

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
 Data File : VY009513.D
 Acq On : 11 Jul 2022 16:18
 Operator : KP/MD
 Sample : N3622-08
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20220497A-SIM-C3A-COMPOSITE

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\82Y070722S.M
 Title : SW846 8260

Signal : TIC: VY009513.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.381	87	92	97	rVB4	2458	5692	1.08%	0.122%
2	3.942	338	348	355	rBV	14861	39181	7.41%	0.839%
3	4.186	378	388	399	rBV	15987	43593	8.25%	0.933%
4	4.704	462	473	488	rBV2	30510	95198	18.01%	2.038%
5	5.735	631	642	654	rBV4	8700	26697	5.05%	0.572%
6	6.972	834	845	861	rBV	21384	68070	12.88%	1.457%
7	7.710	955	966	972	rBV2	70851	172356	32.60%	3.690%
8	7.783	972	978	989	rVB	150809	330793	62.57%	7.083%
9	8.137	1025	1036	1049	rBV	63055	140813	26.64%	3.015%
10	8.313	1059	1065	1077	rVB	14392	33293	6.30%	0.713%
11	8.685	1117	1126	1136	rBV	229151	450970	85.31%	9.656%
12	9.173	1203	1206	1213	rVB5	4256	7942	1.50%	0.170%
13	9.606	1271	1277	1284	rBV3	8287	17050	3.23%	0.365%
14	9.740	1291	1299	1306	rBV3	6230	13305	2.52%	0.285%
15	10.106	1355	1359	1364	rVB2	3924	6600	1.25%	0.141%
16	10.173	1364	1370	1378	rBV	199700	343331	64.95%	7.351%
17	10.801	1468	1473	1479	rVB5	6640	11219	2.12%	0.240%
18	10.898	1481	1489	1491	rBV4	4546	8952	1.69%	0.192%
19	10.941	1491	1496	1505	rVV3	16305	35605	6.74%	0.762%
20	11.032	1507	1511	1515	rVV3	4031	6393	1.21%	0.137%
21	11.087	1515	1520	1525	rVV2	9250	15937	3.01%	0.341%
22	11.136	1525	1528	1532	rVV4	4299	6558	1.24%	0.140%
23	11.197	1532	1538	1543	rVB5	5775	9739	1.84%	0.209%
24	11.295	1550	1554	1563	rVB7	3993	9472	1.79%	0.203%
25	11.484	1578	1585	1595	rBV	322664	528646	100.00%	11.319%
26	11.618	1605	1607	1611	rVB5	4153	5422	1.03%	0.116%
27	11.679	1611	1617	1620	rBV5	7260	14433	2.73%	0.309%
28	11.733	1622	1626	1637	rVB5	14511	39511	7.47%	0.846%
29	11.831	1637	1642	1647	rBV6	5461	12157	2.30%	0.260%
30	11.892	1647	1652	1655	rBV7	4423	7037	1.33%	0.151%
31	11.929	1655	1658	1662	rVB4	4392	6233	1.18%	0.133%
32	11.996	1662	1669	1676	rBV8	17782	53005	10.03%	1.135%
33	12.124	1685	1690	1694	rVB	29246	43693	8.27%	0.936%
34	12.197	1694	1702	1704	rBV6	26379	48948	9.26%	1.048%
35	12.233	1704	1708	1713	rVB4	29779	56040	10.60%	1.200%
36	12.319	1713	1722	1726	rBV7	10084	25862	4.89%	0.554%

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37	12.368	1727	1730	1736	rVB4	16763	31271	5.92%	0.670%
38	12.477	1742	1748	1755	rVB	228277	369162	69.83%	7.904%
39	12.569	1755	1763	1767	rBV8	12755	36236	6.85%	0.776%
40	12.642	1770	1775	1781	rVB4	38714	73451	13.89%	1.573%
41	12.733	1782	1790	1794	rBV8	22612	60802	11.50%	1.302%
42	12.813	1795	1803	1808	rBV7	36031	91501	17.31%	1.959%
43	12.910	1816	1819	1820	rBV3	5984	6110	1.16%	0.131%
44	12.947	1822	1825	1828	rVB3	14439	18043	3.41%	0.386%
45	12.989	1828	1832	1836	rBV5	7883	12992	2.46%	0.278%
46	13.123	1851	1854	1857	rBV4	7741	10834	2.05%	0.232%
47	13.166	1857	1861	1867	rVV7	15043	26470	5.01%	0.567%
48	13.245	1871	1874	1877	rVB4	7733	10576	2.00%	0.226%
49	13.288	1877	1881	1883	rBV3	17641	25629	4.85%	0.549%
50	13.319	1883	1886	1889	rVB4	20823	26501	5.01%	0.567%
51	13.422	1897	1903	1909	rBV	294977	461243	87.25%	9.876%
52	13.562	1922	1926	1930	rVB4	13149	18330	3.47%	0.392%
53	13.745	1950	1956	1961	rBV6	40693	79410	15.02%	1.700%
54	13.788	1961	1963	1966	rBV4	6527	9571	1.81%	0.205%
55	13.928	1981	1986	1988	rBV4	10191	19290	3.65%	0.413%
56	13.959	1989	1991	1997	rVB4	19579	26796	5.07%	0.574%
57	14.068	2006	2009	2015	rBV7	12758	23872	4.52%	0.511%
58	14.135	2015	2020	2026	rVB8	15385	34220	6.47%	0.733%
59	14.203	2026	2031	2033	rBV5	8847	15876	3.00%	0.340%
60	14.257	2035	2040	2050	rVB9	33799	81263	15.37%	1.740%
61	14.379	2056	2060	2062	rBV4	10939	16852	3.19%	0.361%
62	14.416	2063	2066	2071	rVB3	25530	37942	7.18%	0.812%
63	14.617	2095	2099	2103	rBV6	10762	18898	3.57%	0.405%
64	14.672	2104	2108	2114	rVV4	24081	54278	10.27%	1.162%
65	14.727	2114	2117	2123	rVB6	22199	41482	7.85%	0.888%
66	14.940	2149	2152	2156	rVB5	17940	23651	4.47%	0.506%
67	15.117	2178	2181	2183	rBV4	7385	9791	1.85%	0.210%
68	15.208	2192	2196	2203	rBV6	24830	47950	9.07%	1.027%
69	15.605	2257	2261	2265	rVB5	20670	34516	6.53%	0.739%
70	16.007	2325	2327	2329	rBV3	6188	7041	1.33%	0.151%
71	16.153	2347	2351	2357	rVB2	23095	40179	7.60%	0.860%
72	16.470	2399	2403	2409	rBV9	16009	28648	5.42%	0.613%

