

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD010721\
 Data File : VD068031.D
 Acq On : 07 Jan 2021 13:51
 Operator : VA/SY
 Sample : M1023-01
 Misc : 7.00G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 SU-04-010621

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_D\Method\82D122220S.M
 Title : SW846 8260

Signal : TIC: VD068031.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.320	61	68	71	rBV	22312	37595	2.01%	0.291%
2	4.967	509	518	525	rBV5	6312	19670	1.05%	0.152%
3	7.920	1006	1020	1025	rBV2	245672	607896	32.51%	4.711%
4	7.985	1025	1031	1041	rVB	390226	879949	47.07%	6.819%
5	8.338	1080	1091	1101	rBV2	232479	528298	28.26%	4.094%
6	8.867	1172	1181	1193	rBV	625414	1277758	68.34%	9.902%
7	9.361	1259	1265	1270	rVB4	9684	20321	1.09%	0.157%
8	10.344	1423	1432	1439	rBV	1065778	1869603	100.00%	14.489%
9	10.514	1454	1461	1469	rVB4	14801	35567	1.90%	0.276%
10	10.679	1484	1489	1497	rVB3	22314	42966	2.30%	0.333%
11	11.243	1579	1585	1592	rVB2	54149	92421	4.94%	0.716%
12	11.449	1615	1620	1629	rVB4	22221	43857	2.35%	0.340%
13	11.649	1644	1654	1664	rBV	891012	1602494	85.71%	12.419%
14	11.785	1672	1677	1680	rVB4	13236	21270	1.14%	0.165%
15	11.855	1680	1689	1692	rVV5	30966	80216	4.29%	0.622%
16	11.891	1692	1695	1707	rVB7	34428	97871	5.23%	0.758%
17	12.055	1716	1723	1732	rVB10	11681	37327	2.00%	0.289%
18	12.155	1732	1740	1748	rBV5	47116	137191	7.34%	1.063%
19	12.267	1757	1759	1763	rVB3	19572	25024	1.34%	0.194%
20	12.379	1763	1778	1785	rBV5	46442	183558	9.82%	1.423%
21	12.467	1785	1793	1796	rBV9	15242	38051	2.04%	0.295%
22	12.632	1815	1821	1830	rBV	689490	1102019	58.94%	8.540%
23	12.726	1830	1837	1840	rBV9	19594	42286	2.26%	0.328%
24	12.796	1845	1849	1856	rVB4	73821	133873	7.16%	1.037%
25	12.879	1856	1863	1869	rBV8	36736	96678	5.17%	0.749%
26	12.949	1871	1875	1882	rBV6	61229	139103	7.44%	1.078%
27	13.096	1896	1900	1905	rBV6	31437	49242	2.63%	0.382%
28	13.143	1905	1908	1911	rVV4	14717	19883	1.06%	0.154%
29	13.185	1911	1915	1921	rBV2	54174	86303	4.62%	0.669%
30	13.273	1927	1930	1933	rVB4	21662	25500	1.36%	0.198%
31	13.314	1933	1937	1940	rVB4	16327	20848	1.12%	0.162%
32	13.461	1955	1962	1966	rBV9	37659	81508	4.36%	0.632%
33	13.502	1966	1969	1973	rVV4	34835	49002	2.62%	0.380%
34	13.573	1975	1981	1990	rVB	721623	1263733	67.59%	9.794%
35	13.637	1990	1992	1995	rBV3	17481	21626	1.16%	0.168%
36	13.714	2000	2005	2010	rBV8	36348	65866	3.52%	0.510%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	13.808	2018	2021	2023	rBV3	15355	22193	1.19%	0.172%
38	13.896	2030	2036	2042	rBV4	142536	238878	12.78%	1.851%
39	14.008	2051	2055	2056	rBV4	25194	30329	1.62%	0.235%
40	14.114	2070	2073	2077	rVB3	41010	51401	2.75%	0.398%
41	14.220	2086	2091	2096	rBV7	52179	94060	5.03%	0.729%
42	14.284	2097	2102	2108	rVB7	52998	110681	5.92%	0.858%
43	14.367	2108	2116	2118	rBV6	57292	132834	7.10%	1.029%
44	14.408	2119	2123	2128	rVV5	64203	108537	5.81%	0.841%
45	14.526	2139	2143	2145	rBV4	41419	61656	3.30%	0.478%
46	14.573	2145	2151	2155	rVB6	75452	148843	7.96%	1.154%
47	14.755	2178	2182	2187	rVB6	54277	96452	5.16%	0.747%
48	14.832	2187	2195	2197	rBV6	82506	181501	9.71%	1.407%
49	14.867	2197	2201	2209	rVB2	142402	287205	15.36%	2.226%
50	15.202	2254	2258	2263	rVB8	29794	55363	2.96%	0.429%
51	15.367	2280	2286	2292	rBV2	112667	214819	11.49%	1.665%
52	15.779	2352	2356	2363	rVB8	59443	108512	5.80%	0.841%
53	16.343	2447	2452	2458	rVB5	43200	83846	4.48%	0.650%

