

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062824\
 Data File : VY018732.D
 Acq On : 28 Jun 2024 16:37
 Operator : SY/MD
 Sample : P3115-14
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20071

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\82Y061324S.M
 Title : SW846 8260

Signal : TIC: VY018732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.710	956	966	971	rBV2	66236	155568	1.60%	0.557%
2	7.777	971	977	988	rVB	118533	262398	2.70%	0.940%
3	8.130	1024	1035	1045	rBV2	52657	123136	1.27%	0.441%
4	8.679	1117	1125	1136	rBV	164413	322109	3.31%	1.153%
5	10.173	1363	1370	1377	rBV	169634	289785	2.98%	1.038%
6	11.484	1577	1585	1595	rBV	79382	138802	1.43%	0.497%
7	11.703	1612	1621	1631	rBV4	41440	108192	1.11%	0.387%
8	12.642	1767	1775	1782	rVB4	41456	98799	1.02%	0.354%
9	12.727	1782	1789	1795	rBV7	47354	142792	1.47%	0.511%
10	12.800	1795	1801	1807	rVV	965555	1422980	14.63%	5.096%
11	12.855	1807	1810	1816	rVB4	62857	113594	1.17%	0.407%
12	12.947	1821	1825	1829	rBV3	80848	131379	1.35%	0.470%
13	13.002	1829	1834	1835	rBV2	97039	129096	1.33%	0.462%
14	13.038	1835	1840	1846	rVB	776592	1110269	11.42%	3.976%
15	13.105	1846	1851	1852	rBV2	71307	101755	1.05%	0.364%
16	13.166	1857	1861	1865	rBV	166345	262949	2.70%	0.942%
17	13.221	1865	1870	1878	rVB2	296622	579888	5.96%	2.077%
18	13.319	1878	1886	1889	rBV3	579147	1205466	12.39%	4.317%
19	13.361	1889	1893	1896	rVV2	544147	837855	8.61%	3.000%
20	13.398	1896	1899	1901	rVV	399237	560738	5.77%	2.008%
21	13.428	1901	1904	1908	rVV	673534	895656	9.21%	3.207%
22	13.501	1912	1916	1921	rVB2	497738	685693	7.05%	2.456%
23	13.562	1922	1926	1930	rBV3	228652	361231	3.71%	1.294%
24	13.672	1940	1944	1946	rBV3	140071	234855	2.41%	0.841%
25	13.751	1950	1957	1961	rBV	7622104	9725565	100.00%	34.828%
26	13.794	1961	1964	1967	rVB3	293115	416221	4.28%	1.491%
27	13.916	1980	1984	1989	rVB4	322786	499857	5.14%	1.790%
28	14.014	1997	2000	2004	rVB	295640	380302	3.91%	1.362%
29	14.075	2005	2010	2015	rBV3	355830	630784	6.49%	2.259%
30	14.142	2015	2021	2027	rBV6	180067	465922	4.79%	1.669%
31	14.190	2027	2029	2032	rBV3	77033	99285	1.02%	0.356%
32	14.257	2032	2040	2046	rBV8	566514	1494245	15.36%	5.351%
33	14.379	2055	2060	2063	rBV3	270131	445403	4.58%	1.595%
34	14.422	2063	2067	2070	rVB2	254458	380395	3.91%	1.362%
35	14.611	2090	2098	2102	rVB2	414895	683621	7.03%	2.448%
36	14.672	2103	2108	2114	rVV4	148605	398348	4.10%	1.427%

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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\82Y061324S.M

Title : SW846 8260

37	14.727	2114	2117	2124	rVB3	166002	271299	2.79%	0.972%
38	14.873	2138	2141	2148	rVB3	130219	204943	2.11%	0.734%
39	14.940	2148	2152	2156	rVB2	139026	192889	1.98%	0.691%
40	15.001	2157	2162	2173	rBV3	385075	777883	8.00%	2.786%
41	15.276	2203	2207	2210	rBV2	79186	140300	1.44%	0.502%
42	16.470	2399	2403	2412	rVB5	122768	274085	2.82%	0.982%
43	16.757	2445	2450	2455	rVB5	82427	168165	1.73%	0.602%

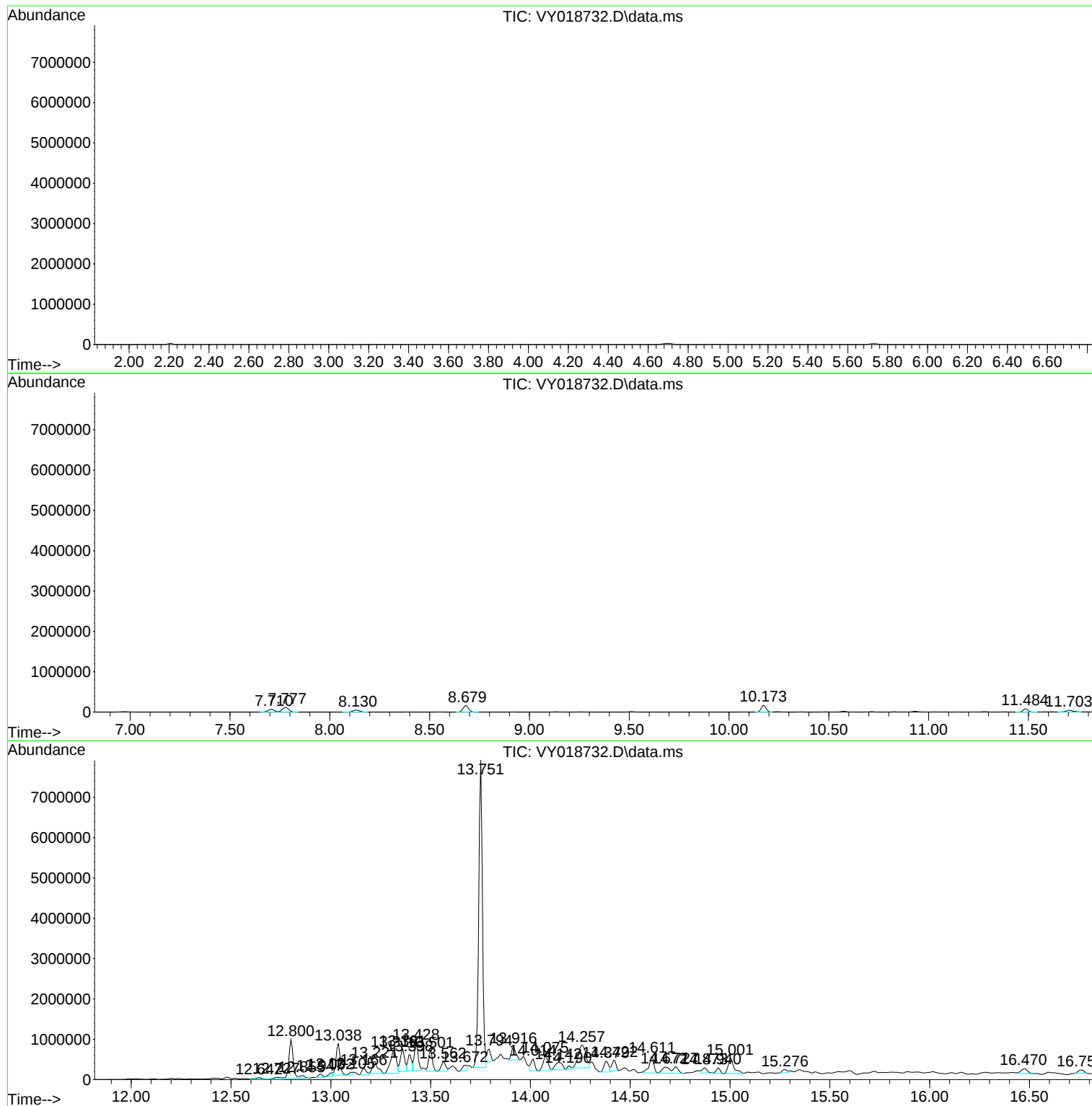
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y061324S.M
Quant Title : SW846 8260

