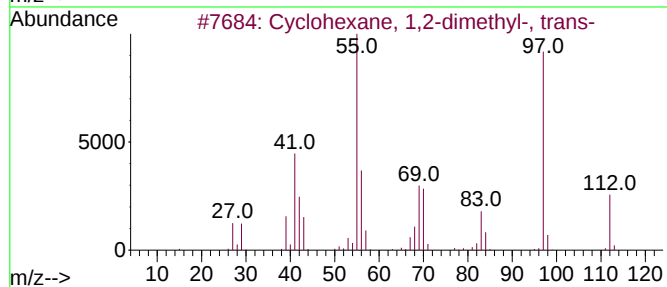
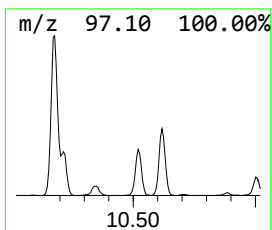
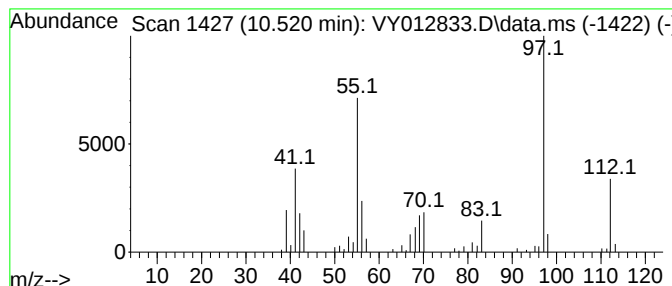
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 4 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.520	12.91 ug/l	105927	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	91
2			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	91
3			Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	91
4			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	91
5			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	90



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Operator : KP/MD
Sample : 01742-01
Misc : 4.99g/5.0mL/MSVOA_Y/SoIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR251669

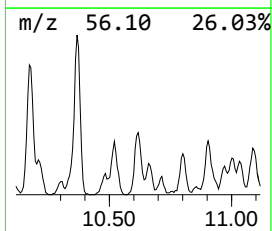
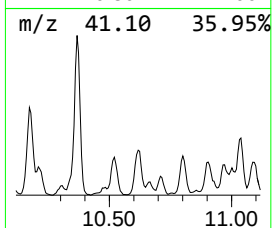