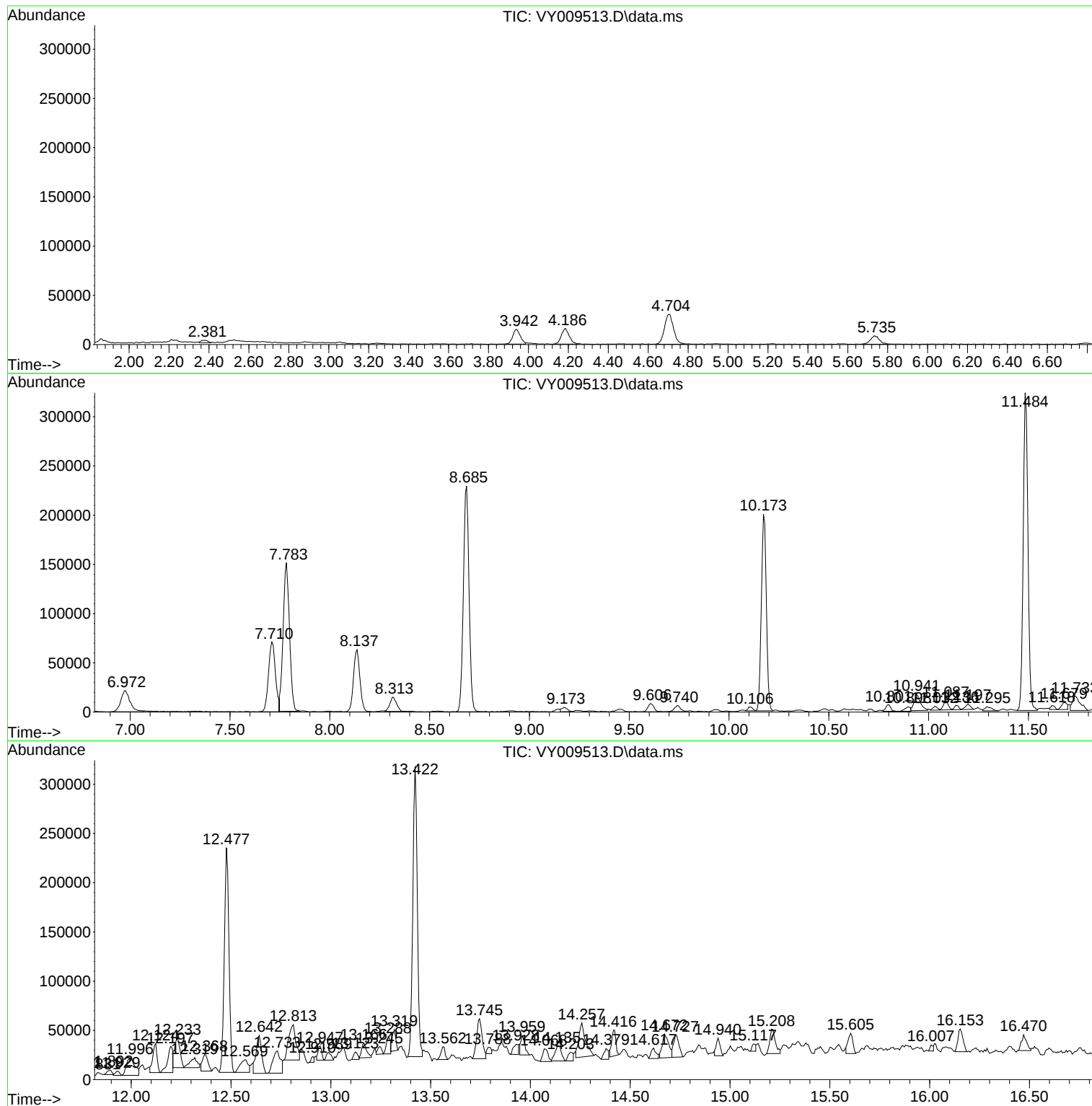
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220497A-SIM-C3A-COMPOSITE