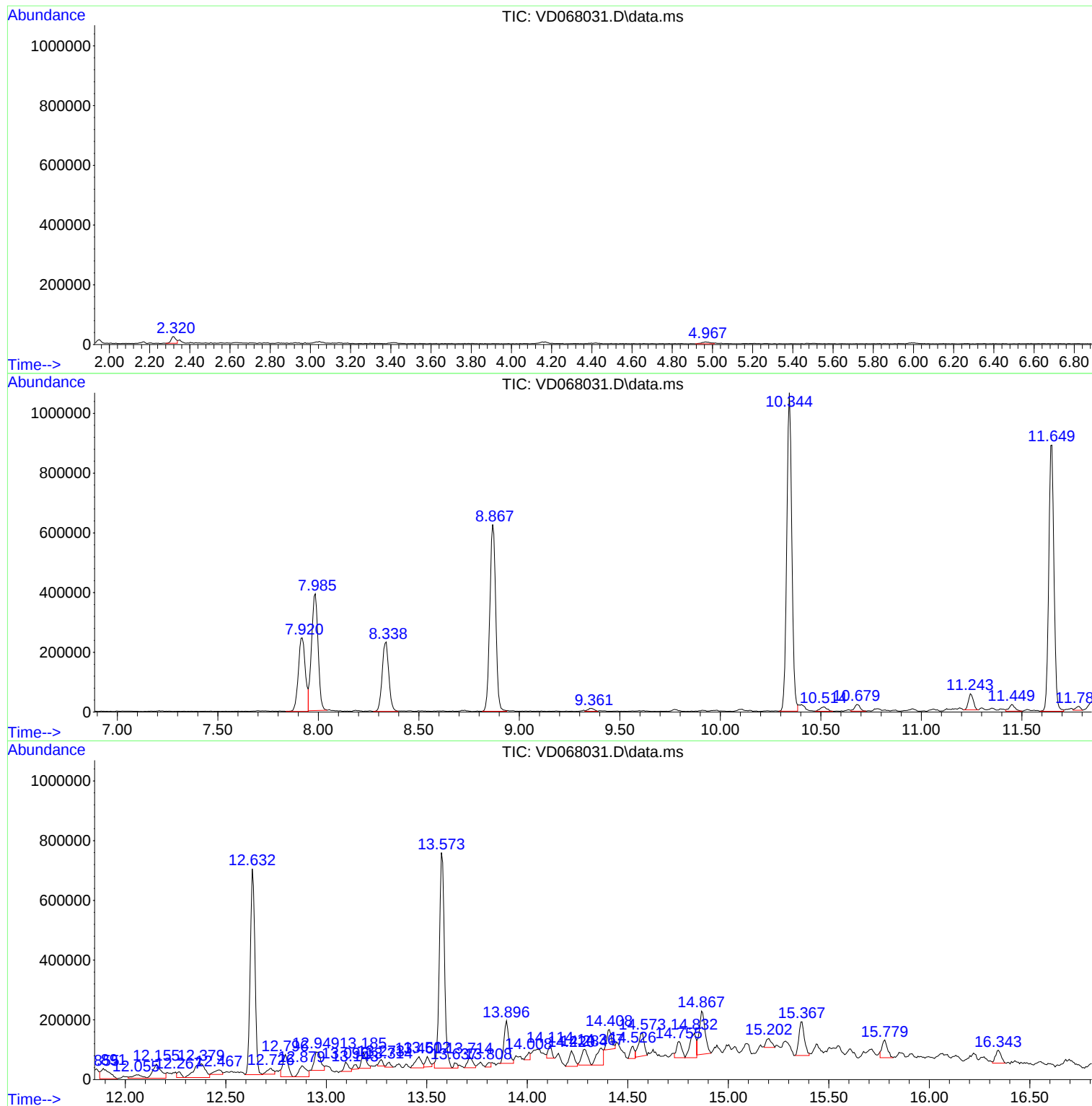
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D122220S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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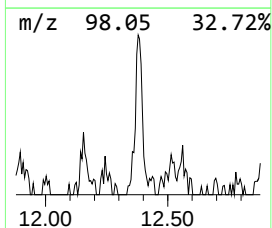
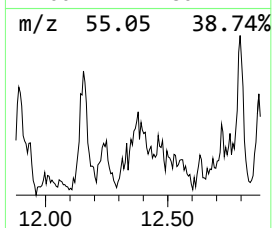
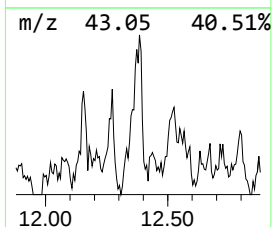
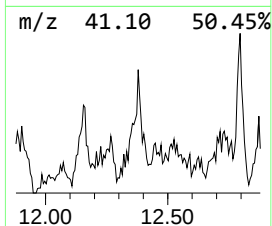
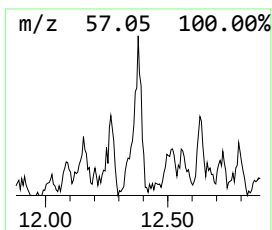
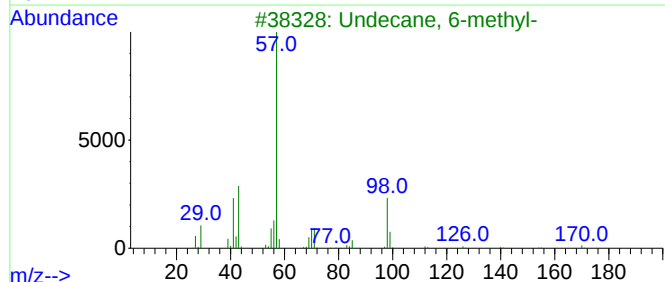
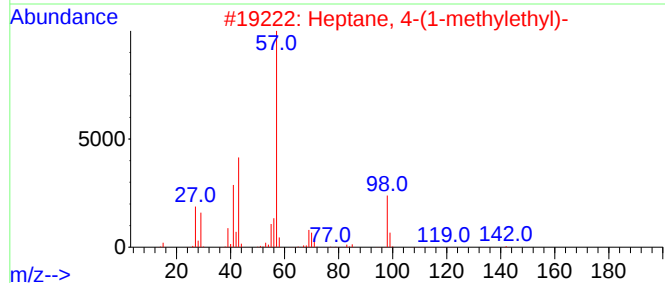
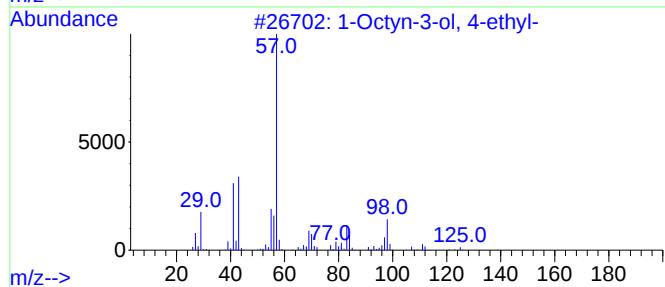
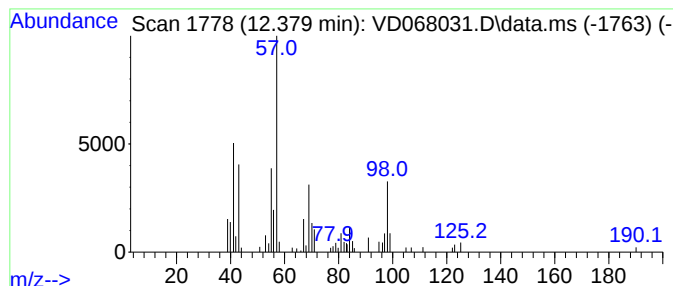
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D12220S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Octyn-3-ol, 4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.379	5.73 ug/l	183558	Chlorobenzene-d5	11.649