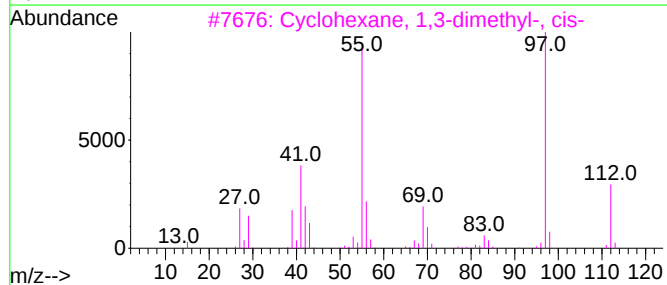
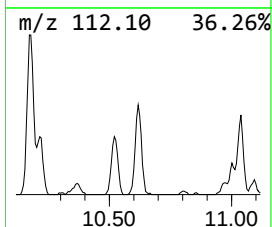
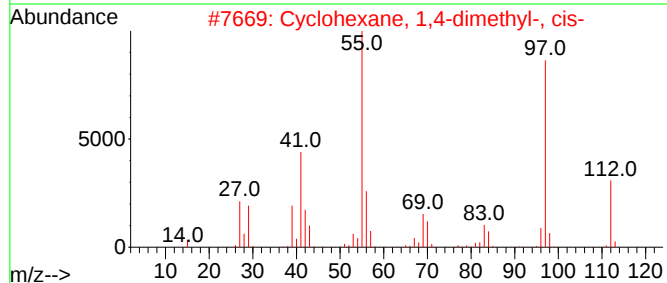
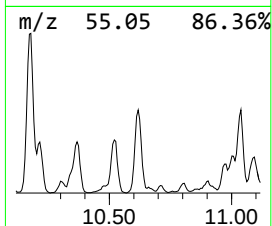
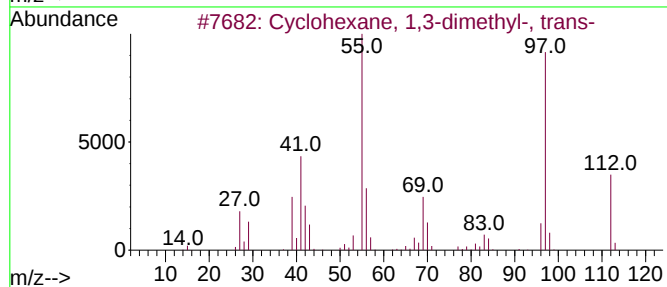
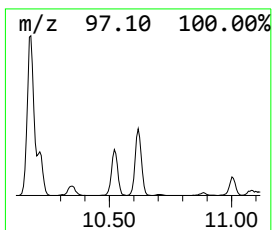
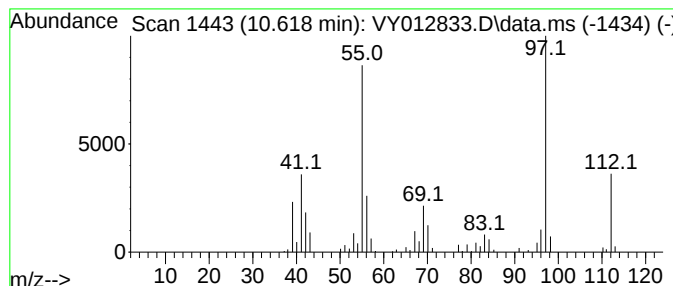
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.618	18.21 ug/l	149431	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	96
2			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	93
3			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	93
4			Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	91
5			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030623\
Data File : VY012833.D
Acq On : 06 Mar 2023 18:52
Operator : KP/MD
Sample : 01742-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR251669