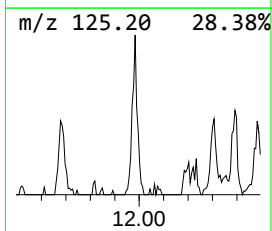
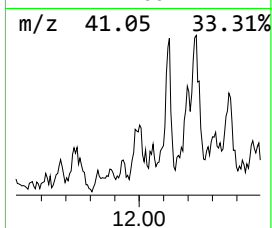
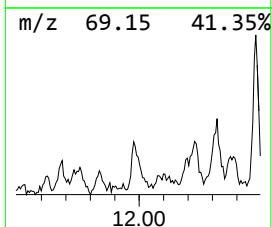
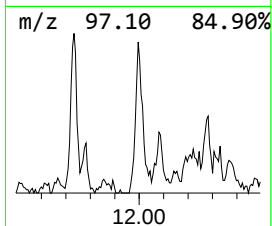
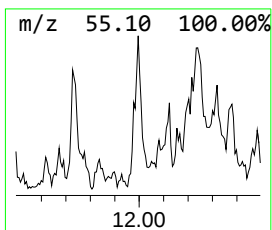
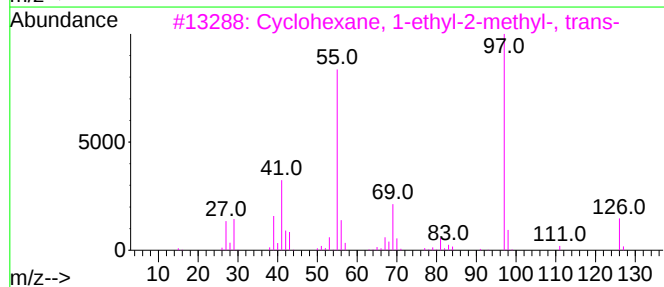
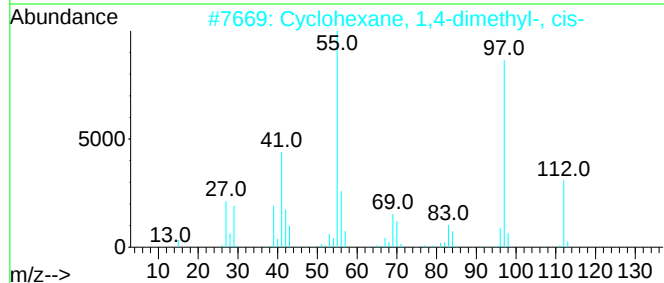
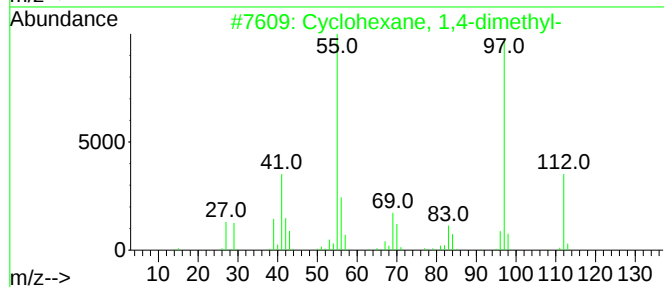
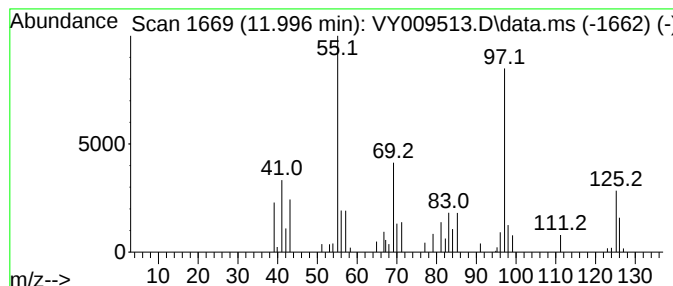
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, 1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.996	5.01 ug/l	53005	Chlorobenzene-d5	11.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	59
2			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	59
3			Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	58
4			4,4-Dimethyl-oct-5-enal	154	C10H18O	1010143-73-6	50
5			3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	47



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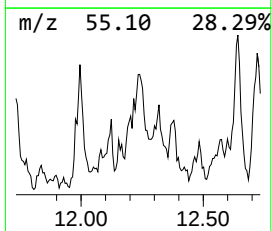
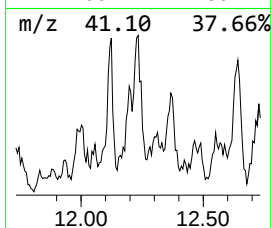
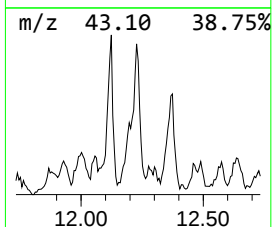
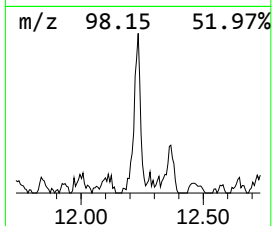
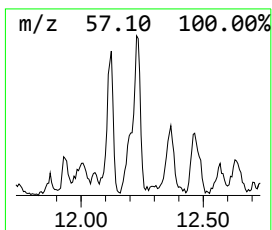
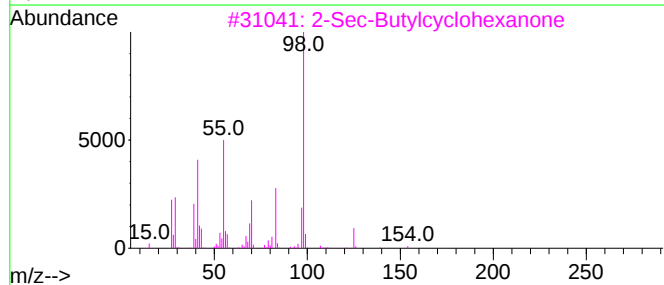
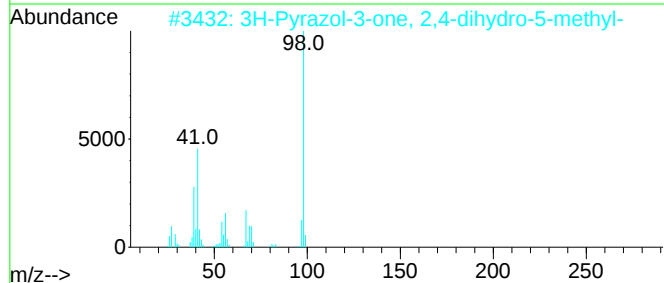
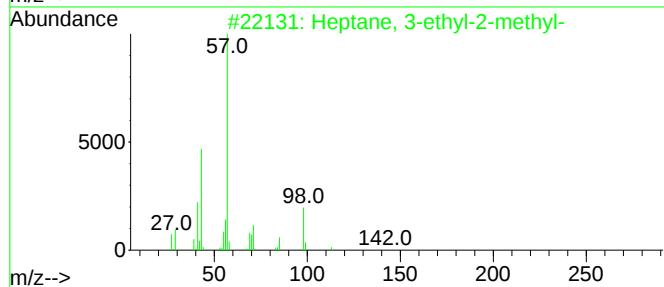
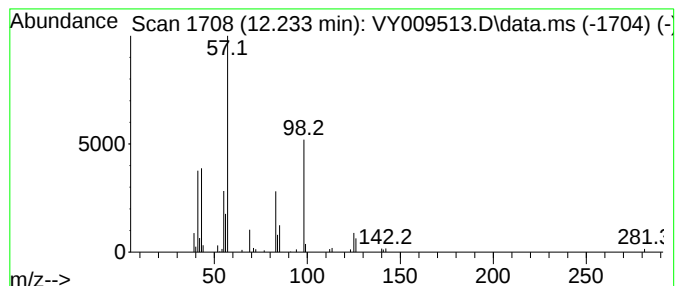
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.233 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	5.30 ug/l	56040	Chlorobenzene-d5	11.483

