

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091521\
 Data File : VY006032.D
 Acq On : 15 Sep 2021 18:23
 Operator : SY/MD
 Sample : M3733-03
 Misc : 7.07G/5ML/MSVOA_Y/SOIL
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SUP-UST-02-(5-7)

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\82Y091421S.M

Title : SW846 8260

Signal : TIC: VY006032.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.965	1325	1336	1348	rBV2	269395	781854	1.83%	0.145%
2	10.179	1365	1371	1375	rBV2	623641	1117866	2.61%	0.207%
3	10.349	1394	1399	1410	rVB4	184849	443965	1.04%	0.082%
4	10.526	1423	1428	1436	rVB	552227	978274	2.29%	0.181%
5	10.624	1436	1444	1448	rBV2	314675	698990	1.63%	0.130%
6	10.715	1455	1459	1464	rVB	600586	896368	2.10%	0.166%
7	10.807	1464	1474	1480	rVB	1398960	2321751	5.43%	0.430%
8	10.904	1480	1490	1497	rBV	1336061	2736543	6.40%	0.507%
9	10.977	1497	1502	1508	rBV	959858	1561611	3.65%	0.290%
10	11.038	1508	1512	1516	rVB	815524	1133532	2.65%	0.210%
11	11.093	1516	1521	1526	rBV	2161724	3476741	8.13%	0.645%
12	11.148	1526	1530	1534	rVB	517448	719723	1.68%	0.133%
13	11.209	1534	1540	1544	rBV	2514844	4198839	9.82%	0.778%
14	11.300	1544	1555	1563	rVB3	3045496	10064335	23.53%	1.866%
15	11.380	1563	1568	1573	rBV	2270208	3918400	9.16%	0.726%
16	11.477	1579	1584	1589	rBV	705018	1193509	2.79%	0.221%
17	11.569	1595	1599	1604	rBV2	723654	1092452	2.55%	0.203%
18	11.630	1604	1609	1613	rBV	2255779	3542155	8.28%	0.657%
19	11.678	1613	1617	1622	rBV3	2370059	4315370	10.09%	0.800%
20	11.739	1622	1627	1631	rBV2	8024172	13573535	31.74%	2.516%
21	11.782	1631	1634	1640	rVB	4772114	7398576	17.30%	1.372%
22	11.843	1640	1644	1646	rBV2	693802	1088444	2.54%	0.202%
23	11.880	1646	1650	1652	rBV	1235791	1878109	4.39%	0.348%
24	11.934	1655	1659	1664	rVB2	6955397	10953491	25.61%	2.031%
25	12.014	1664	1672	1678	rBV4	19271490	42768979	100.00%	7.929%
26	12.062	1678	1680	1683	rVB2	3430948	3528184	8.25%	0.654%
27	12.130	1687	1691	1696	rVB	22608179	31326907	73.25%	5.808%
28	12.203	1696	1703	1706	rBV4	12956346	25126326	58.75%	4.658%
29	12.245	1706	1710	1716	rVB2	18957657	34042050	79.60%	6.311%
30	12.331	1721	1724	1726	rVV2	3543333	5497830	12.85%	1.019%
31	12.380	1726	1732	1736	rVV3	14708424	32616094	76.26%	6.047%
32	12.422	1736	1739	1744	rVB2	13052352	19088919	44.63%	3.539%
33	12.495	1744	1751	1755	rBV4	5396460	9571249	22.38%	1.774%
34	12.581	1755	1765	1768	rBV3	7719775	19250815	45.01%	3.569%
35	12.617	1769	1771	1773	rVV	2627586	3524146	8.24%	0.653%
36	12.648	1773	1776	1783	rVB3	13261149	24496662	57.28%	4.541%

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37	12.733	1783	1790	1794	rBV4	6729764	15122961	35.36%	2.804%
38	12.818	1795	1804	1808	rBV3	18869626	41490012	97.01%	7.692%
39	12.867	1808	1812	1817	rVB	12121546	18152174	42.44%	3.365%
40	12.916	1817	1820	1822	rBV3	1290114	1663519	3.89%	0.308%
41	12.959	1822	1827	1830	rBV2	9798275	14166339	33.12%	2.626%
42	13.007	1830	1835	1838	rBV2	8621069	15375534	35.95%	2.850%
43	13.044	1838	1841	1848	rVB	22928523	32496981	75.98%	6.025%
44	13.105	1848	1851	1858	rVB4	4401996	7011207	16.39%	1.300%
45	13.172	1858	1862	1867	rBV2	6127786	8880197	20.76%	1.646%
46	13.227	1867	1871	1873	rBV3	3455438	5107094	11.94%	0.947%
47	13.324	1879	1887	1891	rBV	10889581	20097604	46.99%	3.726%
48	13.361	1891	1893	1898	rVB3	3122041	4009664	9.38%	0.743%
49	13.568	1923	1927	1929	rBV3	557892	945944	2.21%	0.175%
50	13.593	1929	1931	1941	rVB4	1602519	2823635	6.60%	0.523%
51	13.696	1941	1948	1952	rBV2	910326	1914526	4.48%	0.355%
52	13.751	1952	1957	1961	rBV2	4388949	7034509	16.45%	1.304%
53	13.794	1961	1964	1969	rVB3	993587	1399669	3.27%	0.259%
54	13.855	1970	1974	1979	rVB4	693995	1145468	2.68%	0.212%
55	13.916	1980	1984	1989	rBV5	437186	1009470	2.36%	0.187%
56	13.971	1989	1993	1998	rVB	1679176	2604142	6.09%	0.483%
57	14.013	1998	2000	2005	rVB3	471893	646732	1.51%	0.120%
58	14.074	2005	2010	2015	rVB3	552953	998395	2.33%	0.185%
59	14.141	2015	2021	2027	rVB5	491930	1121389	2.62%	0.208%
60	14.263	2036	2041	2056	rVB6	913294	2748481	6.43%	0.510%
61	14.379	2056	2060	2064	rBV3	303658	511849	1.20%	0.095%