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octyn-3-ol, 4-ethyl-	154	C10H18O	005877-42-9	64
2			Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	50
3			Undecane, 6-methyl-	170	C12H26	017302-33-9	43
4			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	43
5			Heptane, 4-propyl-	142	C10H22	003178-29-8	37



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Instrument :
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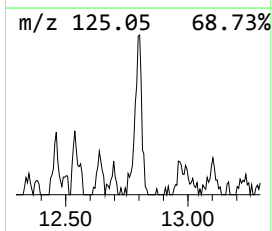
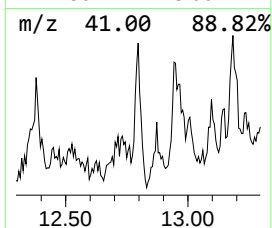
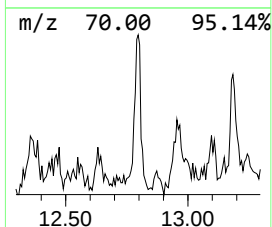
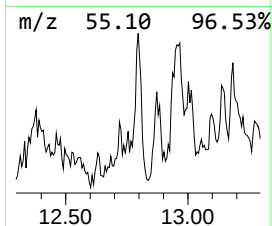
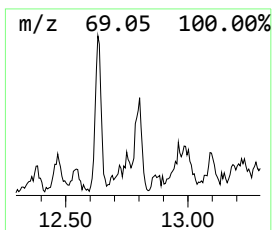
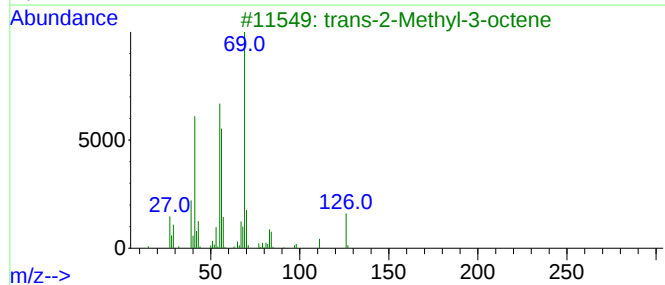
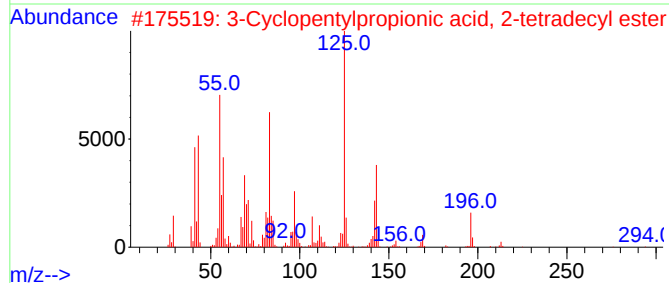
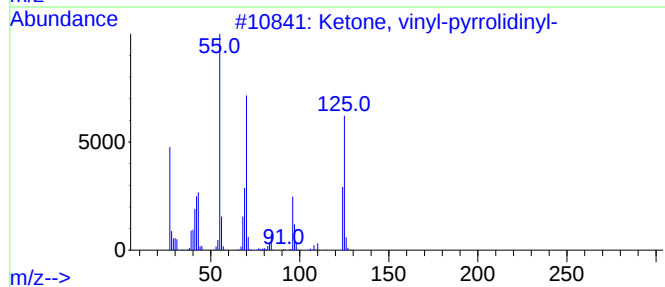
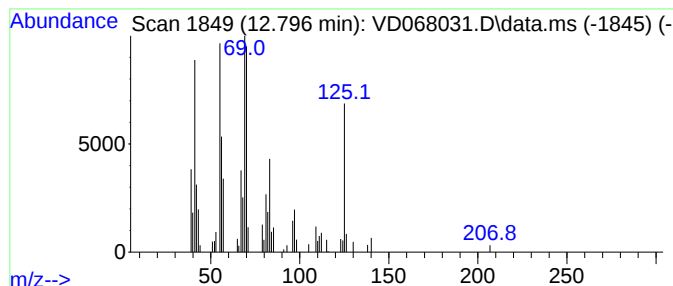
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D122220S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown12.796 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.796	5.30 ug/l	133873	1,4-Dichlorobenzene-d4	13.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ketone, vinyl-pyrrolidinyl-	125	C7H11NO	042104-70-1	38
2			3-Cyclopentylpropionic acid, 2-t...	338	C22H42O2	1000293-57-2	30
3			trans-2-Methyl-3-octene	126	C9H18	052937-36-7	30
4			3-Octene, (Z)-	112	C8H16	014850-22-7	25
5			3-Cyclopentylpropionic acid, 2-t...	324	C21H40O2	1000293-56-9	22