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



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Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
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Instrument :
MSVOA_Y
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20071

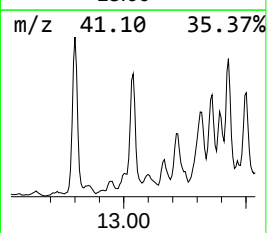
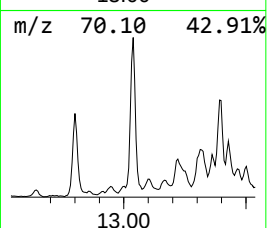
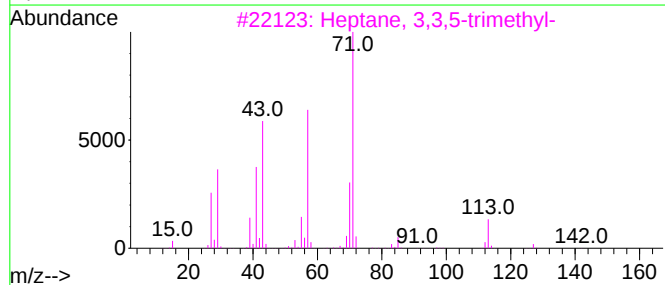
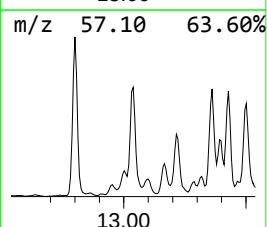
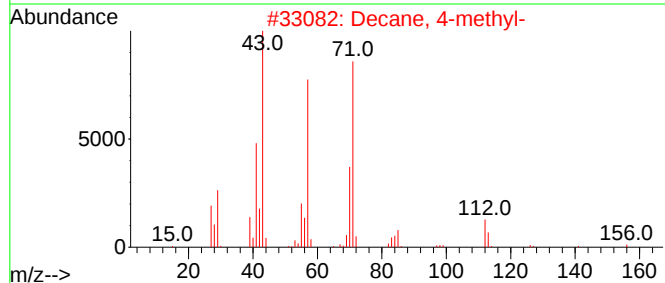
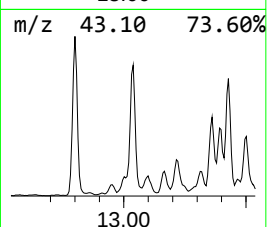
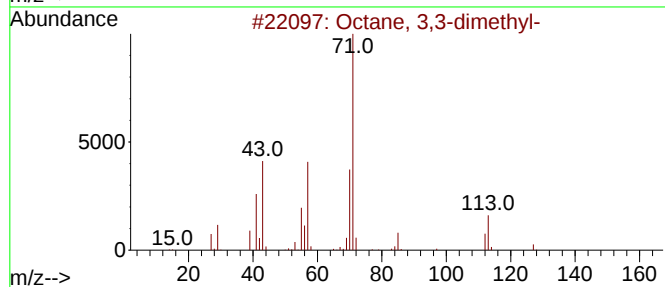
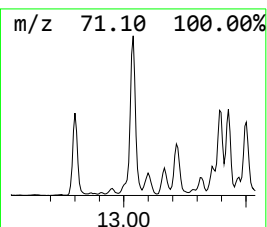
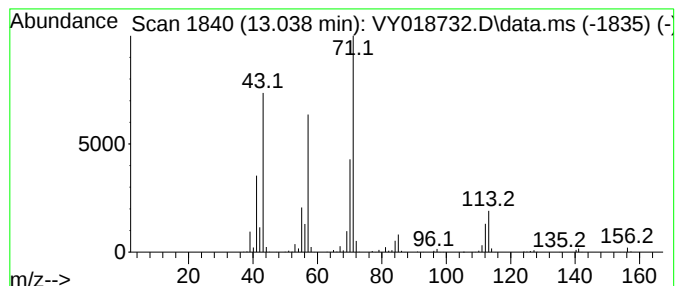
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y061324S.M
Quant Title : SW846 8260

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

Peak Number 1 Octane, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.038	61.98 ug/l	1110270	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	83
2			Decane, 4-methyl-	156	C11H24	002847-72-5	83
3			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	72
4			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59



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Sample : P3115-14
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