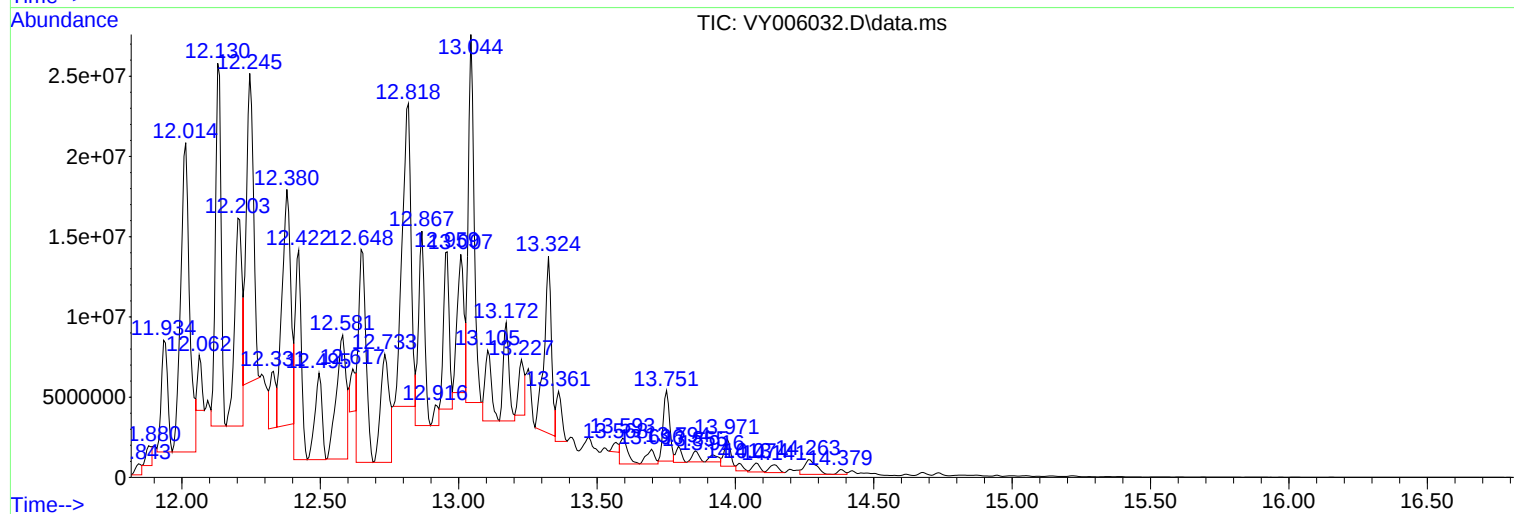
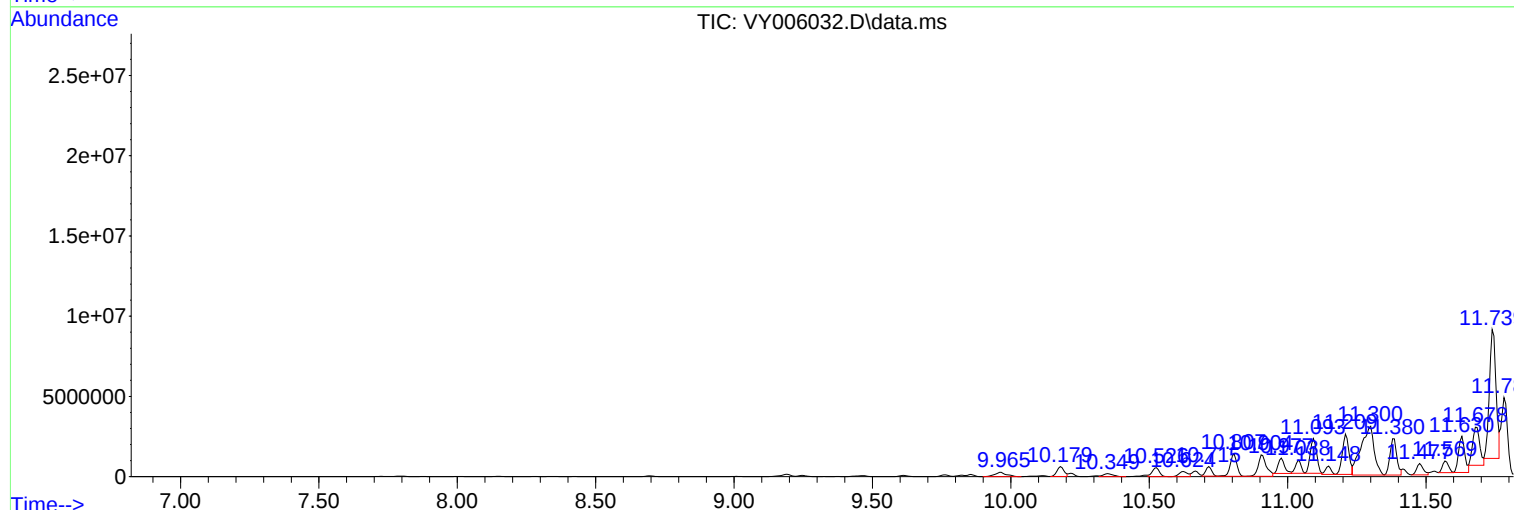
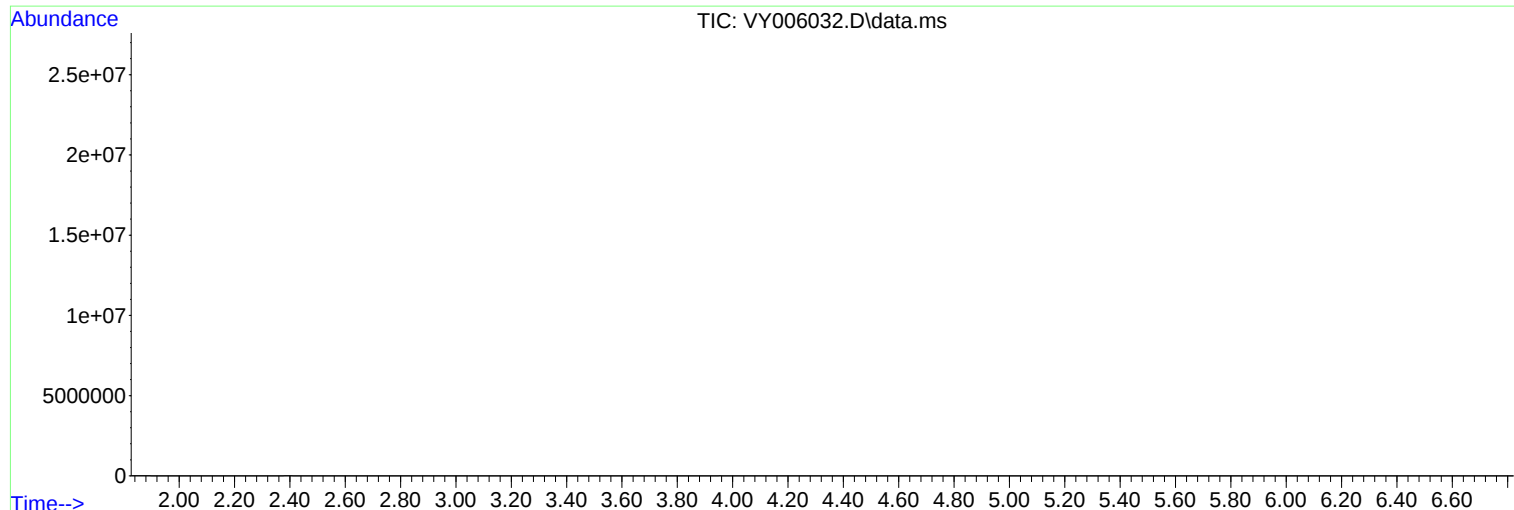
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Instrument :
MSVOA_Y
ClientSampleId :
SUP-UST-02-(5-7)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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