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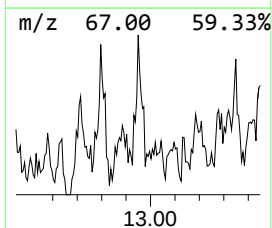
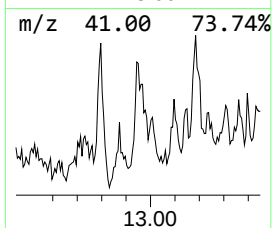
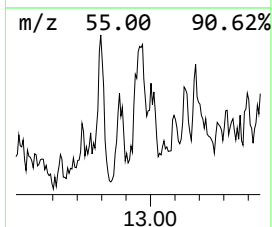
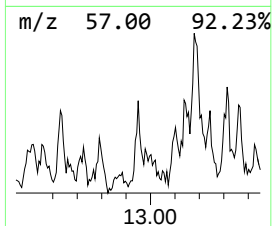
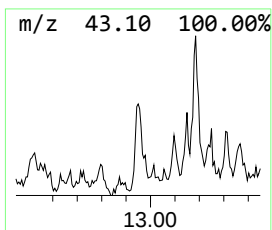
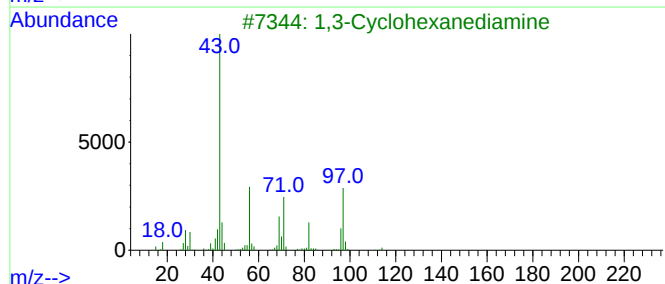
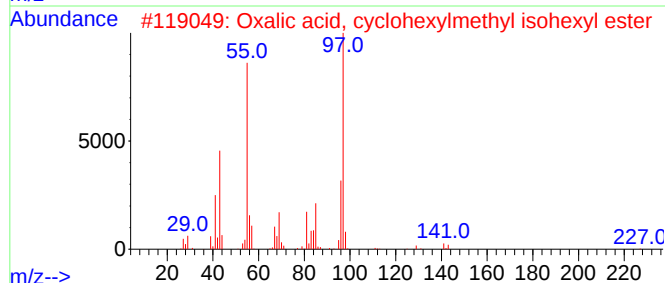
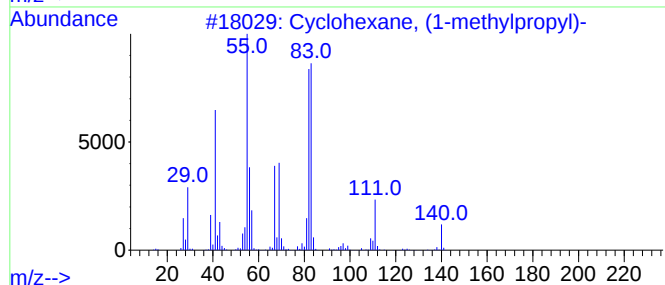
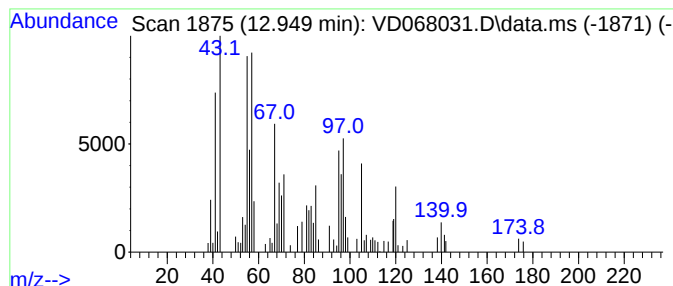
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.949 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.949	5.50 ug/l	139103	1,4-Dichlorobenzene-d4	13.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (1-methylpropyl)-	140	C10H20	007058-01-7	25
2			Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	22
3			1,3-Cyclohexanediamine	114	C6H14N2	003385-21-5	22
4			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	006069-97-2	20
5			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	18



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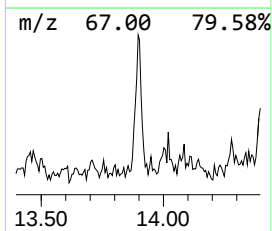
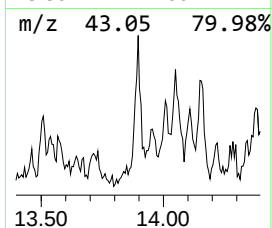
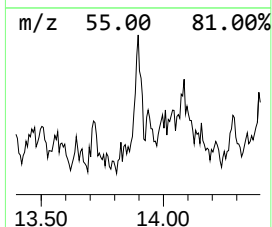
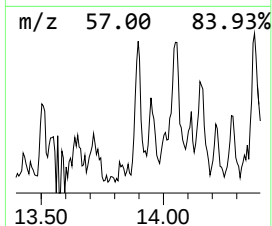
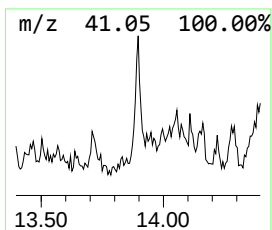
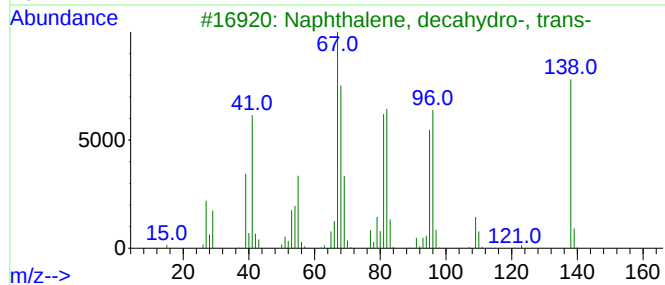
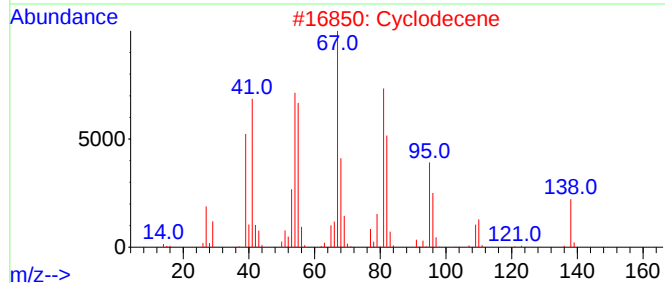
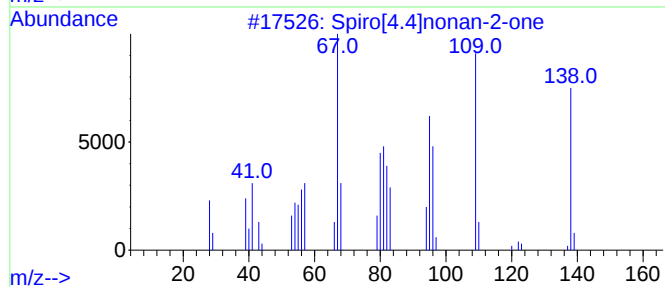
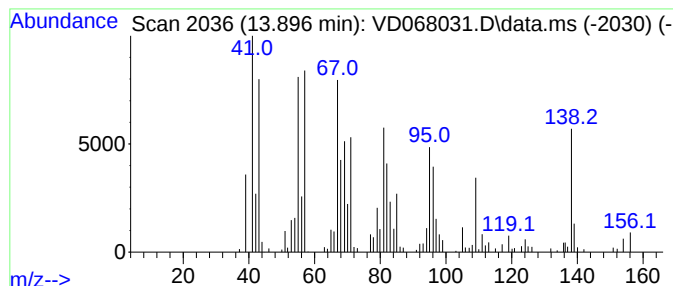
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D12220S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Spiro[4.4]nonan-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.896	9.45 ug/l	238878	1,4-Dichlorobenzene-d4	13.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Spiro[4.4]nonan-2-one	138	C9H14O	034177-18-9	70
2			Cyclodecene	138	C10H18	003618-12-0	62
3			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	62
4			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	58
5			1H-Inden-1-one, octahydro-, trans-	138	C9H14O	016783-22-5	55