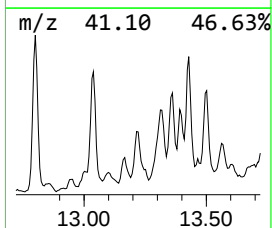
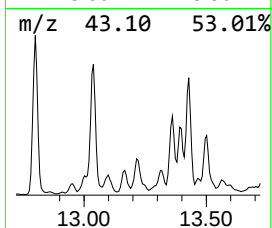
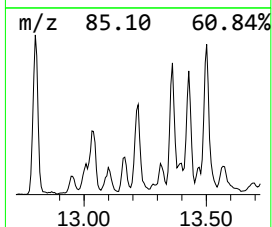
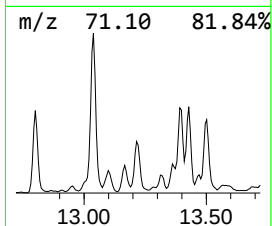
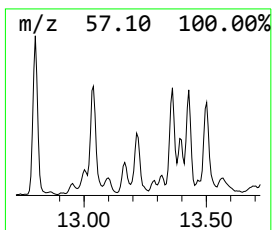
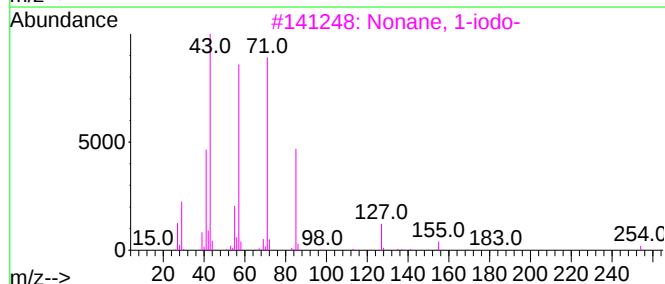
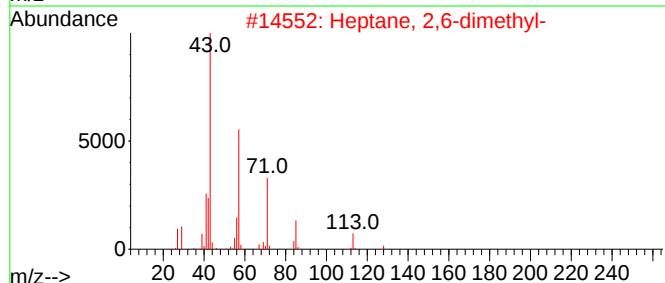
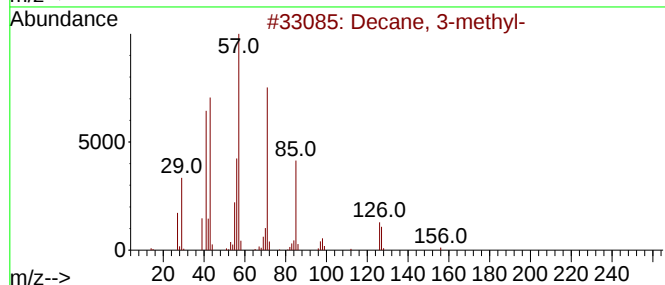
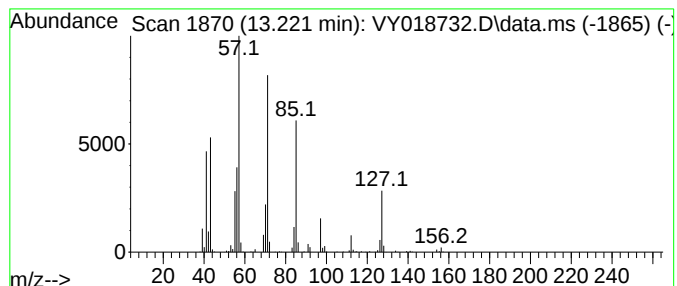
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y061324S.M
Quant Title : SW846 8260

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

Peak Number 2 Decane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.221	32.37 ug/l	579888	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3-methyl-	156	C11H24	013151-34-3	80
2			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	47
3			Nonane, 1-iodo-	254	C9H19I	004282-42-2	47
4			Sulfurous acid, nonyl 2-pentyl e...	278	C14H30O3S	1010309-15-8	47
5			Ether, heptyl hexyl	200	C13H28O	007289-40-9	43



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Data File : VY018732.D
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Operator : SY/MD
Sample : P3115-14
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

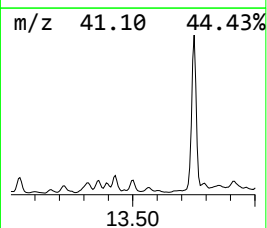
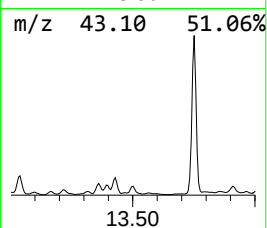
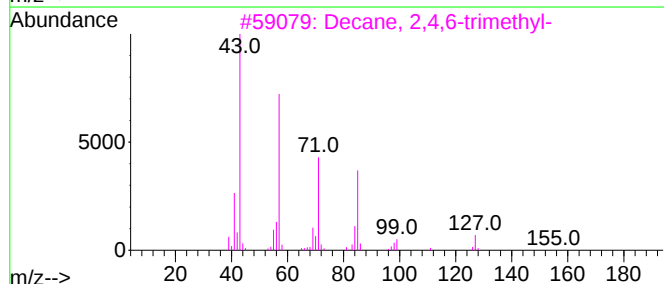
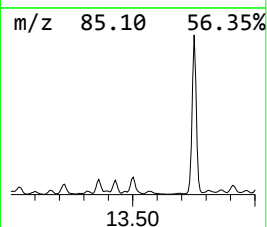
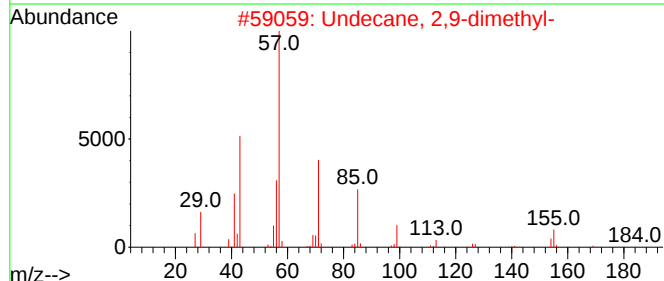
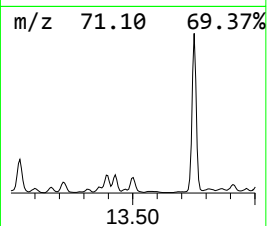
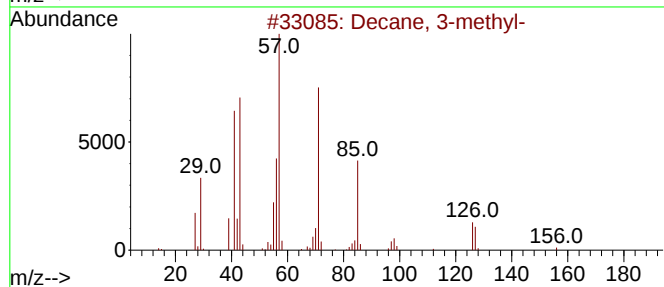
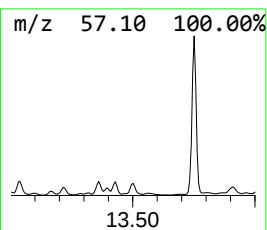
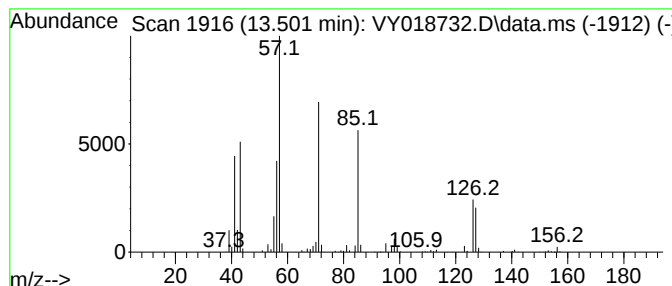
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y061324S.M
Quant Title : SW846 8260