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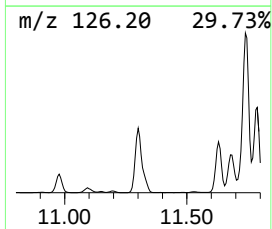
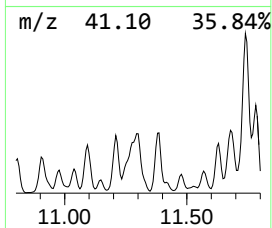
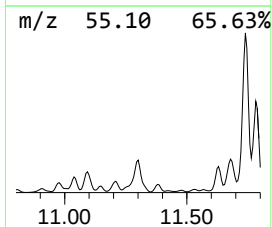
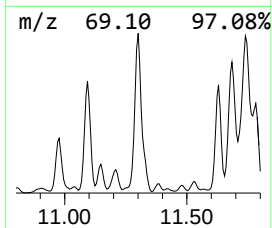
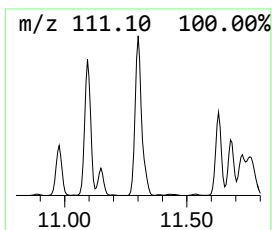
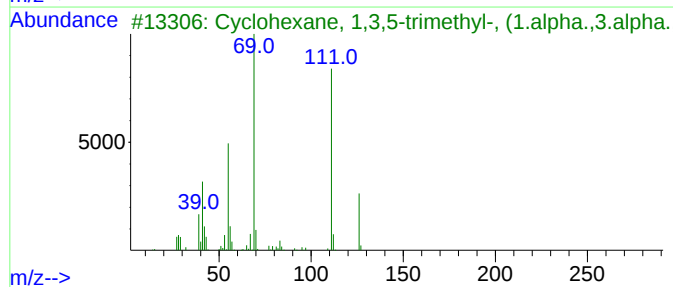
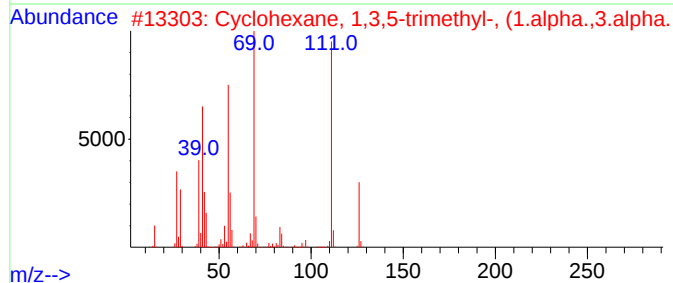
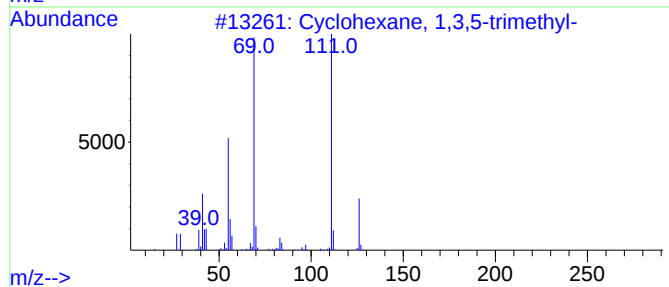
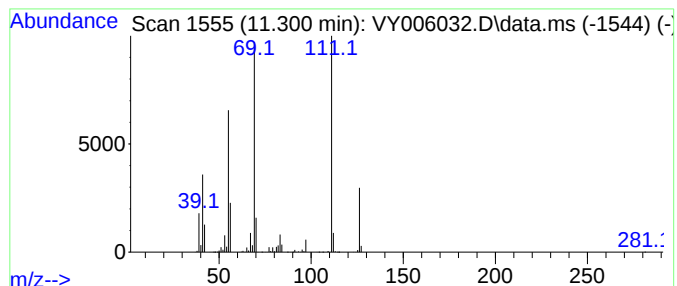
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,3,5-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.300	421.63 ug/l	10064300	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	91
2			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	91
3			Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	90
4			Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	90
5			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	81



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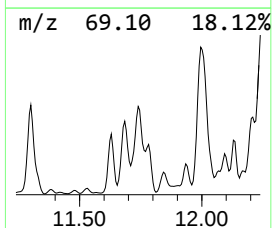
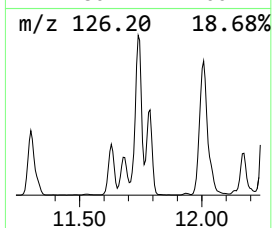
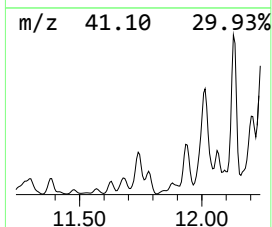
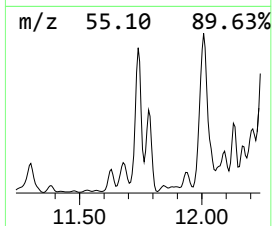
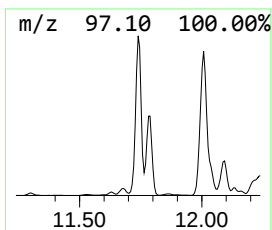
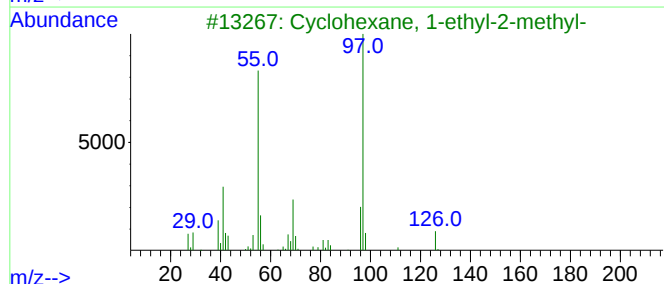
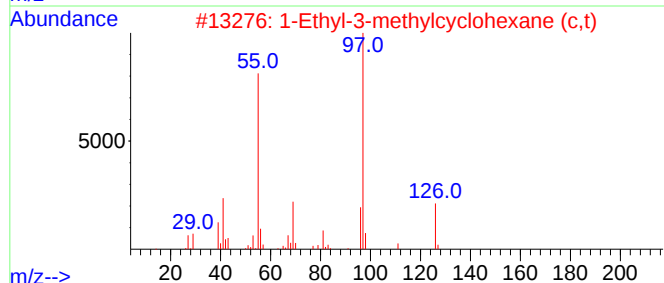
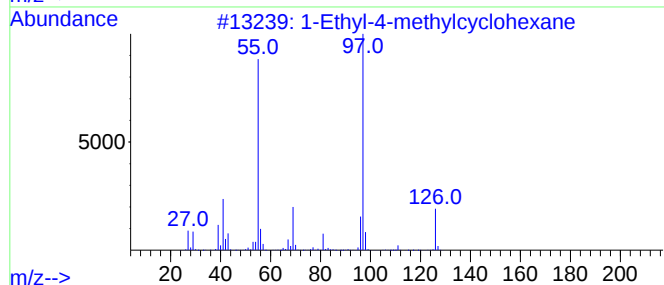
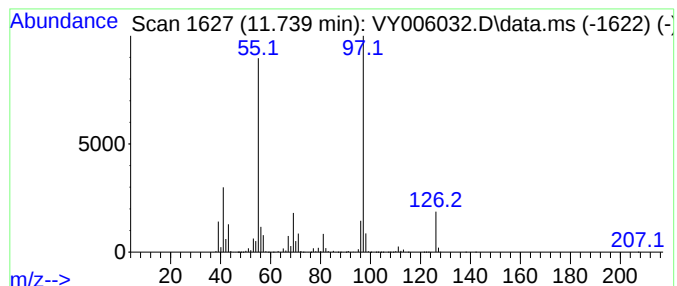
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 2 1-Ethyl-4-methylcyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	568.64 ug/l	13573500	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	95
2			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	94
3			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	91
4			cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	90
5			3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	87