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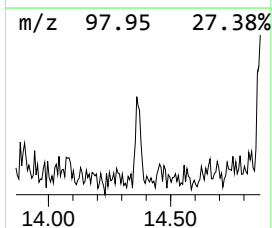
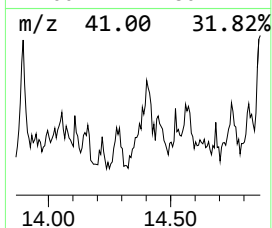
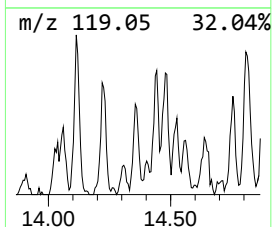
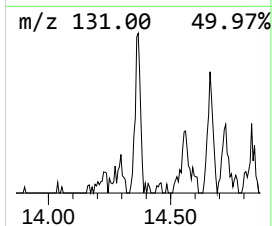
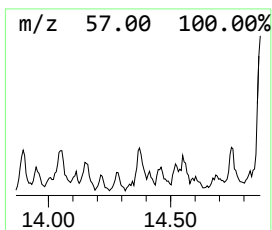
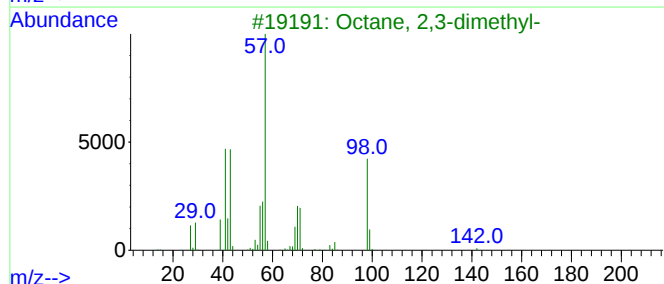
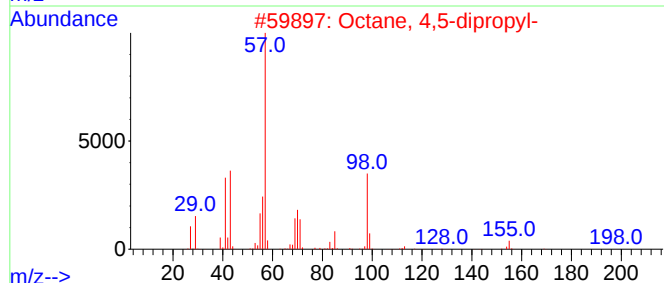
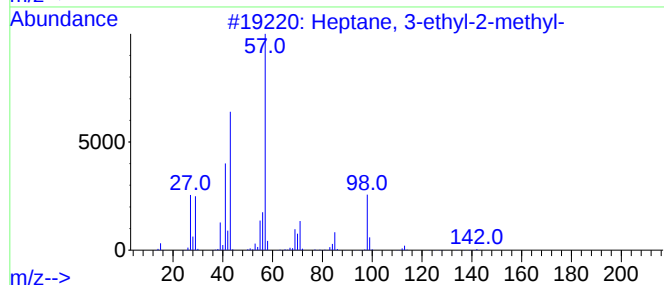
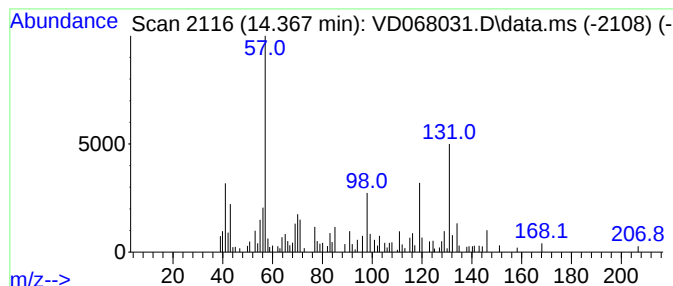
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown14.367 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.367	5.26 ug/l	132834	1,4-Dichlorobenzene-d4	13.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	27
2			Octane, 4,5-dipropyl-	198	C14H30	020905-05-9	27
3			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	22
4			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	18
5			Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD010721\
Data File : VD068031.D
Acq On : 07 Jan 2021 13:51
Operator : VA/SY
Sample : M1023-01
Misc : 7.00G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SU-04-010621