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

Peak Number 3 Undecane, 2,9-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.502	38.28 ug/l	685693	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3-methyl-	156	C11H24	013151-34-3	91
2			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	59
3			Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	50
4			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	50
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	47



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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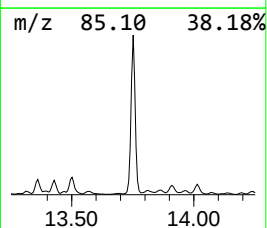
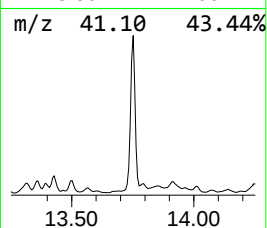
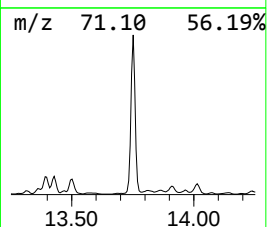
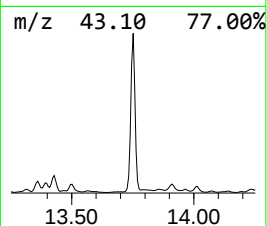
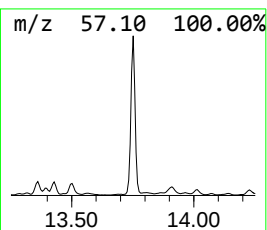
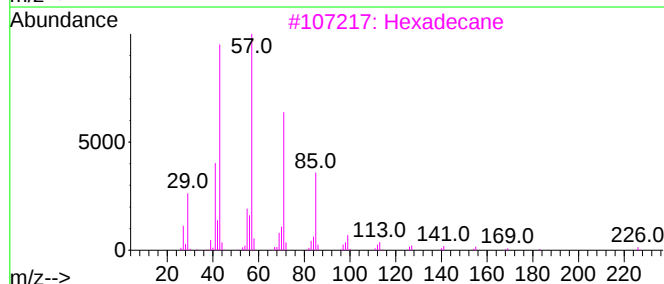
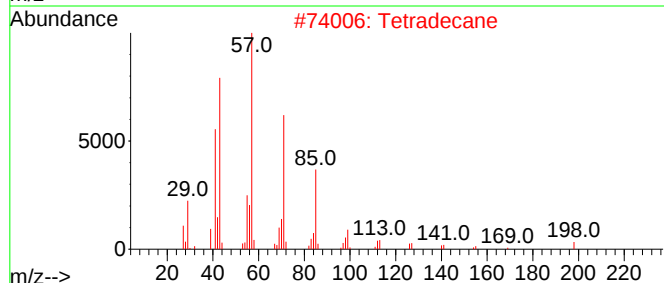
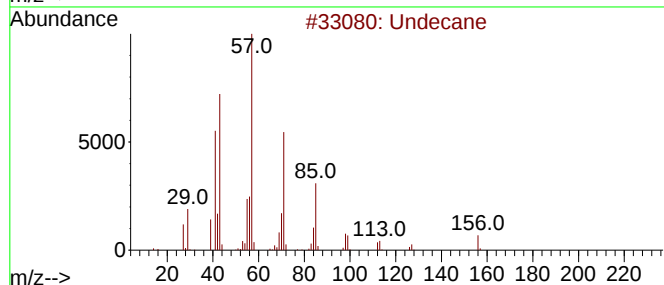
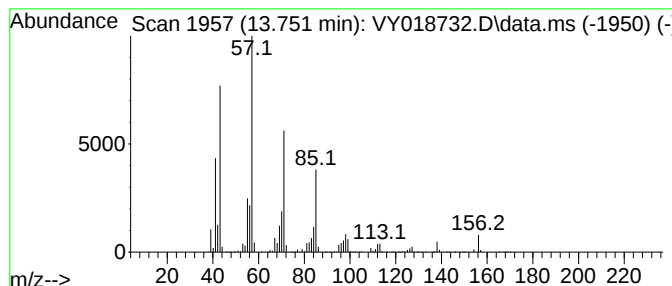
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y061324S.M
Quant Title : SW846 8260

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

Peak Number 4 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	542.93 ug/l	9725570	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Tetradecane			198	C14H30	000629-59-4	86
3	Hexadecane			226	C16H34	000544-76-3	64
4	Decane, 1-iodo-			268	C10H21I	002050-77-3	53
5	Ether, hexyl pentyl			172	C11H24O	032357-83-8	52