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	40
2			3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	38
3			2-Sec-Butylcyclohexanone	154	C10H18O	014765-30-1	38
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	38
5			Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	35



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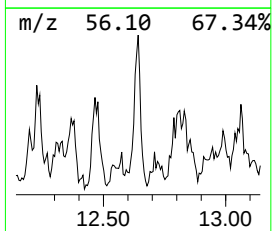
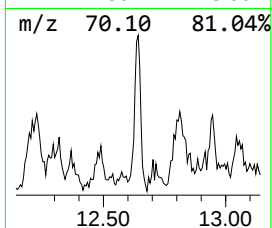
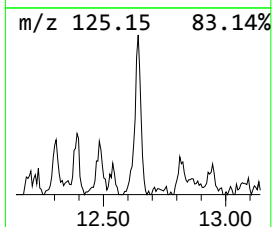
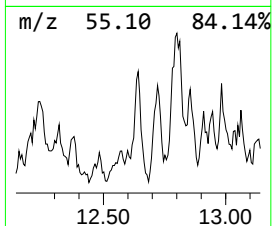
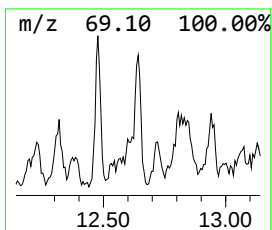
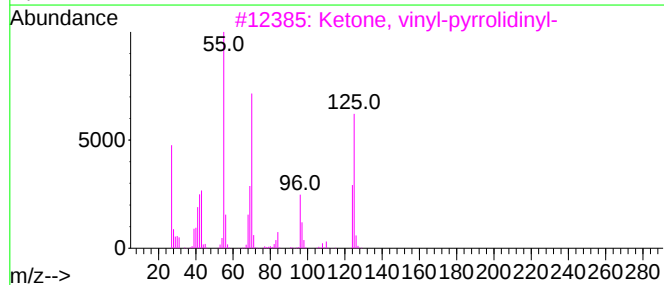
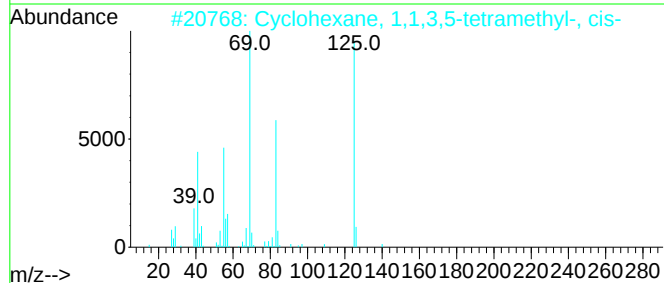
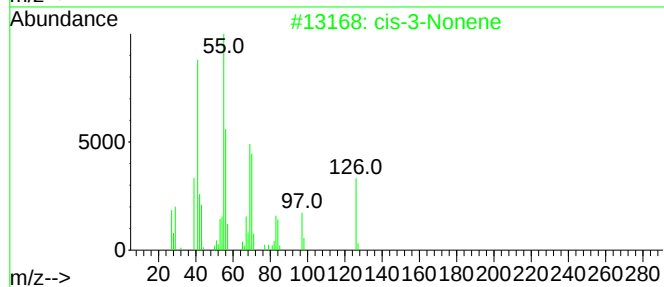
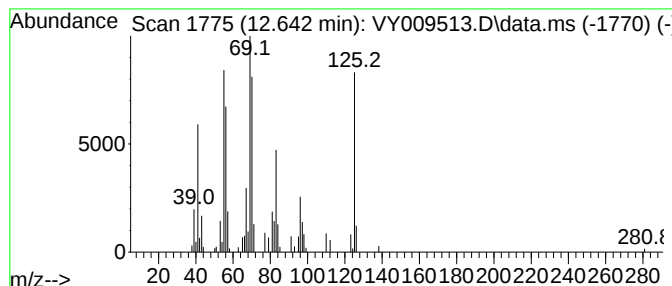
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 cis-3-Nonene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.642	7.96 ug/l	73451	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-3-Nonene	126	C9H18	020237-46-1	52
2			Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	50
3			Ketone, vinyl-pyrrolidinyl-	125	C7H11NO	042104-70-1	46
4			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	43
5			3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	38



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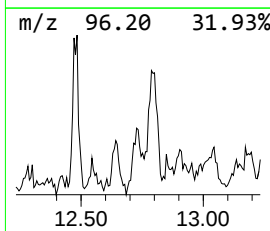
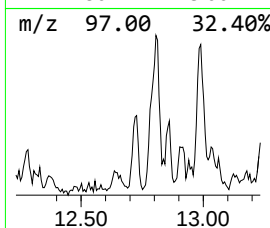
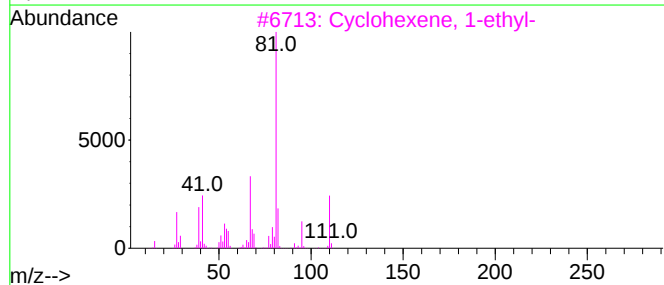
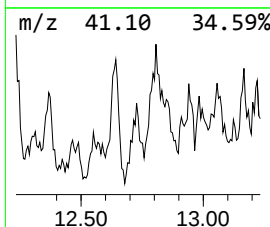
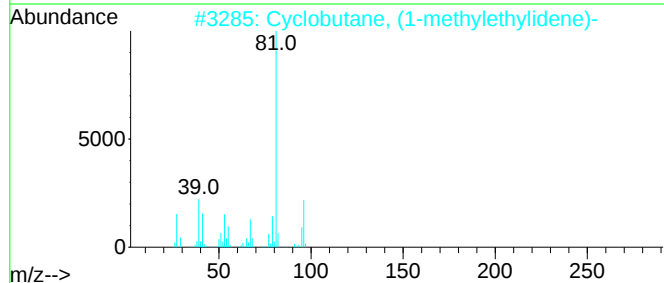
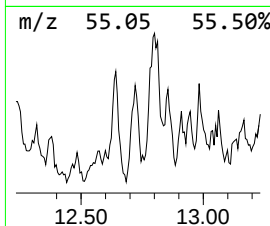
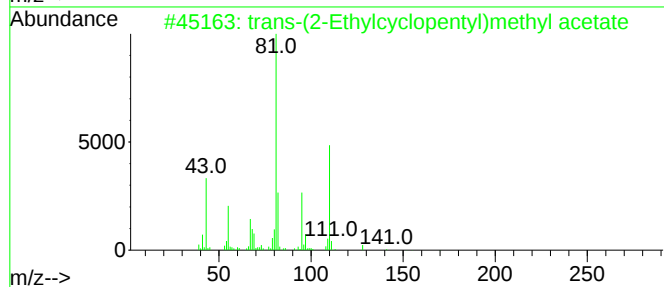
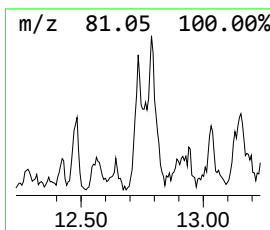
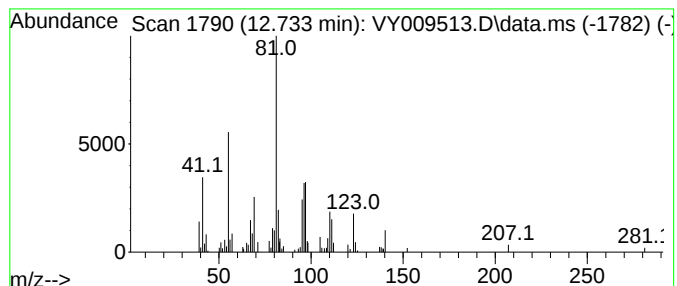
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Quant Title : SW846 8260