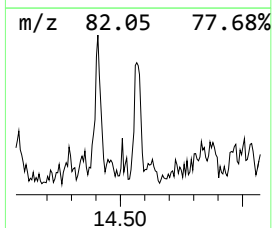
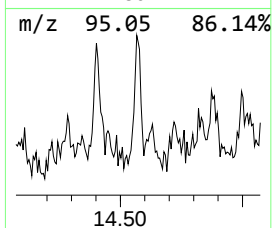
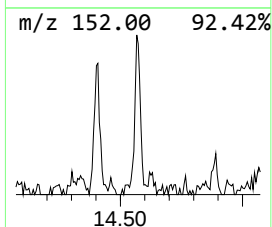
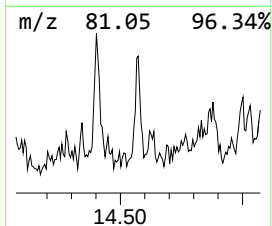
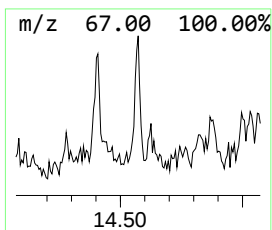
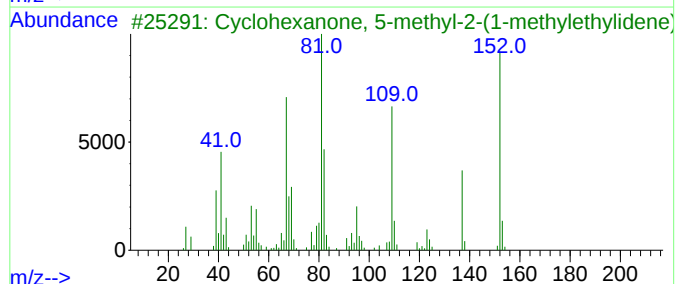
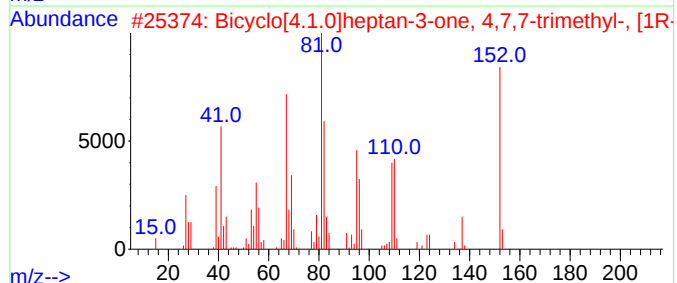
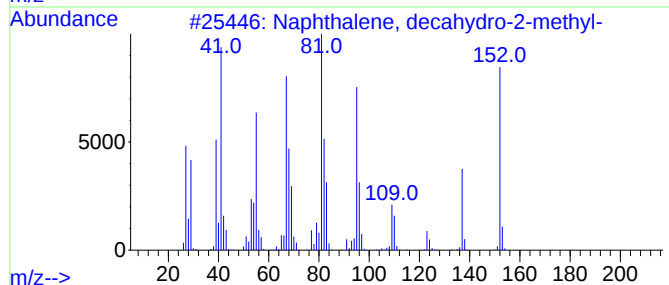
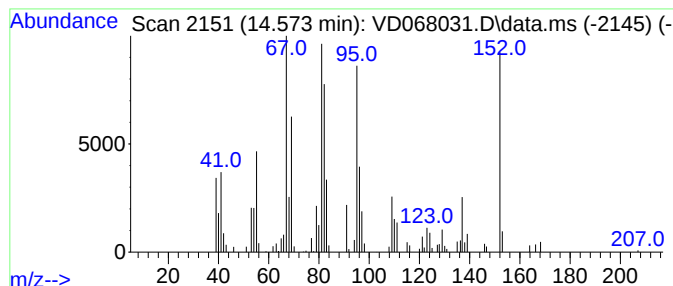
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Naphthalene, decahydro-2-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.573	5.89 ug/l	148843	1,4-Dichlorobenzene-d4	13.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	91
2			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	81
3			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	78
4			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	76
5			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-01-6	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD010721\
Data File : VD068031.D
Acq On : 07 Jan 2021 13:51
Operator : VA/SY
Sample : M1023-01
Misc : 7.00G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SU-04-010621