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Instrument :
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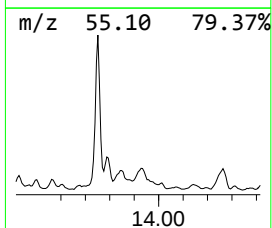
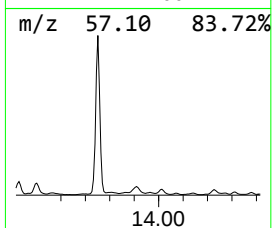
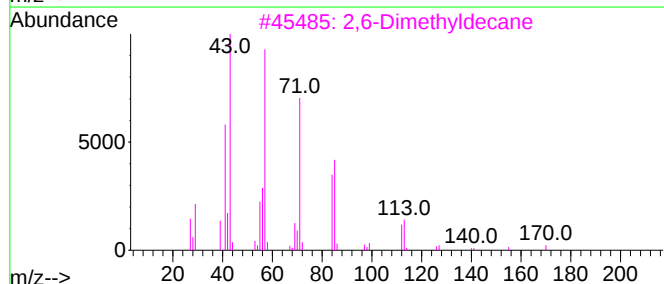
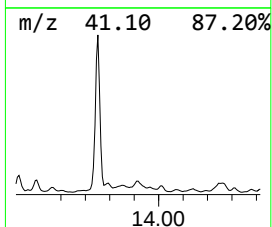
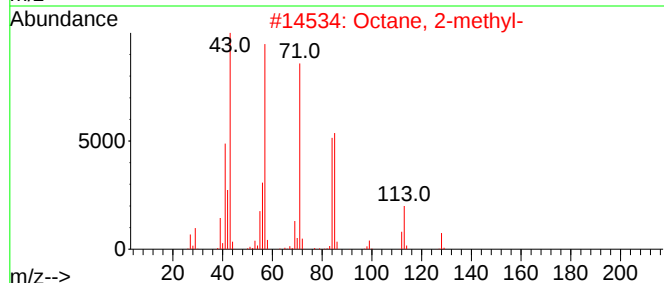
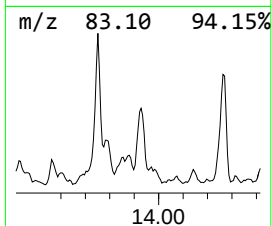
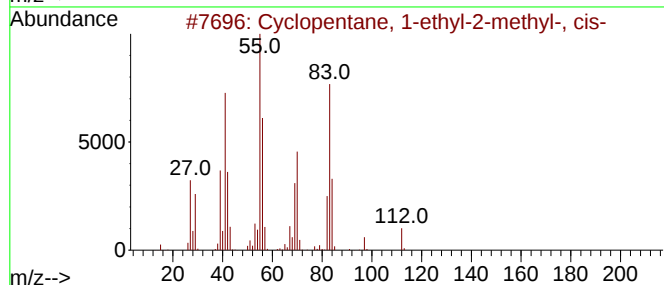
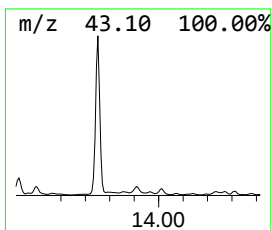
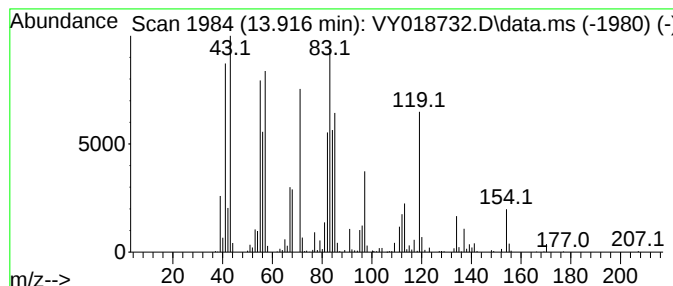
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Quant Title : SW846 8260

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

Peak Number 5 unknown13.916 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	27.90 ug/l	499857	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	35
2			Octane, 2-methyl-	128	C9H20	003221-61-2	35
3			2,6-Dimethyldecane	170	C12H26	013150-81-7	30
4			Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	27
5			Caprolactam	113	C6H11NO	000105-60-2	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062824\
Data File : VY018732.D
Acq On : 28 Jun 2024 16:37
Operator : SY/MD
Sample : P3115-14
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

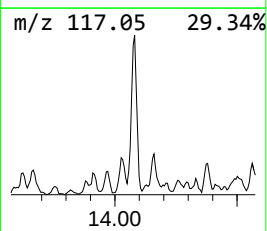
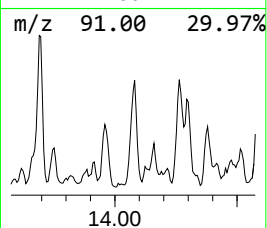
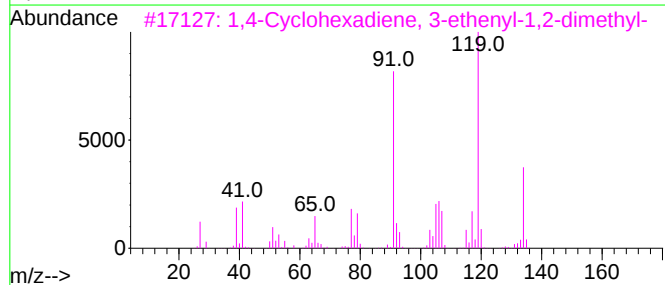
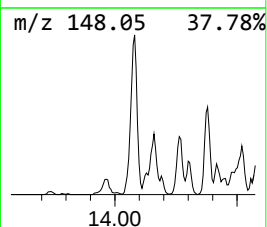
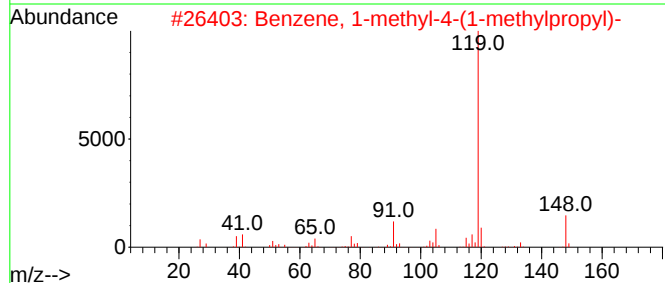
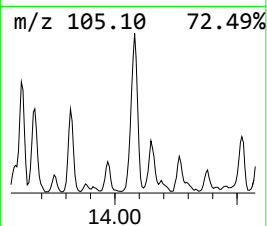
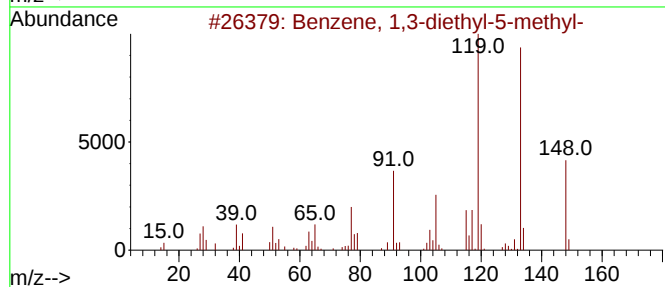
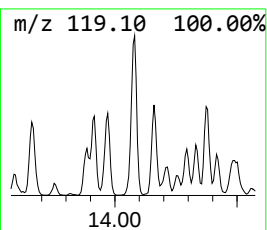
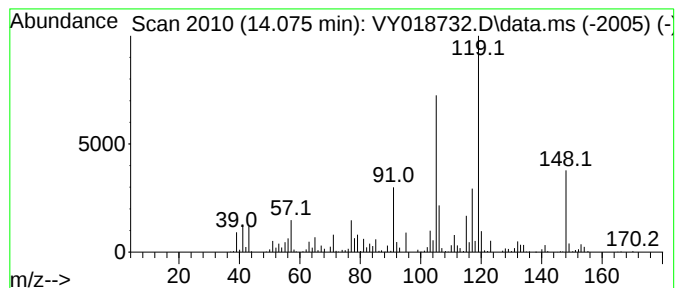
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,3-diethyl-5-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.075	35.21 ug/l	630784	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	70
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	58
3			1,4-Cyclohexadiene, 3-ethenyl-1,...	134	C10H14	062338-57-2	53
4			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	50
5			Propiophenone, 2'-methyl-	148	C10H12O	002040-14-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062824\
Data File : VY018732.D
Acq On : 28 Jun 2024 16:37
Operator : SY/MD
Sample : P3115-14
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