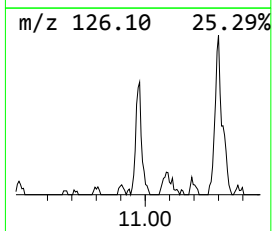
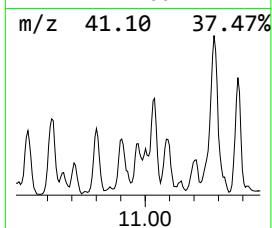
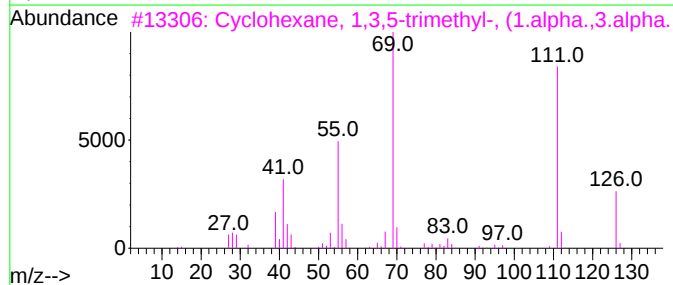
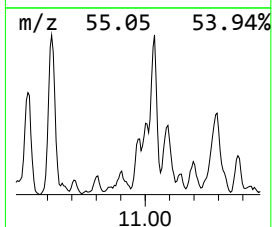
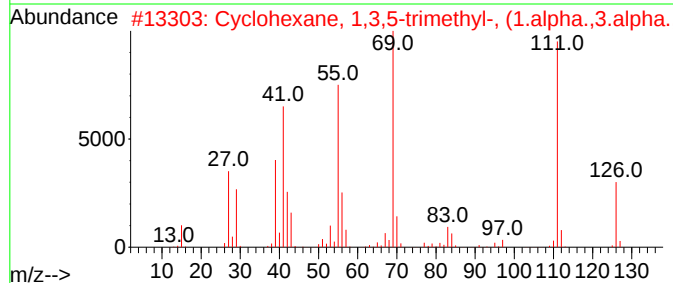
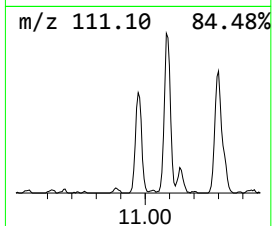
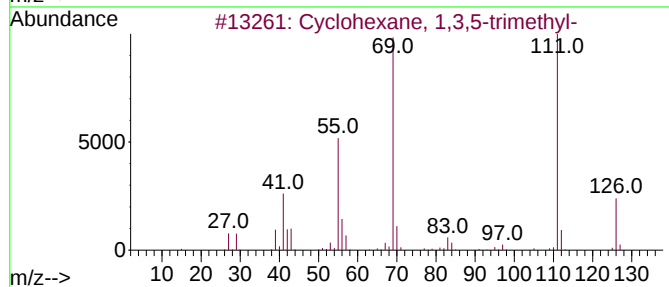
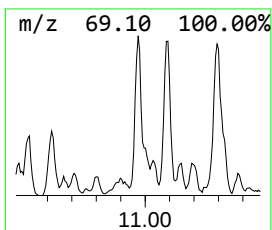
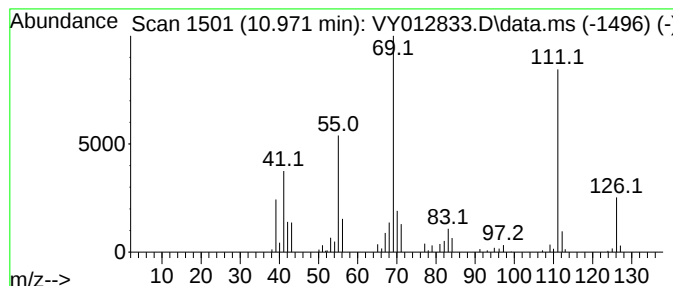
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, 1,3,5-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.971	10.71 ug/l	87871	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	94
2			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	87
3			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	81
4			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	74
5			3-Octen-2-one	126	C8H14O	001669-44-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030623\
Data File : VY012833.D
Acq On : 06 Mar 2023 18:52
Operator : KP/MD
Sample : 01742-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR251669