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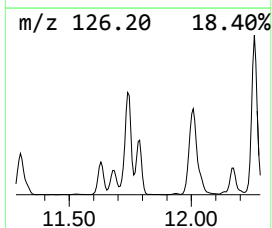
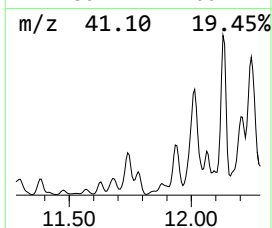
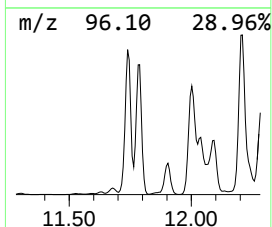
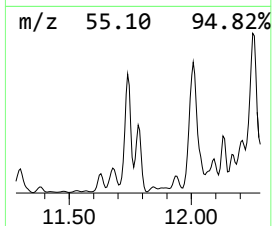
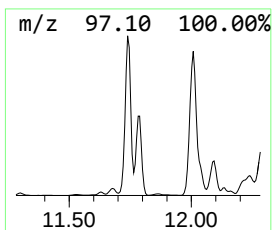
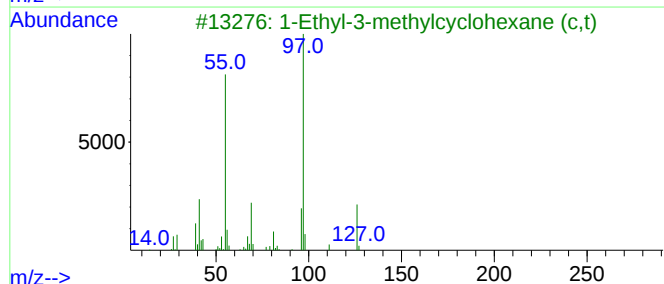
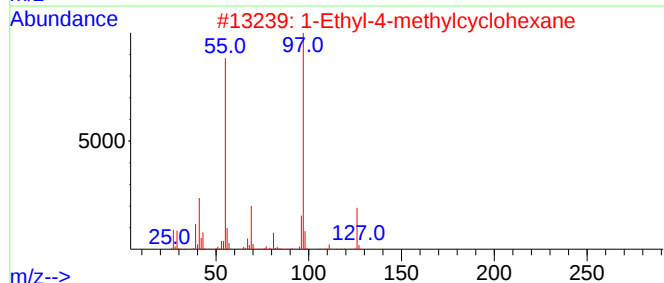
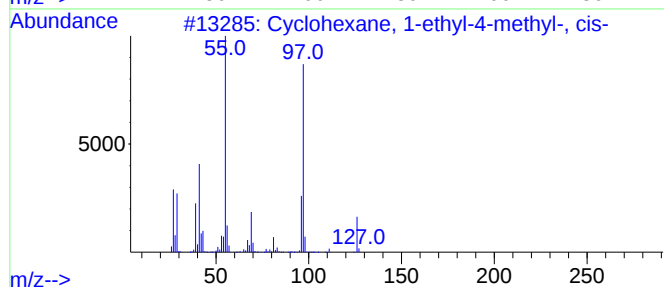
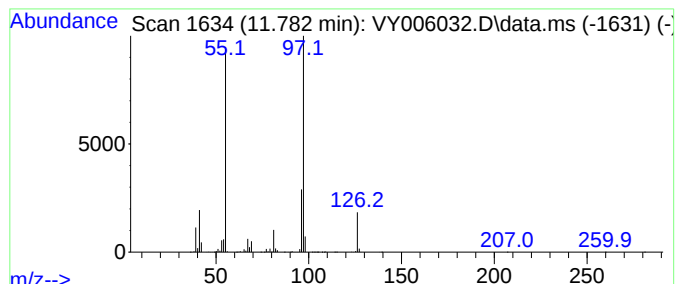
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Quant Title : SW846 8260

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

Peak Number 3 Cyclohexane, 1-ethyl-4-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.782	309.95 ug/l	7398580	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	90
2			1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	87
3			1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	86
4			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	86
5			cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	72



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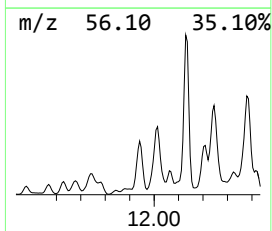
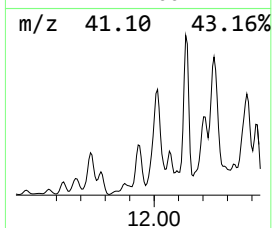
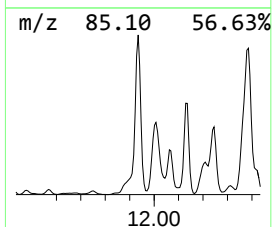
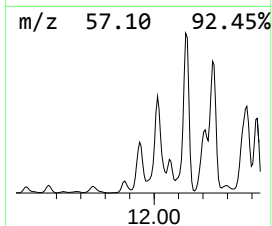
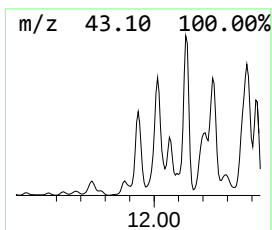
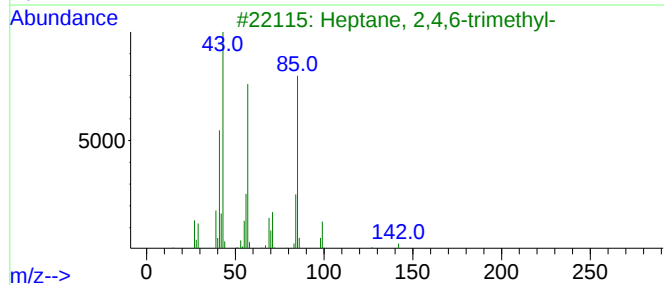
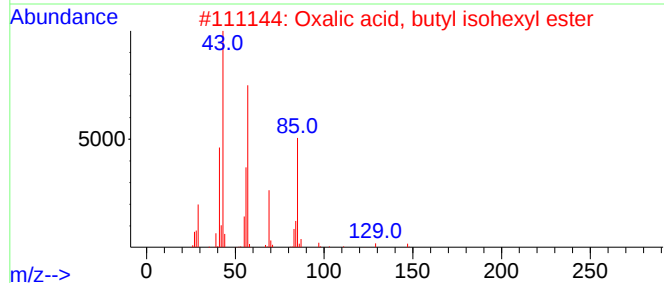
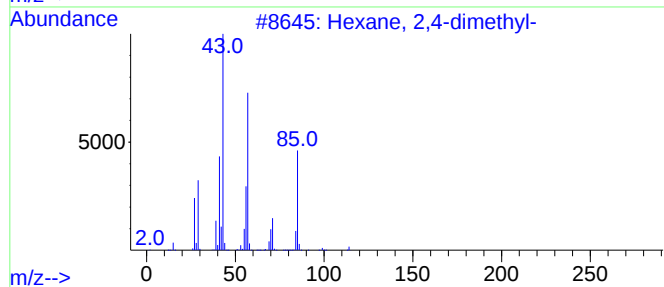
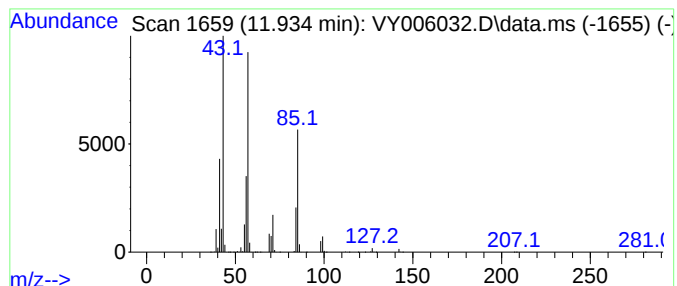
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 4 Hexane, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.935	458.88 ug/l	10953500	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
2			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
3			Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	64
4			Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	59
5			4,4-Dimethyl octane	142	C10H22	015869-95-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091521\
Data File : VY006032.D
Acq On : 15 Sep 2021 18:23
Operator : SY/MD
Sample : M3733-03
Misc : 7.07G/5ML/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SUP-UST-02-(5-7)