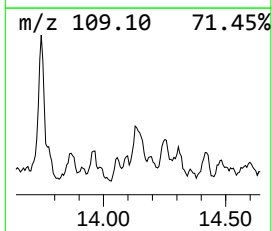
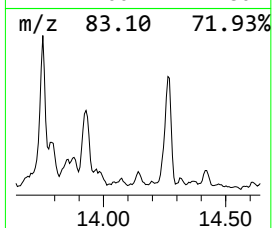
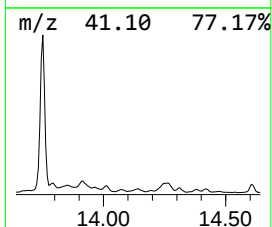
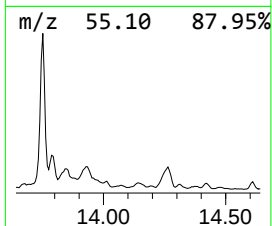
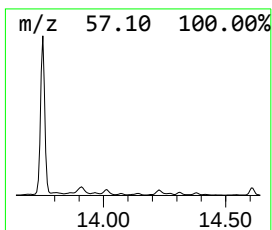
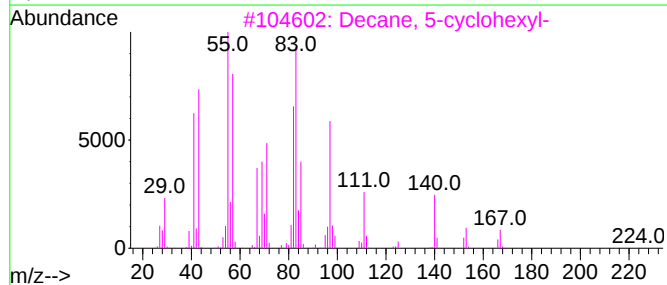
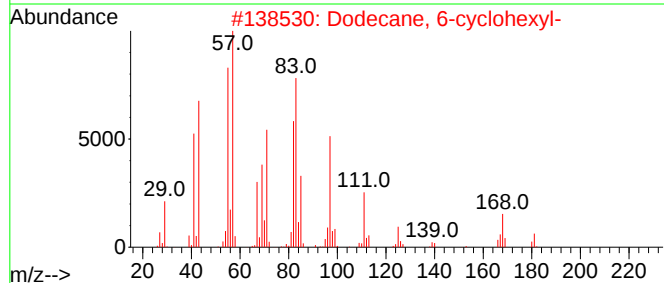
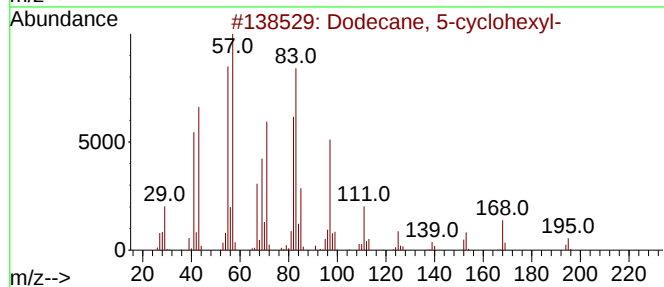
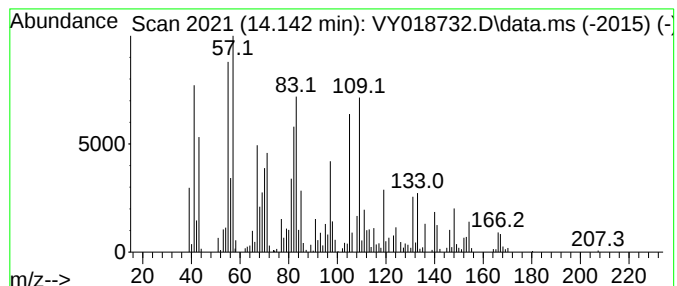
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.142 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.142	26.01 ug/l	465922	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	49
2			Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	46
3			Decane, 5-cyclohexyl-	224	C16H32	013151-76-3	46
4			Undecane, 5-cyclohexyl-	238	C17H34	013151-80-9	46
5			Pentadecafluorooctanoic acid, do...	582	C20H25F15O2	1000406-04-2	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062824\
Data File : VY018732.D
Acq On : 28 Jun 2024 16:37
Operator : SY/MD
Sample : P3115-14
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