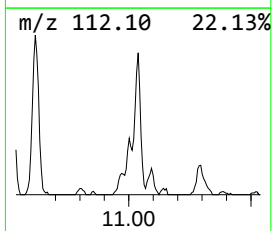
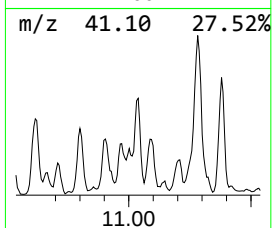
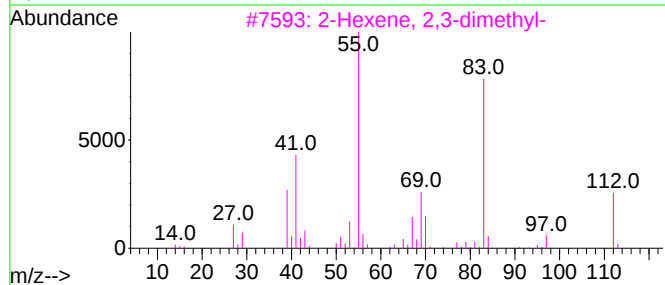
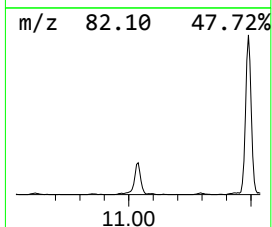
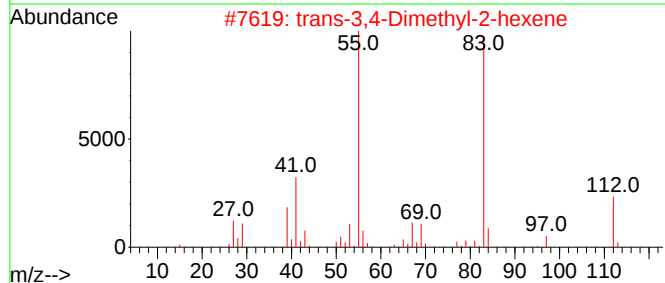
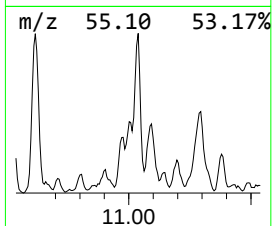
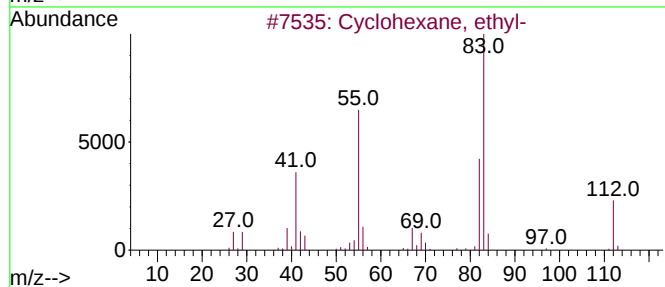
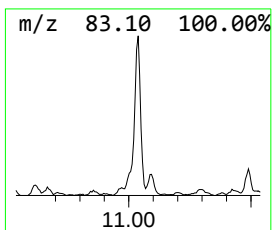
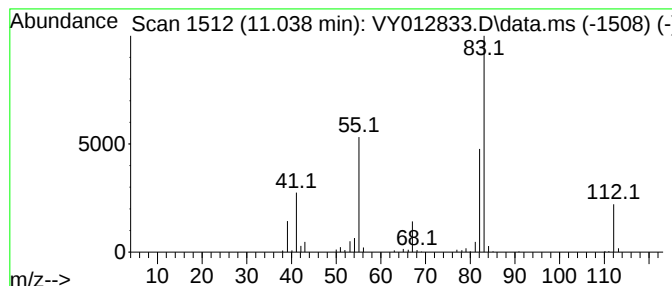
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexane, ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.038	15.31 ug/l	125696	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, ethyl-	112	C8H16	001678-91-7	90
2			trans-3,4-Dimethyl-2-hexene	112	C8H16	019550-82-4	53
3			2-Hexene, 2,3-dimethyl-	112	C8H16	007145-20-2	53
4			trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	53
5			4-Oxohex-2-enal	112	C6H8O2	020697-55-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030623\
Data File : VY012833.D
Acq On : 06 Mar 2023 18:52
Operator : KP/MD
Sample : 01742-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