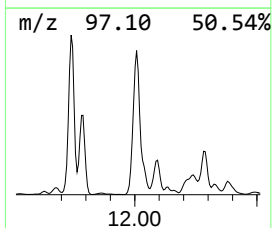
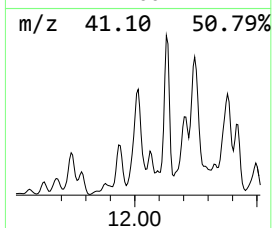
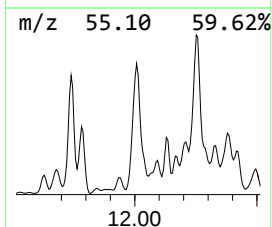
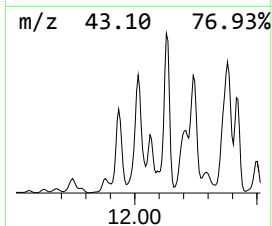
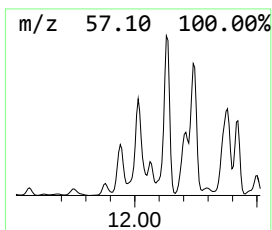
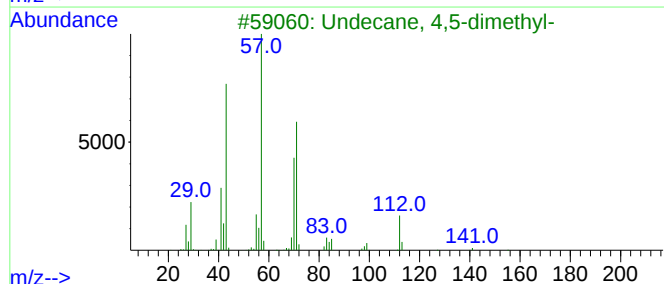
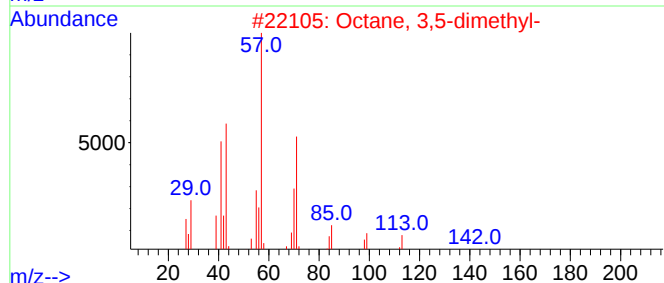
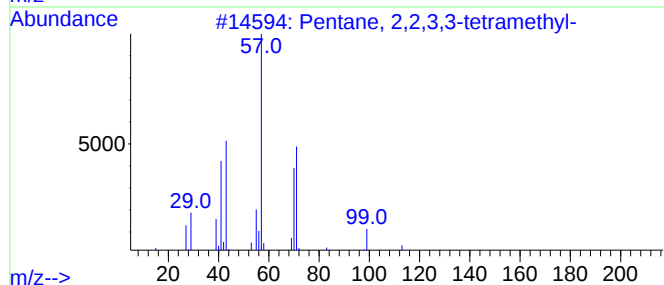
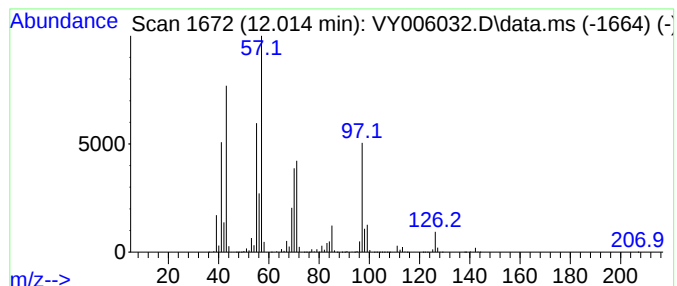
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Quant Title : SW846 8260

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

Peak Number 5 unknown12.014 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.014	1791.73 ug/l	42769000	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	47
2			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	43
3			Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	38
4			Nonane, 4-methyl-	142	C10H22	017301-94-9	38
5			Decane, 3,4-dimethyl-	170	C12H26	017312-45-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091521\
Data File : VY006032.D
Acq On : 15 Sep 2021 18:23
Operator : SY/MD
Sample : M3733-03
Misc : 7.07G/5ML/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SUP-UST-02-(5-7)