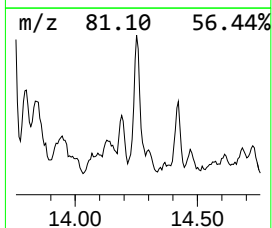
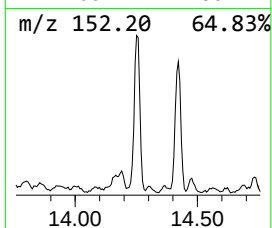
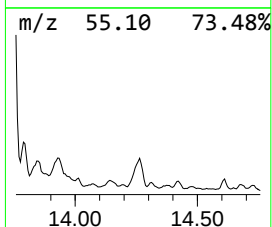
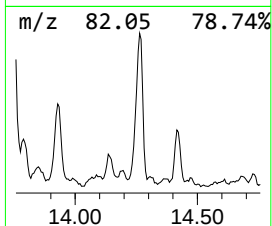
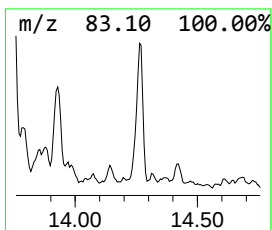
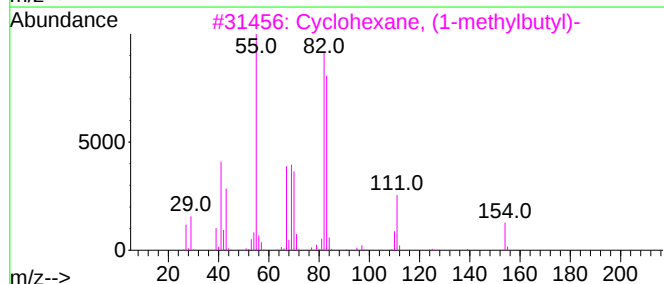
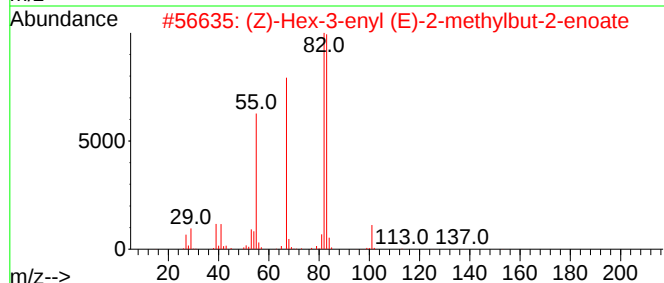
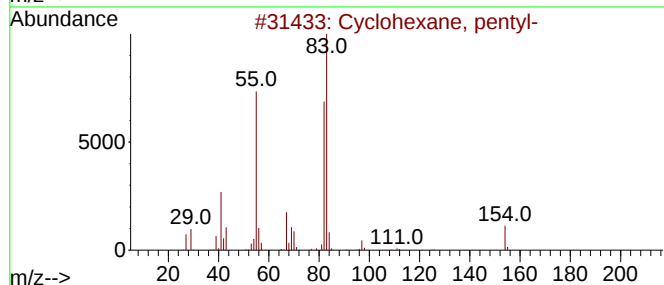
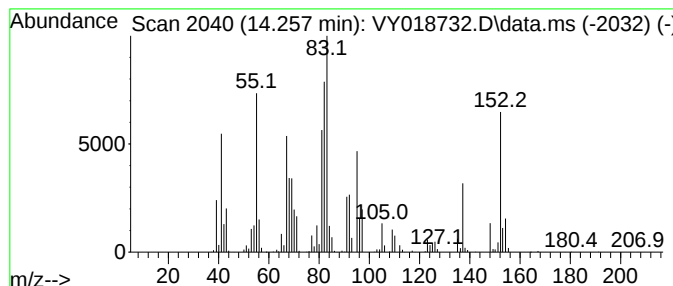
Instrument :
MSVOA_Y
ClientSampleId :
20071

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y061324S.M
Quant Title : SW846 8260

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

Peak Number 8 unknown14.257 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.257	83.42 ug/l	1494250	1,4-Dichlorobenzene-d4	13.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	43
2	(Z)-Hex-3-enyl (E)-2-methylbut-2...	182	C11H18O2	067883-79-8	43
3	Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	43
4	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	38
5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062824\
Data File : VY018732.D
Acq On : 28 Jun 2024 16:37
Operator : SY/MD
Sample : P3115-14
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

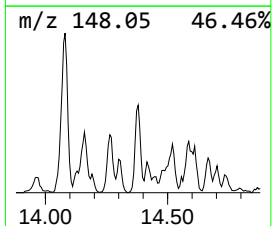
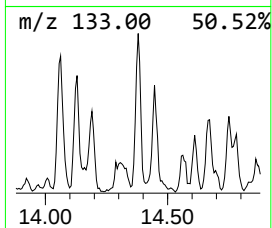
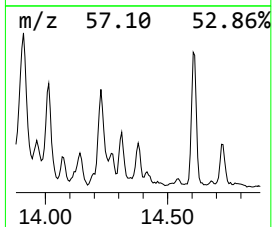
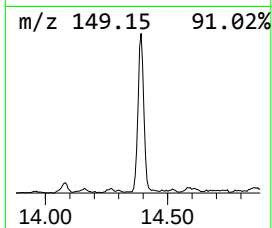
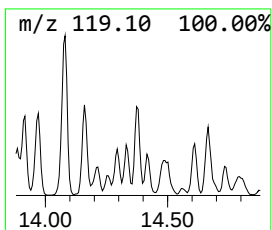
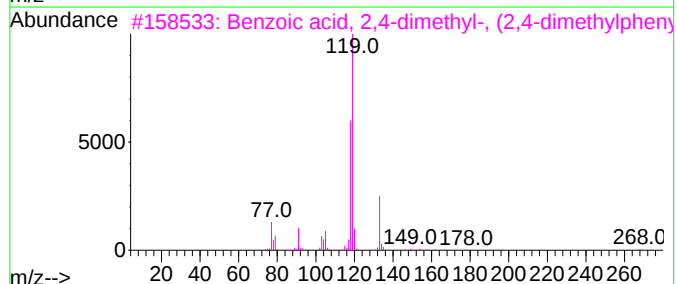
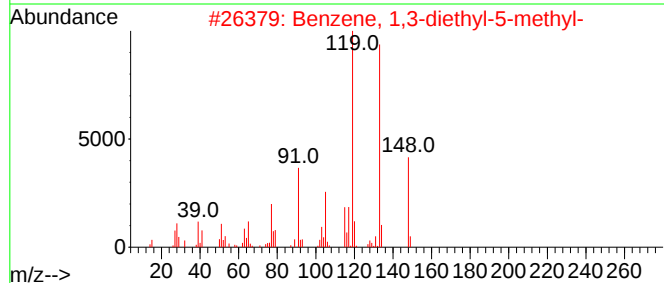
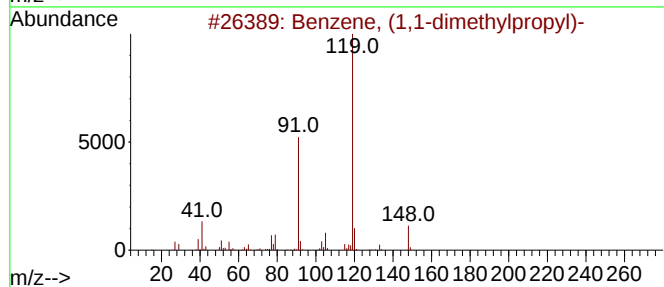
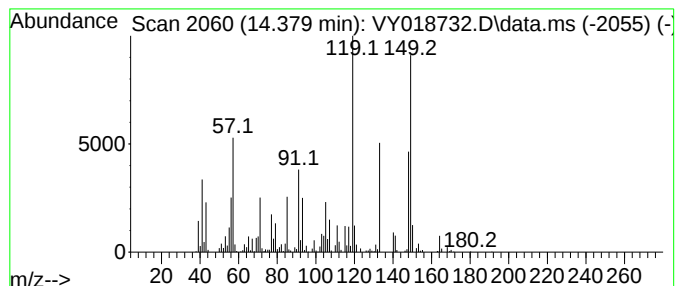
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Quant Title : SW846 8260