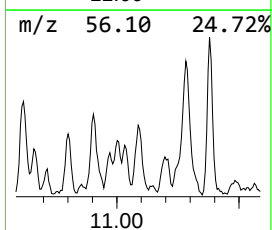
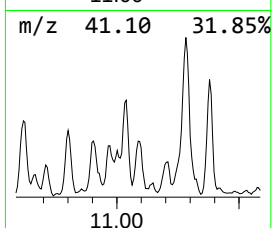
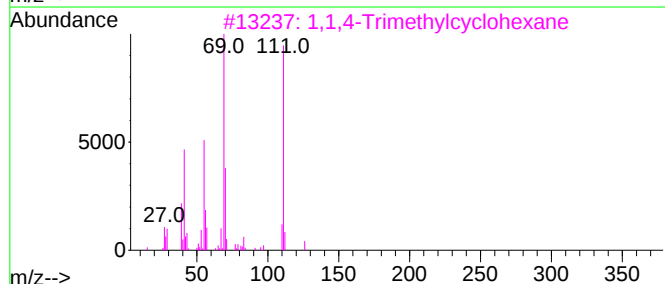
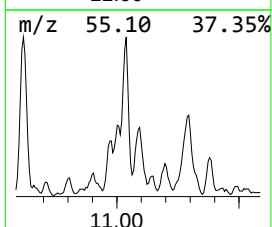
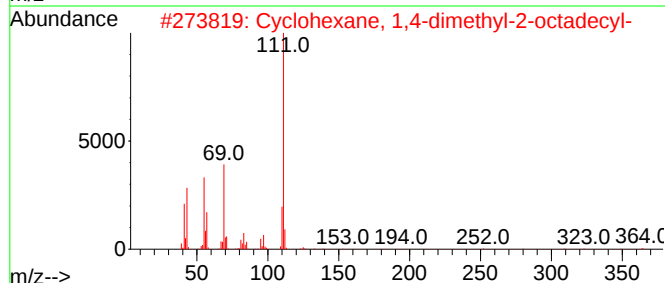
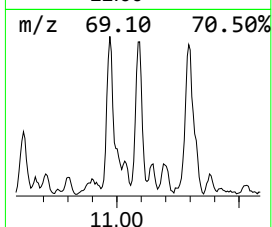
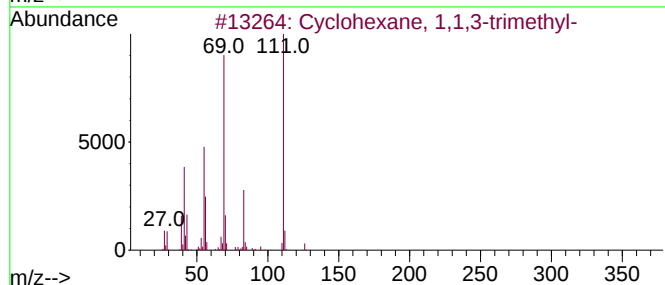
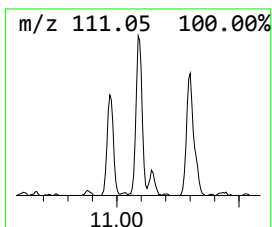
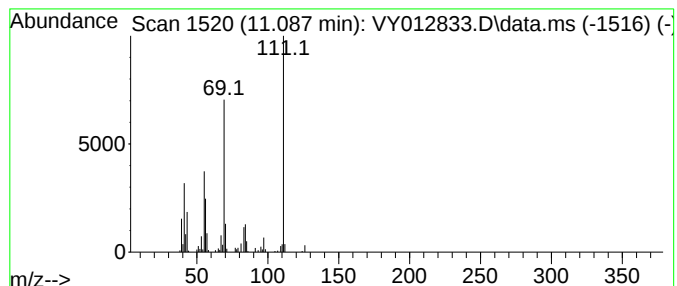
Instrument :
MSVOA_Y
ClientSampleId :
RBR251669