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

Peak Number 4 trans-(2-Ethylcyclopentyl)m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	6.59 ug/l	60802	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-(2-Ethylcyclopentyl)methyl...	170	C10H18O2	1000099-13-9	50
2			Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	46
3			Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	43
4			Cyclohexene, 3-ethyl-	110	C8H14	002808-71-1	43
5			1,4-Hexadiene, 3-ethyl-	110	C8H14	002080-89-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
Data File : VY009513.D
Acq On : 11 Jul 2022 16:18
Operator : KP/MD
Sample : N3622-08
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220497A-SIM-C3A-COMPOSITE

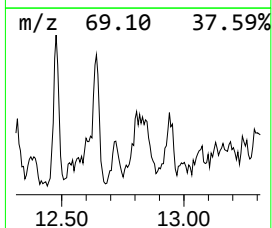
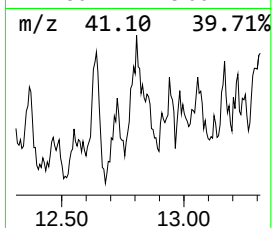
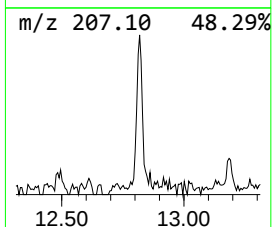
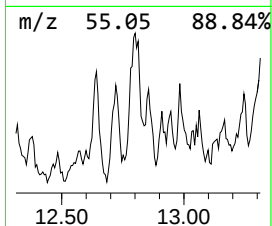
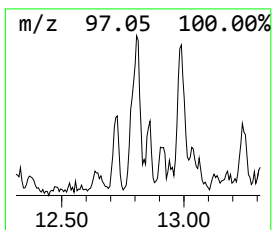
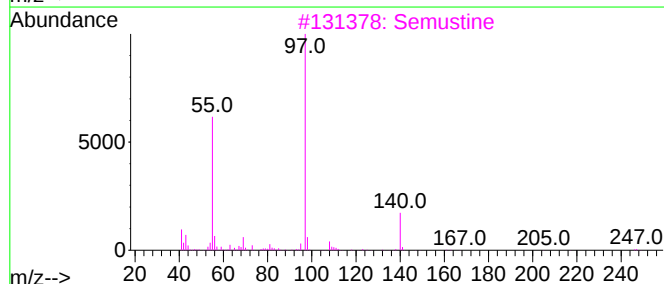
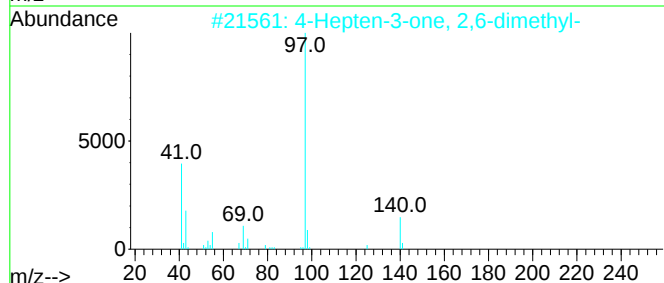
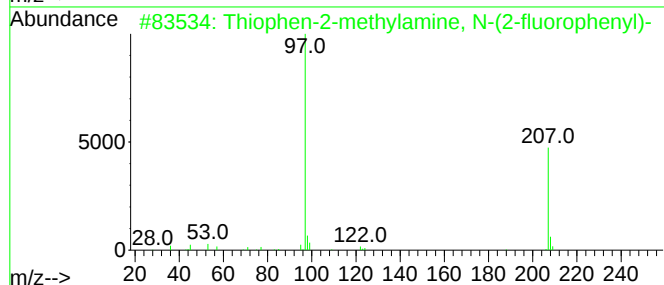
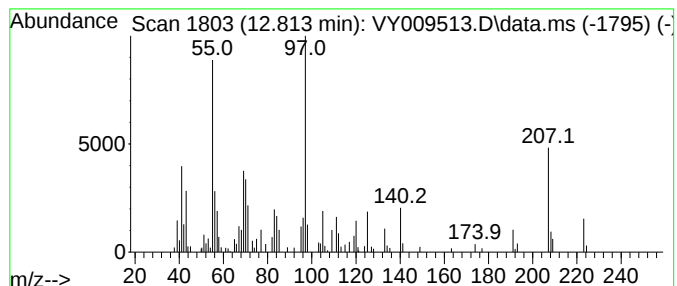
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Quant Title : SW846 8260