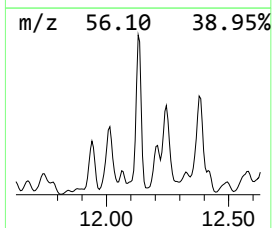
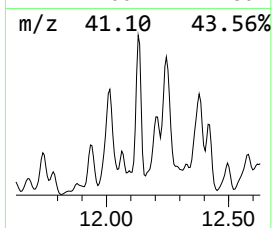
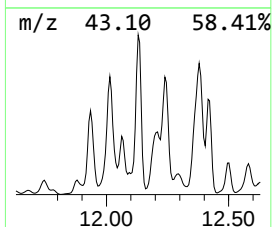
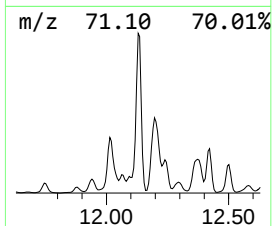
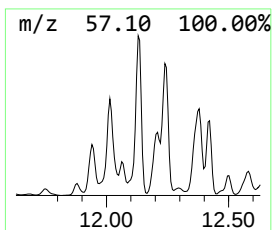
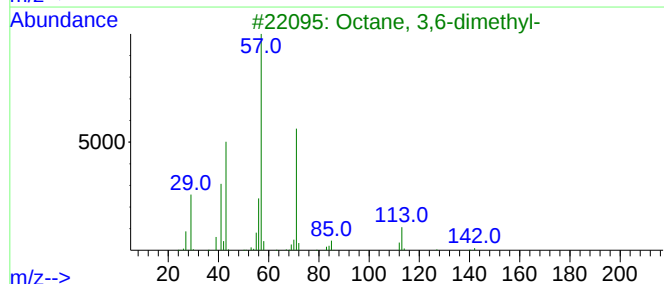
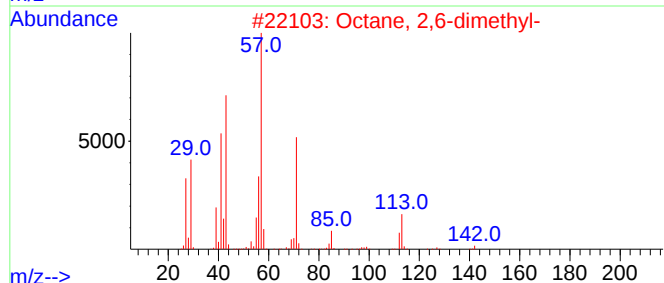
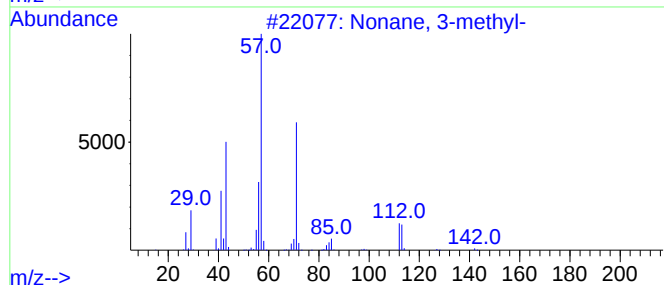
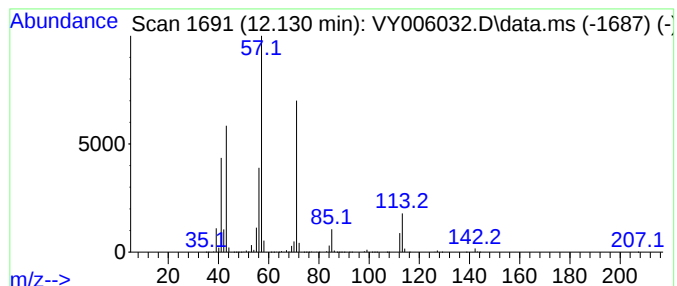
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Quant Title : SW846 8260

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

Peak Number 6 Nonane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.130	1312.39 ug/l	31326900	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 3-methyl-	142	C10H22	005911-04-6	91
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	87
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	59
5			2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091521\
Data File : VY006032.D
Acq On : 15 Sep 2021 18:23
Operator : SY/MD
Sample : M3733-03
Misc : 7.07G/5ML/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SUP-UST-02-(5-7)

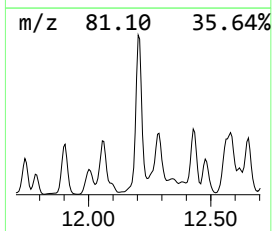
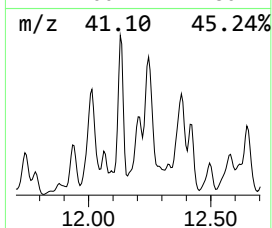
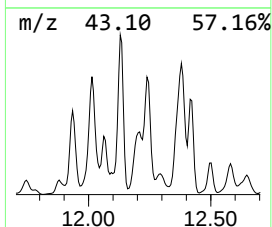
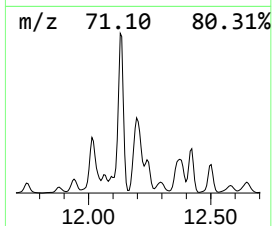
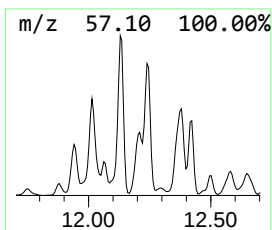
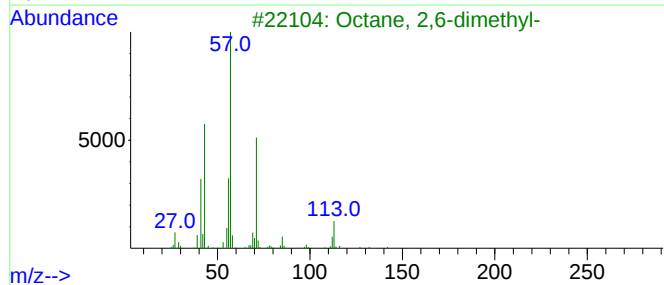
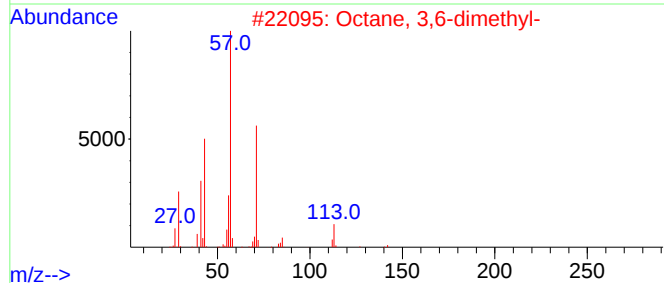
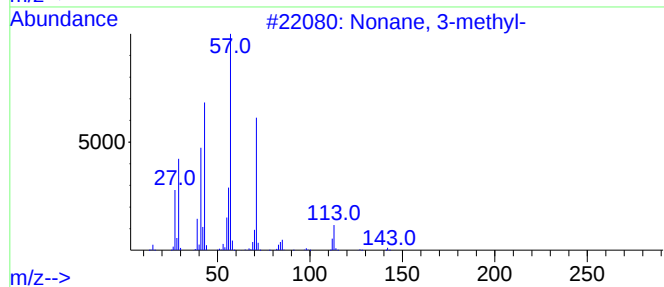
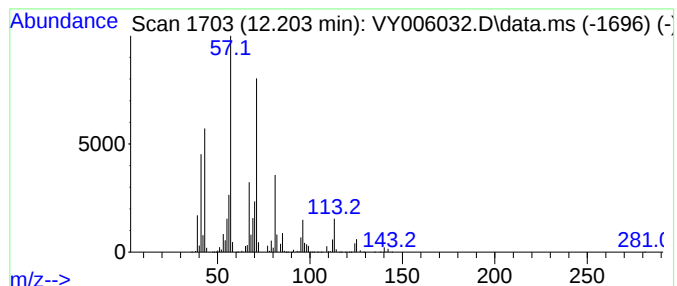
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Quant Title : SW846 8260

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

Peak Number 7 Octane, 3,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.203	1052.62 ug/l	25126300	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-			142	C10H22	005911-04-6	70
2	Octane, 3,6-dimethyl-			142	C10H22	015869-94-0	70
3	Octane, 2,6-dimethyl-			142	C10H22	002051-30-1	58
4	Butane, 2,2-dimethyl-			86	C6H14	000075-83-2	47
5	6-Methyl-2-heptanol, 2-methylpro...			200	C12H24O2	1000447-36-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091521\
Data File : VY006032.D
Acq On : 15 Sep 2021 18:23
Operator : SY/MD
Sample : M3733-03
Misc : 7.07G/5ML/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