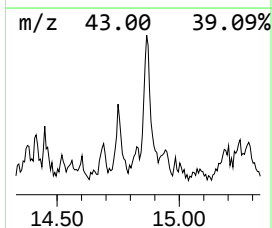
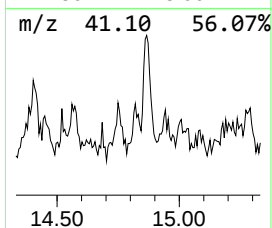
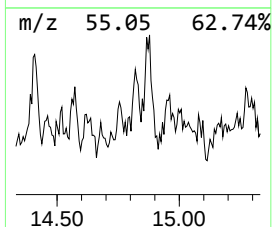
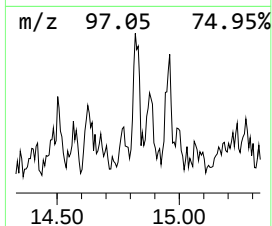
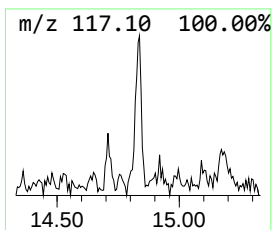
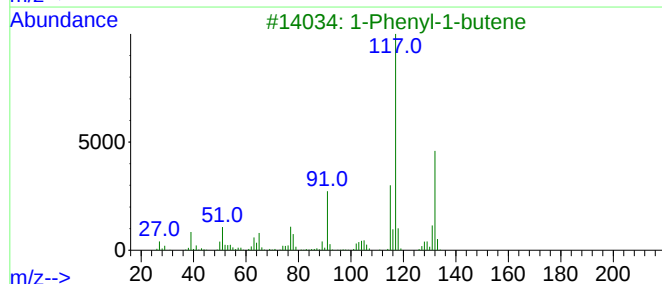
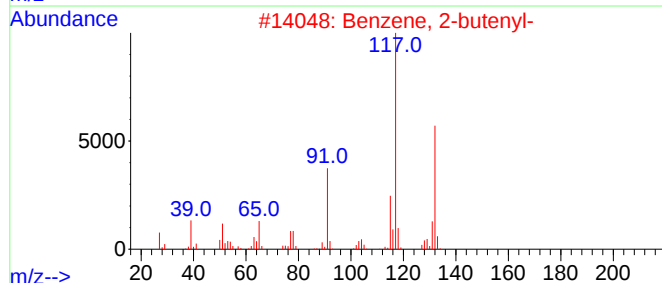
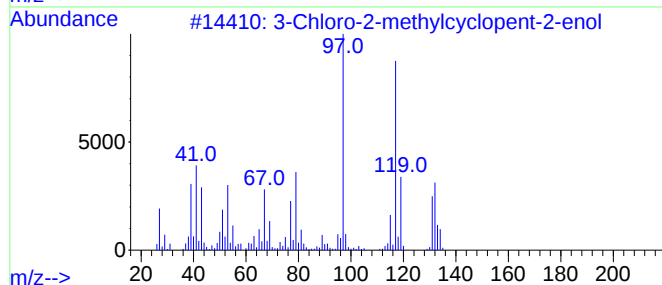
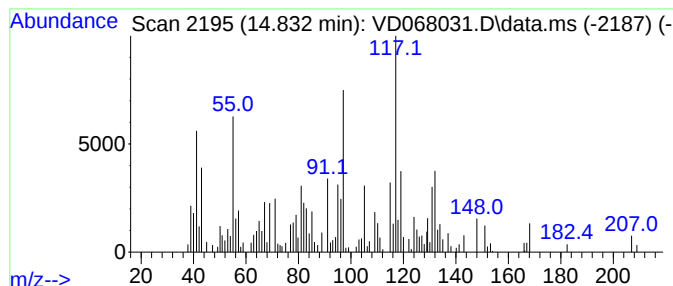
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 3-Chloro-2-methylcyclopent-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.832	7.18 ug/l	181501	1,4-Dichlorobenzene-d4	13.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-2-methylcyclopent-2-enol	132	C6H9ClO	1000192-84-7	53
2			Benzene, 2-butenyl-	132	C10H12	001560-06-1	38
3			1-Phenyl-1-butene	132	C10H12	000824-90-8	38
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	38
5			Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD010721\
Data File : VD068031.D
Acq On : 07 Jan 2021 13:51
Operator : VA/SY
Sample : M1023-01
Misc : 7.00G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SU-04-010621

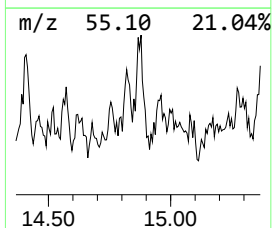
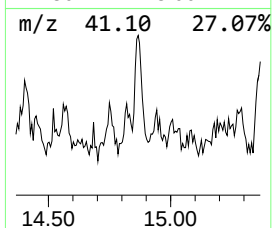
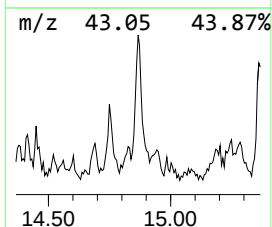
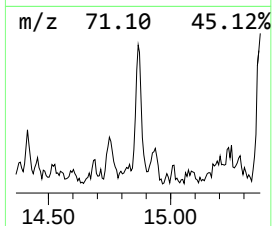
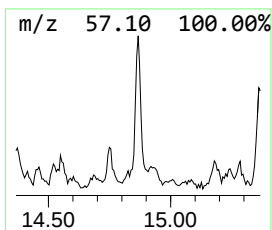
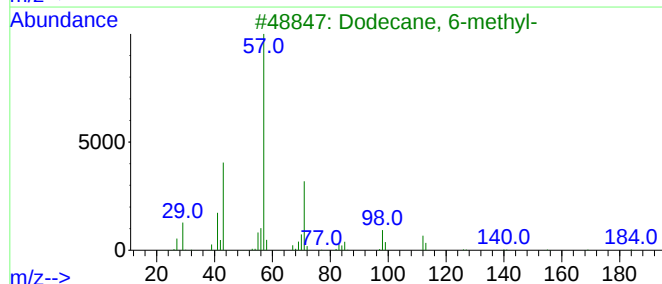
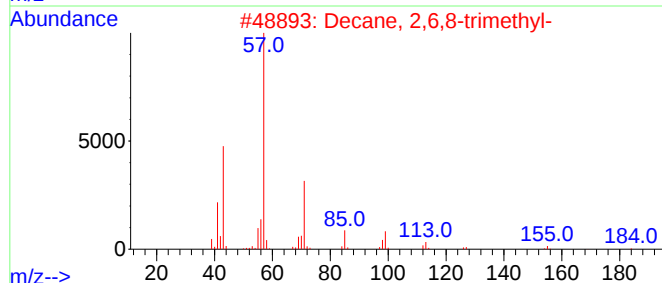
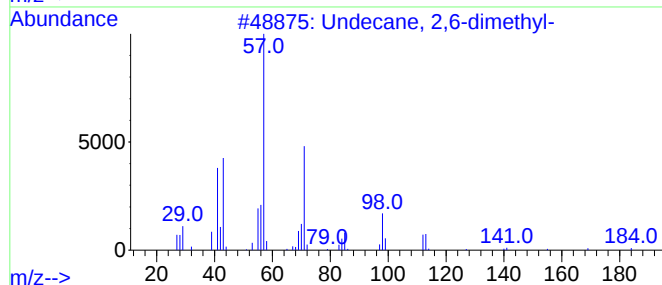
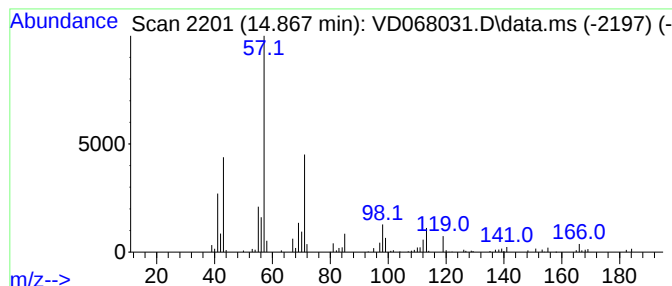
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Undecane, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.867	11.36 ug/l	287205	1,4-Dichlorobenzene-d4	13.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	91
2			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	72
3			Dodecane, 6-methyl-	184	C13H28	006044-71-9	72
4			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	59
5			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD010721\
Data File : VD068031.D
Acq On : 07 Jan 2021 13:51
Operator : VA/SY
Sample : M1023-01
Misc : 7.00G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SU-04-010621