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

Peak Number 9 unknown14.379 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.379	24.86 ug/l	445403	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	35
2			Benzene, 1,3-diethyl-5-methyl-	148	C11H16	002050-24-0	30
3			Benzoic acid, 2,4-dimethyl-, (2,...	268	C18H20O2	055000-43-6	22
4			Benzene, 4-(chloromethyl)-1,2-di...	154	C9H11Cl	000102-46-5	20
5			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	20



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062824\
Data File : VY018732.D
Acq On : 28 Jun 2024 16:37
Operator : SY/MD
Sample : P3115-14
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

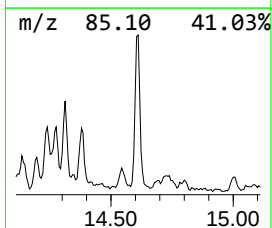
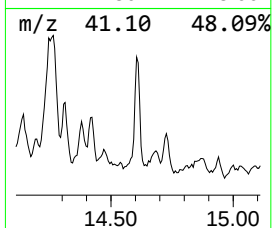
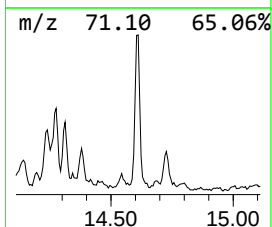
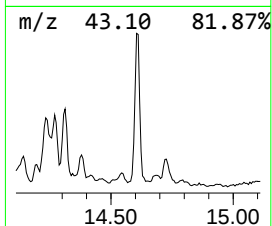
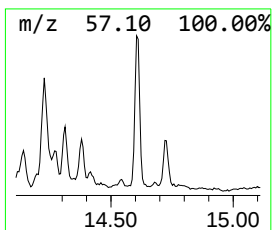
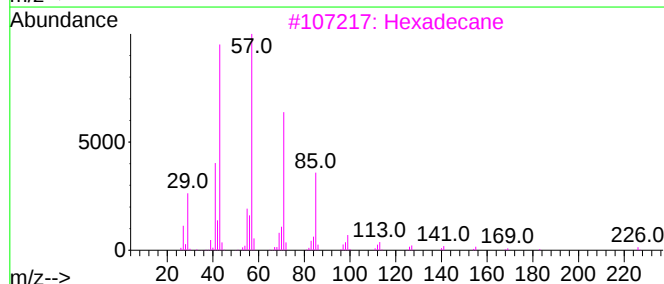
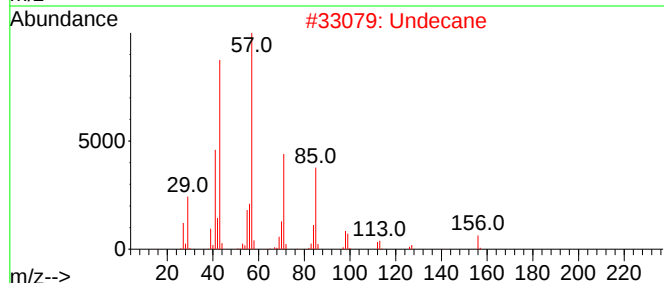
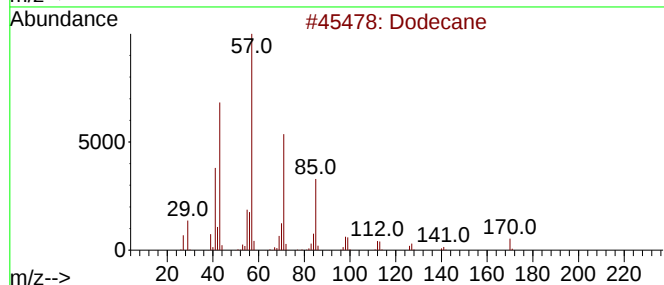
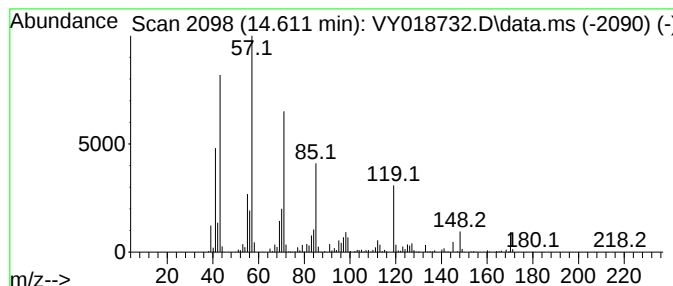
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Quant Title : SW846 8260

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

Peak Number 10 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.611	38.16 ug/l	683621	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Undecane	156	C11H24	001120-21-4	59
3			Hexadecane	226	C16H34	000544-76-3	58
4			Ether, hexyl pentyl	172	C11H24O	032357-83-8	49
5			Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY062824\
Data File : VY018732.D
Acq On : 28 Jun 2024 16:37
Operator : SY/MD
Sample : P3115-14
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
20071

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y061324S.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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Decane, 3-methyl-	13.221	32.4	ug/l	579888	4	13.422	895656	50.0
Undecane, 2,9-d...	13.502	38.3	ug/l	685693	4	13.422	895656	50.0
Undecane	13.751	542.9	ug/l	9725570	4	13.422	895656	50.0
unknown13.916	13.916	27.9	ug/l	499857	4	13.422	895656	50.0
Benzene, 1,3-di...	14.075	35.2	ug/l	630784	4	13.422	895656	50.0
unknown14.142	14.142	26.0	ug/l	465922	4	13.422	895656	50.0
unknown14.257	14.257	83.4	ug/l	1494250	4	13.422	895656	50.0
unknown14.379	14.379	24.9	ug/l	445403	4	13.422	895656	50.0
Dodecane	14.611	38.2	ug/l	683621	4	13.422	895656	50.0