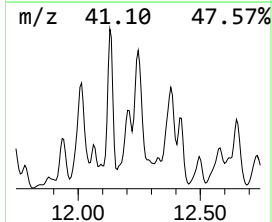
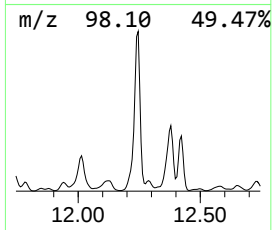
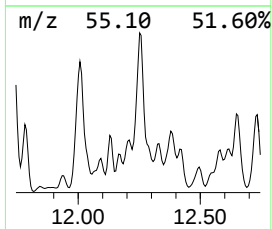
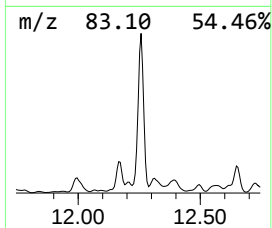
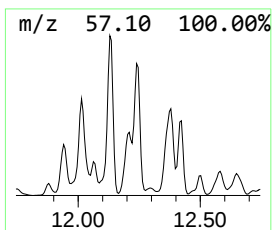
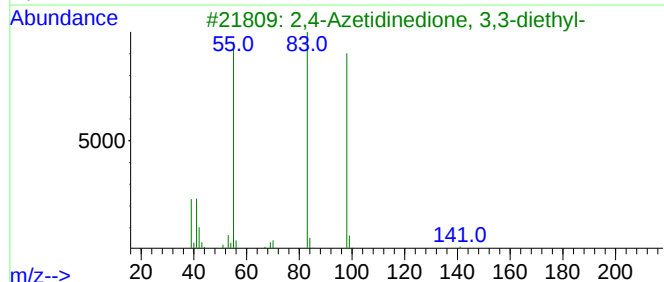
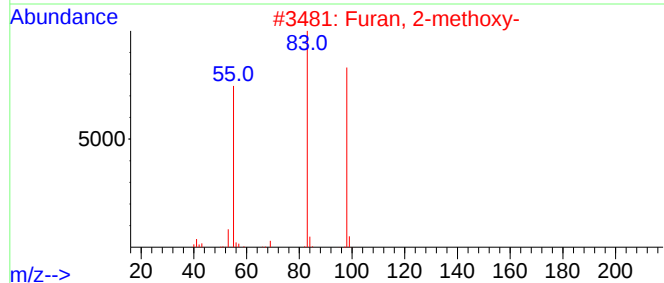
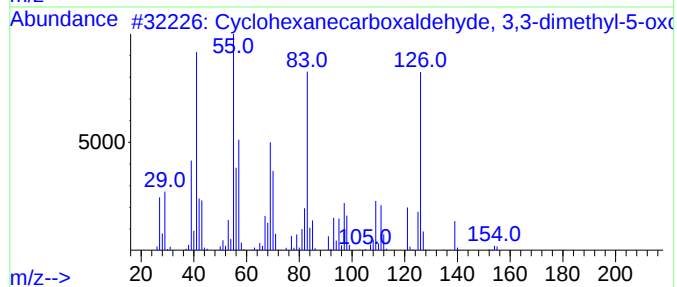
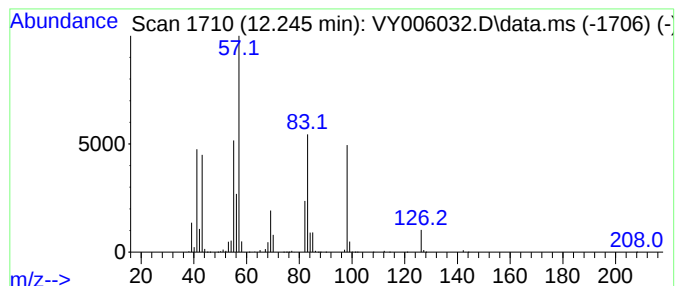
Instrument :
MSVOA_Y
ClientSampleId :
SUP-UST-02-(5-7)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.M
Quant Title : SW846 8260

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

Peak Number 8 unknown12.245 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.245	1426.13 ug/l	34042100	Chlorobenzene-d5	11.496	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxaldehyde, 3,3-d...	154	C9H14O2	065080-66-2	47
2	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	43
3	2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	43
4	Cyclohexane, propyl-	126	C9H18	001678-92-8	38
5	1H-Pyrazole, 3-ethyl-4,5-dihydro-	98	C5H10N2	005920-29-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091521\
Data File : VY006032.D
Acq On : 15 Sep 2021 18:23
Operator : SY/MD
Sample : M3733-03
Misc : 7.07G/5ML/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SUP-UST-02-(5-7)

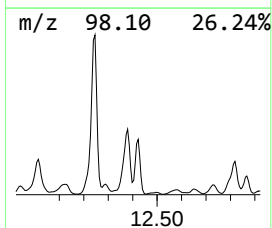
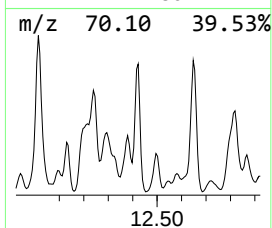
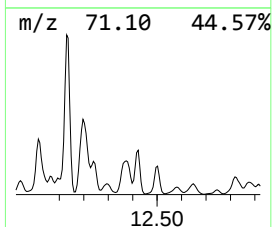
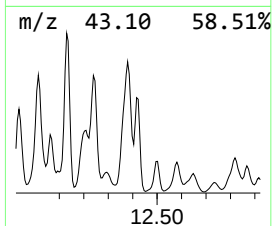
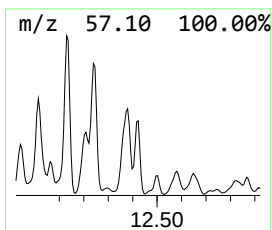
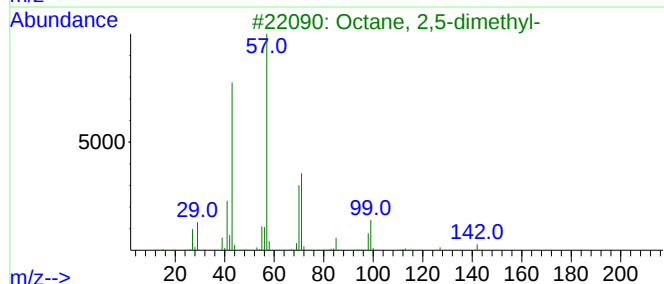
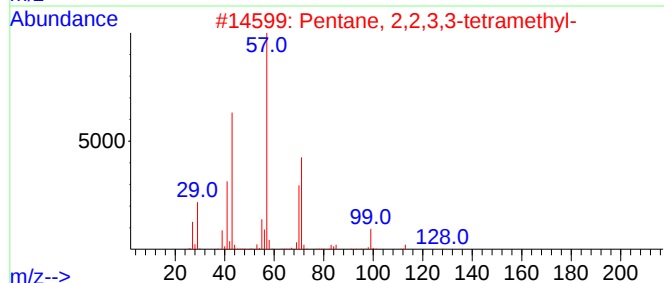
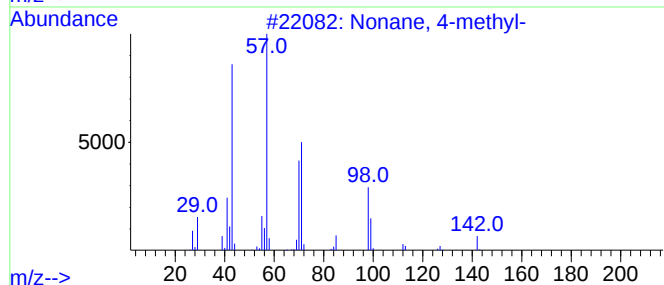
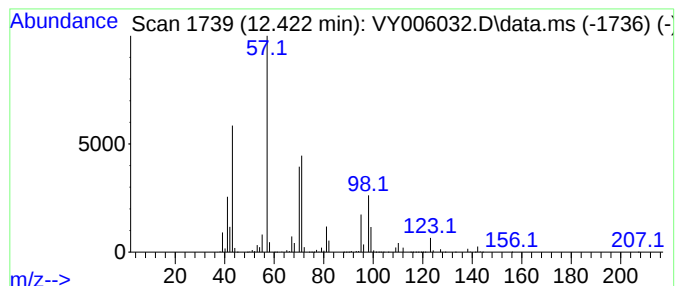
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Quant Title : SW846 8260