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.M
Quant Title : SW846 8260

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

Peak Number 8 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.087	11.83 ug/l	97065	Chlorobenzene-d5	11.489	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	74
2	Cyclohexane, 1,4-dimethyl-2-octa...	364	C26H52	055282-02-5	50
3	1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	50
4	Cyclooctane, butyl-	168	C12H24	016538-93-5	47
5	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030623\
Data File : VY012833.D
Acq On : 06 Mar 2023 18:52
Operator : KP/MD
Sample : 01742-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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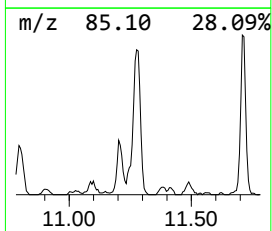
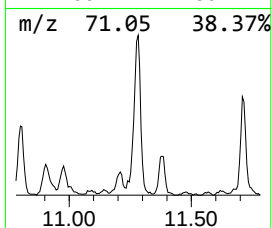
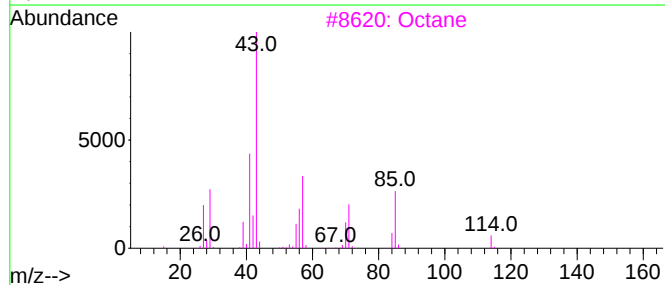
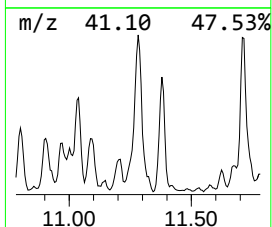
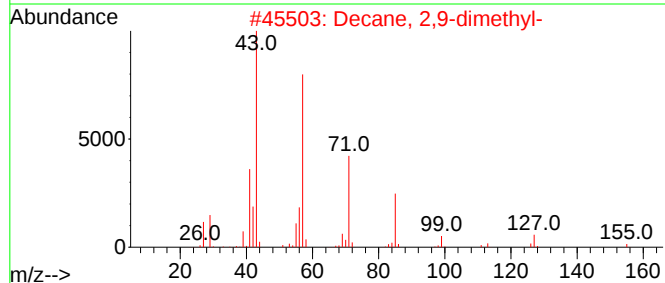
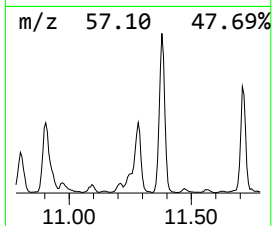
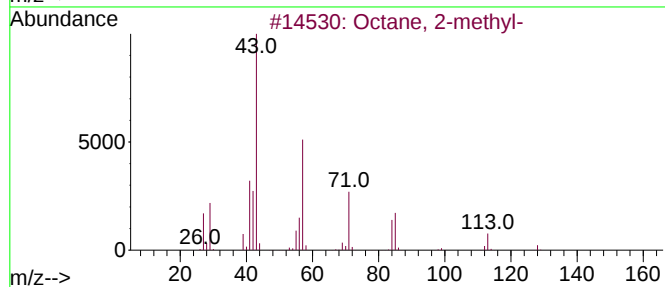
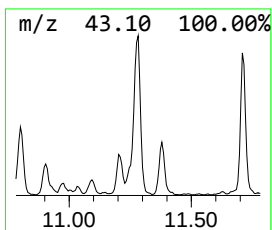
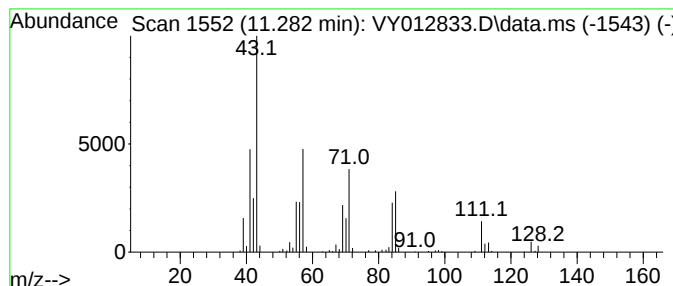
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Quant Title : SW846 8260

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

Peak Number 9 Octane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.282	36.41 ug/l	298829	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-methyl-	128	C9H20	003221-61-2	72
2			Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	53
3			Octane	114	C8H18	000111-65-9	50
4			Octane, 4-methyl-	128	C9H20	002216-34-4	47
5			Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030623\
Data File : VY012833.D
Acq On : 06 Mar 2023 18:52
Operator : KP/MD
Sample : 01742-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR251669