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

Peak Number 5 unknown12.813 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.813	9.92 ug/l	91501	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophen-2-methylamine, N-(2-flu...	207	C11H10FNS	1000310-35-2	47
2			4-Hepten-3-one, 2,6-dimethyl-	140	C9H16O	056259-14-4	38
3			Semustine	247	C10H18ClN3O2	013909-09-6	35
4			2(5H)-Furanone, 5-(7-hydroxy-6-m...	226	C13H22O3	1206874-24-9	27
5			Oxalic acid, cyclohexylmethyl oc...	298	C17H30O4	1000309-68-4	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
Data File : VY009513.D
Acq On : 11 Jul 2022 16:18
Operator : KP/MD
Sample : N3622-08
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220497A-SIM-C3A-COMPOSITE

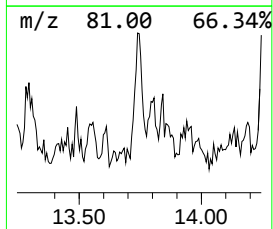
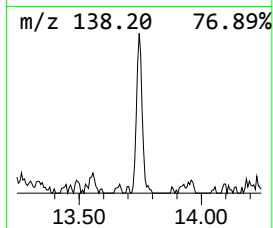
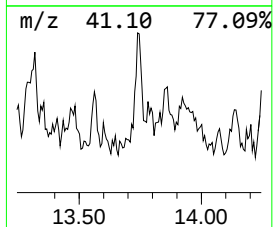
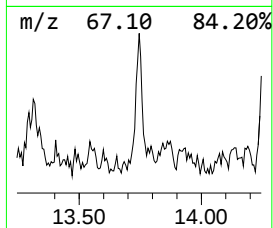
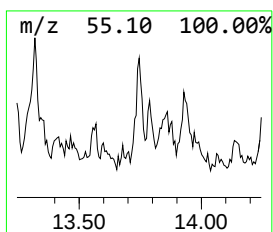
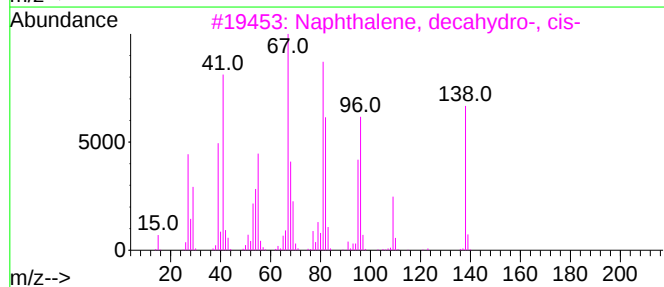
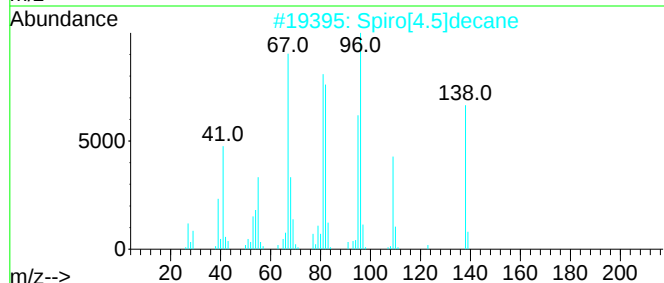
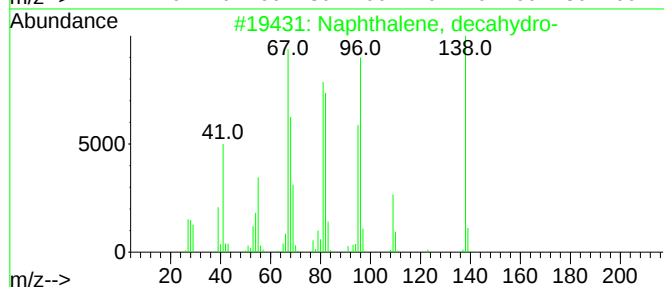
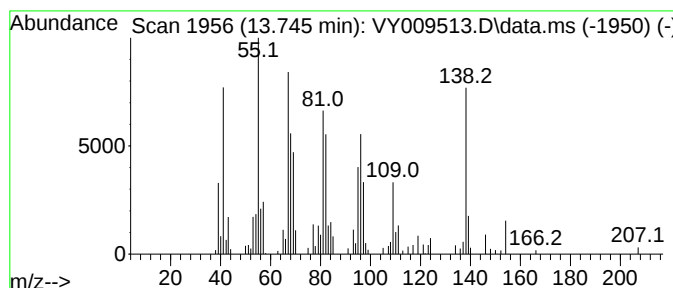
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, decahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	8.61 ug/l	79410	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	96
2			Spiro[4.5]decane	138	C10H18	000176-63-6	94
3			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	91
4			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	90
5			Bicyclo[5.3.0]decane	138	C10H18	005661-80-3	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
Data File : VY009513.D
Acq On : 11 Jul 2022 16:18
Operator : KP/MD
Sample : N3622-08
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220497A-SIM-C3A-COMPOSITE