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

Peak Number 9 Nonane, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.422	799.70 ug/l	19088900	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 4-methyl-	142	C10H22	017301-94-9	58
2			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	50
3			Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	47
4			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	38
5			Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091521\
Data File : VY006032.D
Acq On : 15 Sep 2021 18:23
Operator : SY/MD
Sample : M3733-03
Misc : 7.07G/5ML/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SUP-UST-02-(5-7)

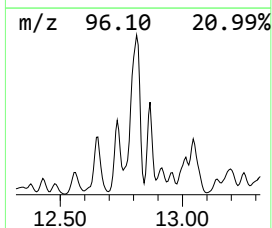
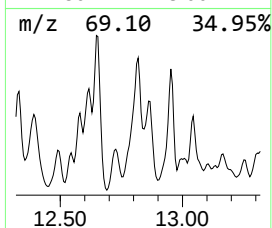
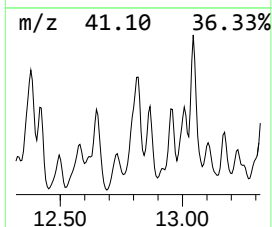
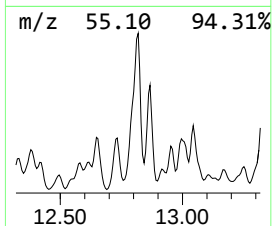
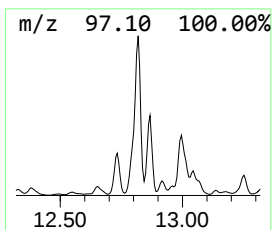
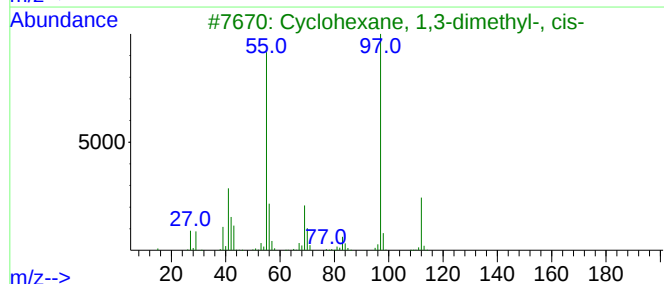
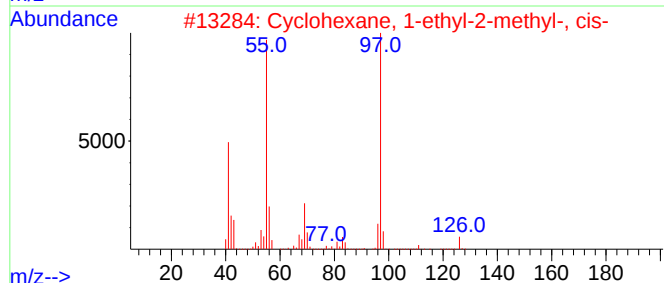
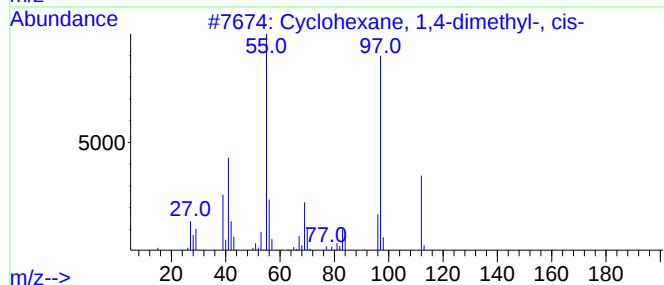
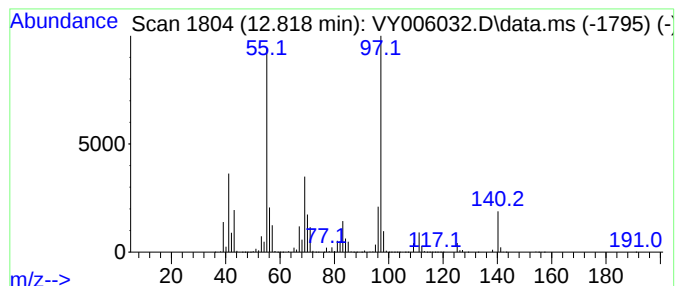
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Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.818	517.38 ug/l	41490000	1,4-Dichlorobenzene-d4	13.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	64
2			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-77-7	64
3			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	53
4			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	52
5			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091521\
Data File : VY006032.D
Acq On : 15 Sep 2021 18:23
Operator : SY/MD
Sample : M3733-03
Misc : 7.07G/5ML/MSVOA_Y/SOIL
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SUP-UST-02-(5-7)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091421S.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
Cyclohexane, 1,...	11.300	421.6	ug/l	10064300	3	11.496	1193510	50.0
1-Ethyl-4-methy...	11.739	568.6	ug/l	13573500	3	11.496	1193510	50.0
Cyclohexane, 1-...	11.782	309.9	ug/l	7398580	3	11.496	1193510	50.0
Hexane, 2,4-dim...	11.935	458.9	ug/l	10953500	3	11.496	1193510	50.0
unknown12.014	12.014	1791.7	ug/l	42769000	3	11.496	1193510	50.0
Nonane, 3-methyl-	12.130	1312.4	ug/l	31326900	3	11.496	1193510	50.0
Octane, 3,6-dim...	12.203	1052.6	ug/l	25126300	3	11.496	1193510	50.0
unknown12.245	12.245	1426.1	ug/l	34042100	3	11.496	1193510	50.0
Nonane, 4-methyl-	12.422	799.7	ug/l	19088900	3	11.496	1193510	50.0
Cyclohexane, 1,...	12.818	517.4	ug/l	41490000	4	13.404	4009660	50.0