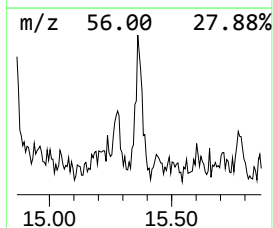
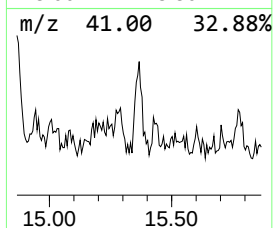
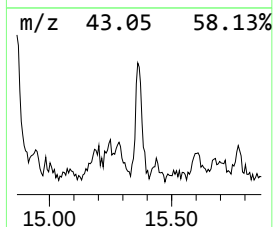
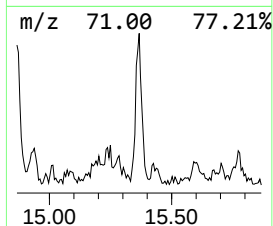
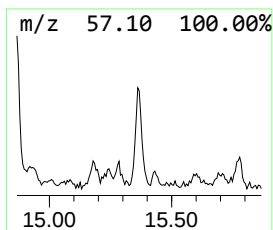
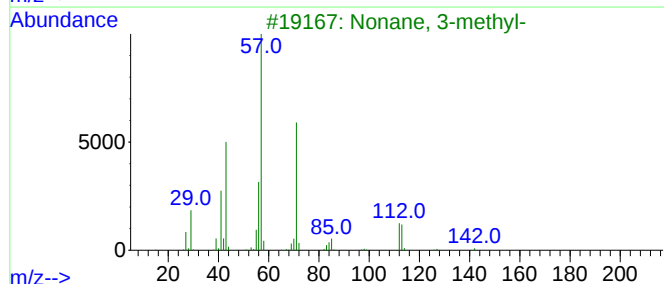
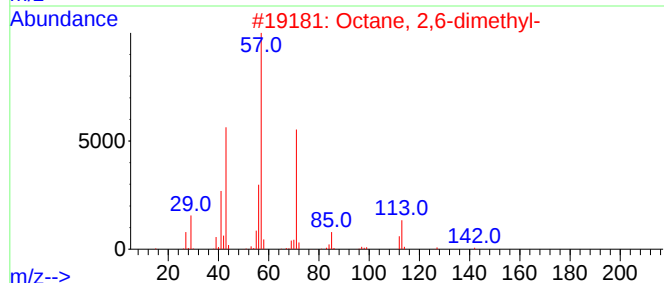
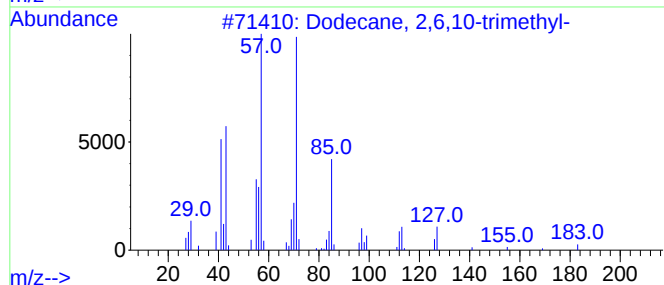
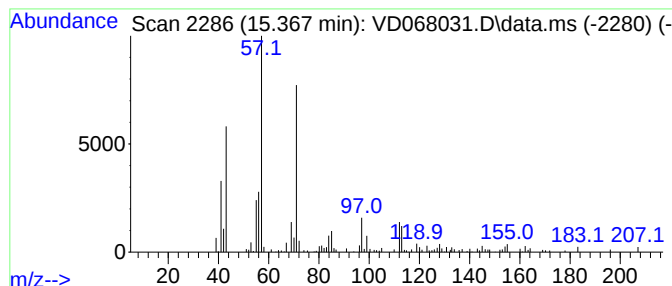
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D12220S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Dodecane, 2,6,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.367	8.50 ug/l	214819	1,4-Dichlorobenzene-d4	13.579

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	72
4			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	72
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD010721\
Data File : VD068031.D
Acq On : 07 Jan 2021 13:51
Operator : VA/SY
Sample : M1023-01
Misc : 7.00G/5.00ml/MSVOA_D/SOIL
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
SU-04-010621

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D122220S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown12.796	12.796	5.3	ug/l	133873	4	13.579	1263730	50.0
unknown12.949	12.949	5.5	ug/l	139103	4	13.579	1263730	50.0
Spiro[4.4]nonan...	13.896	9.4	ug/l	238878	4	13.579	1263730	50.0
unknown14.367	14.367	5.3	ug/l	132834	4	13.579	1263730	50.0
Naphthalene, de...	14.573	5.9	ug/l	148843	4	13.579	1263730	50.0
3-Chloro-2-meth...	14.832	7.2	ug/l	181501	4	13.579	1263730	50.0
Undecane, 2,6-d...	14.867	11.4	ug/l	287205	4	13.579	1263730	50.0
Dodecane, 2,6,1...	15.367	8.5	ug/l	214819	4	13.579	1263730	50.0