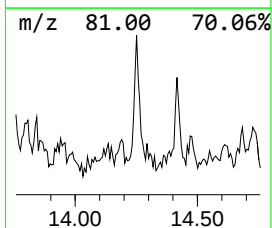
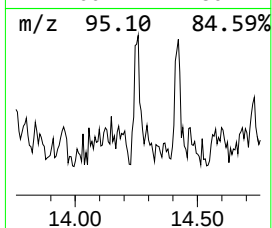
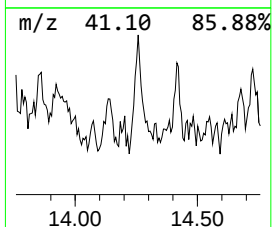
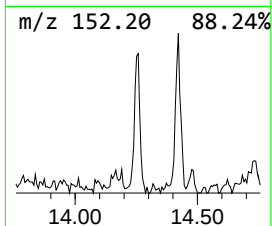
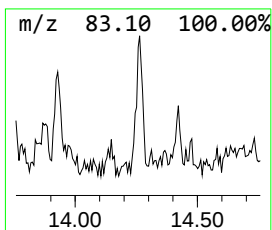
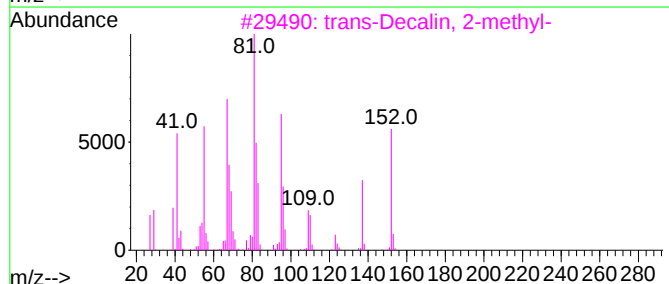
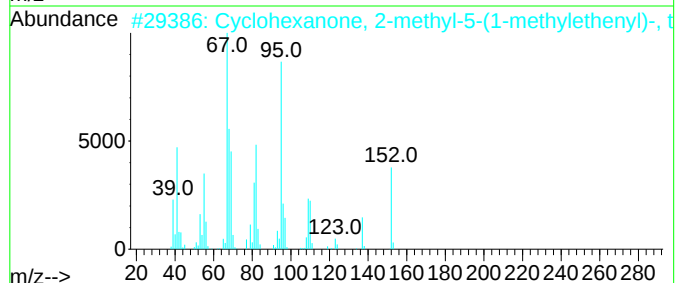
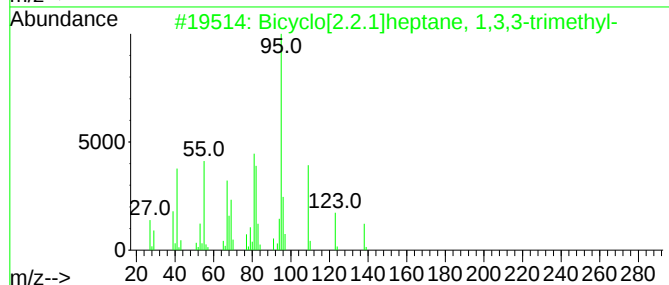
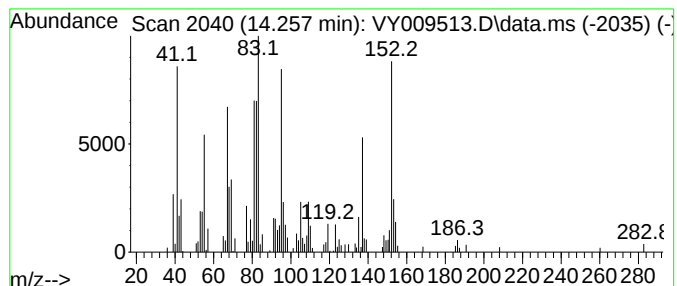
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Quant Title : SW846 8260

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

Peak Number 7 Bicyclo[2.2.1]heptane, 1,3,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	8.81 ug/l	81263	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	87
2			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	64
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	62
4			6,6-Dimethyl-cyclooct-4-enone	152	C10H16O	1000194-10-0	58
5			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
Data File : VY009513.D
Acq On : 11 Jul 2022 16:18
Operator : KP/MD
Sample : N3622-08
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220497A-SIM-C3A-COMPOSITE

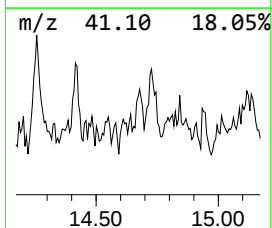
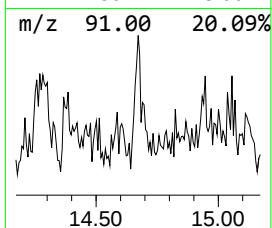
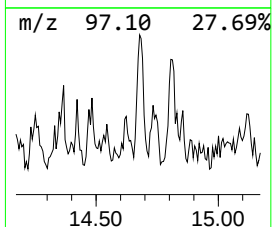
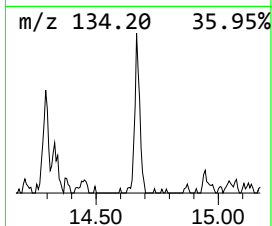
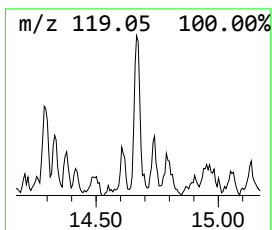
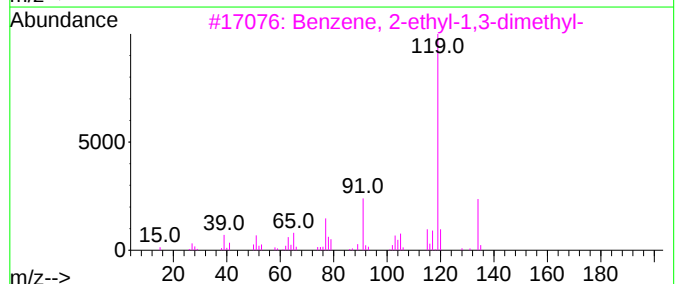
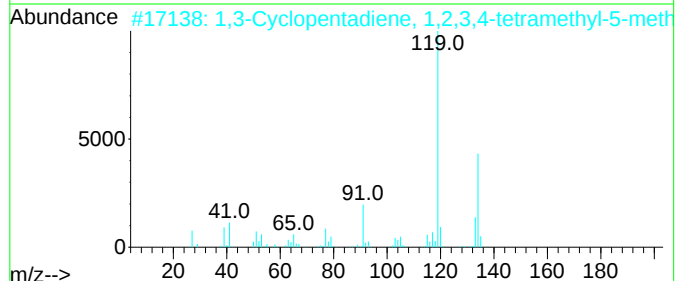
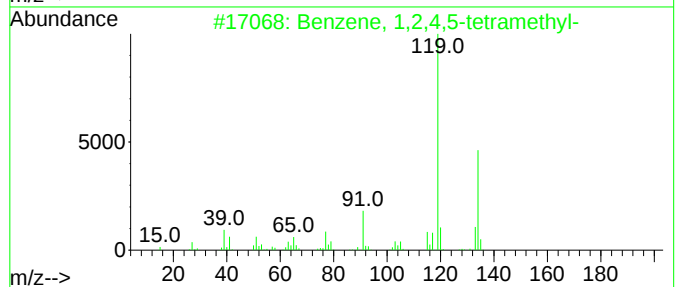
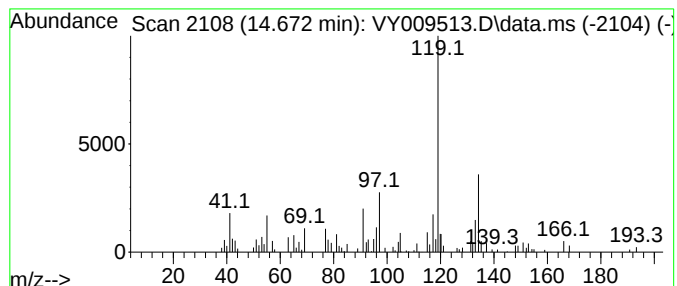
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.672	5.88 ug/l	54278	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	76
2			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	70
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	64
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	64
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
Data File : VY009513.D
Acq On : 11 Jul 2022 16:18
Operator : KP/MD
Sample : N3622-08
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220497A-SIM-C3A-COMPOSITE