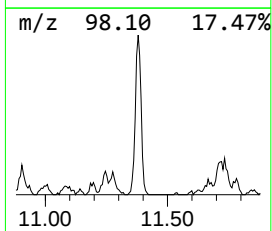
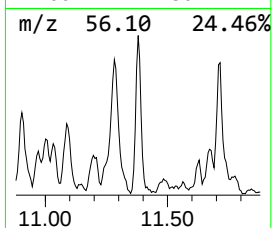
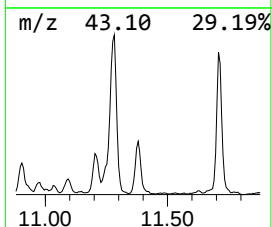
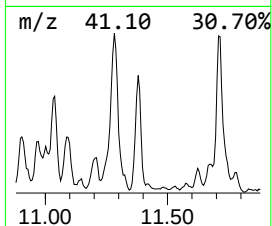
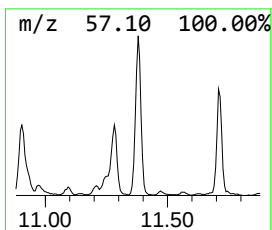
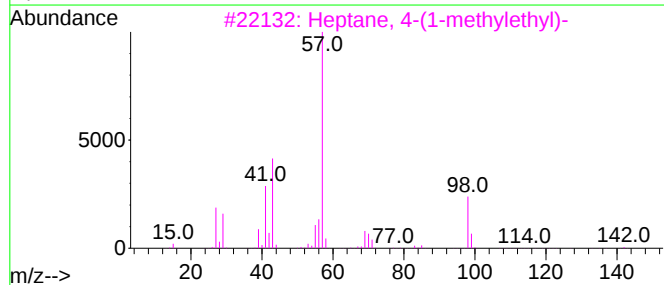
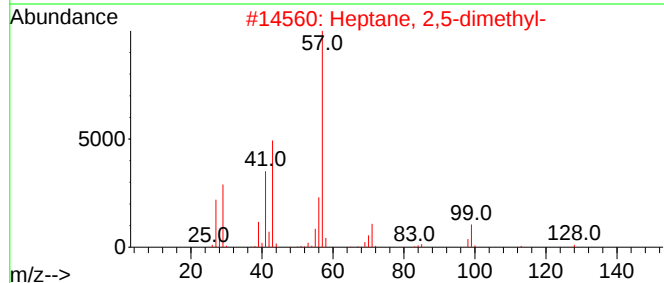
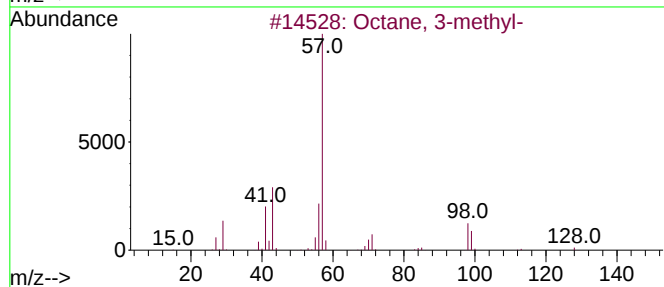
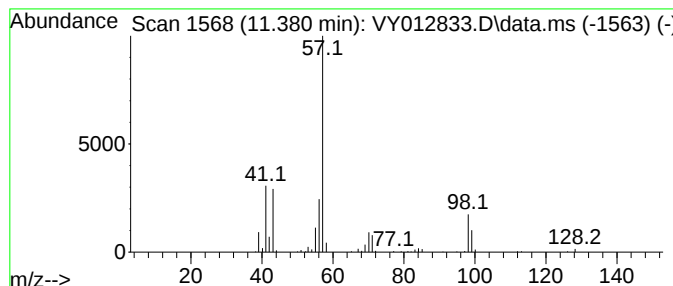
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Quant Title : SW846 8260

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

Peak Number 10 Octane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.380	15.23 ug/l	124973	Chlorobenzene-d5	11.489

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 3-methyl-	128	C9H20	002216-33-3	91
2		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	74
3		Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	59
4		Undecane, 6-methyl-	170	C12H26	017302-33-9	50
5		Aziridine, 1-acetyl-2-methyl-	99	C5H9NO	013416-47-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY030623\
Data File : VY012833.D
Acq On : 06 Mar 2023 18:52
Operator : KP/MD
Sample : 01742-01
Misc : 4.99g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RBR251669

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030223S.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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Heptane, 3-methyl-	9.959	22.9	ug/l	172339	2	8.691	375723	50.0
Octane	10.368	37.3	ug/l	305776	3	11.489	410375	50.0
Cyclohexane, 1,...	10.520	12.9	ug/l	105927	3	11.489	410375	50.0
Cyclohexane, 1,...	10.618	18.2	ug/l	149431	3	11.489	410375	50.0
Cyclohexane, 1,...	10.971	10.7	ug/l	87871	3	11.489	410375	50.0
Cyclohexane, et...	11.038	15.3	ug/l	125696	3	11.489	410375	50.0
Cyclohexane, 1,...	11.087	11.8	ug/l	97065	3	11.489	410375	50.0
Octane, 2-methyl-	11.282	36.4	ug/l	298829	3	11.489	410375	50.0
Octane, 3-methyl-	11.380	15.2	ug/l	124973	3	11.489	410375	50.0