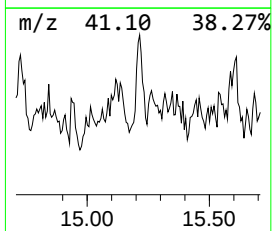
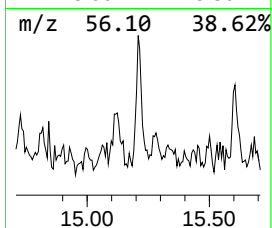
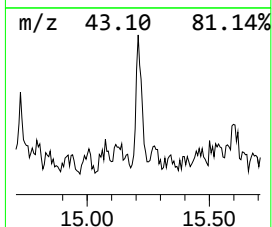
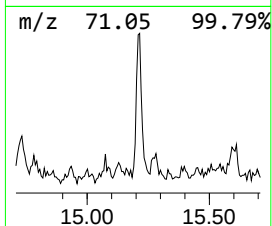
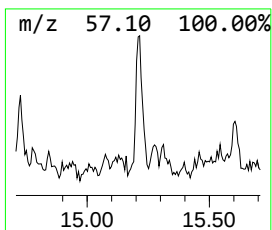
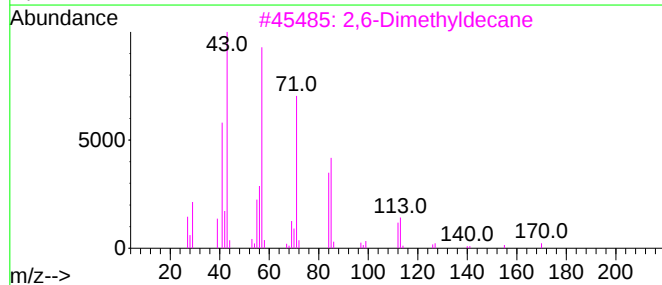
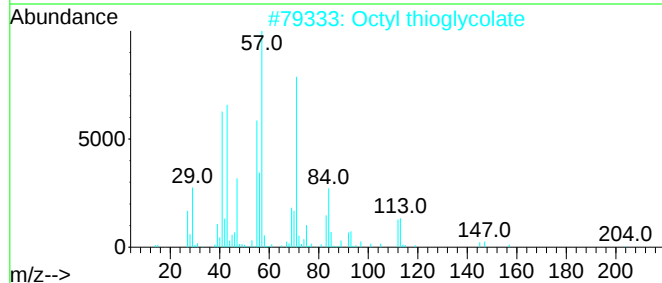
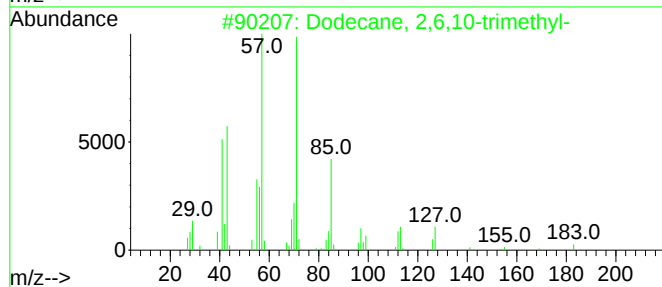
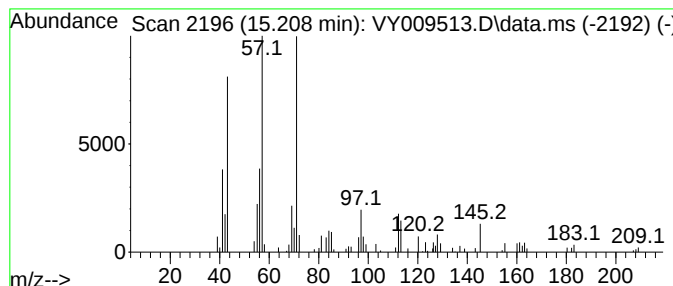
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Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 2,6,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.209	5.20 ug/l	47950	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80
2			Octyl thioglycolate	204	C10H20O2S	007664-80-4	64
3			2,6-Dimethyldecane	170	C12H26	013150-81-7	59
4			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	59
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY071122\
Data File : VY009513.D
Acq On : 11 Jul 2022 16:18
Operator : KP/MD
Sample : N3622-08
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20220497A-SIM-C3A-COMPOSITE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y070722S.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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unknown12.233	12.233	5.3	ug/l	56040	3	11.483	528646	50.0
cis-3-Nonene	12.642	8.0	ug/l	73451	4	13.422	461243	50.0
trans-(2-Ethylc...	12.733	6.6	ug/l	60802	4	13.422	461243	50.0
unknown12.813	12.813	9.9	ug/l	91501	4	13.422	461243	50.0
Naphthalene, de...	13.745	8.6	ug/l	79410	4	13.422	461243	50.0
Bicyclo[2.2.1]h...	14.257	8.8	ug/l	81263	4	13.422	461243	50.0
Benzene, 1,2,4,...	14.672	5.9	ug/l	54278	4	13.422	461243	50.0
Dodecane, 2,6,1...	15.209	5.2	ug/l	47950	4	13.422	461243	50.0