

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052024\
 Data File : VY018334.D
 Acq On : 20 May 2024 14:51
 Operator : SY/MD
 Sample : P2511-02
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 510-D

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\82Y050724S.M

Title : SW846 8260

Signal : TIC: VY018334.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.211	59	64	73	rBV3	11247	27219	1.08%	0.310%
2	3.936	335	347	360	rBV	57120	160978	6.39%	1.834%
3	6.966	834	844	857	rBV4	12794	44606	1.77%	0.508%
4	7.710	957	966	967	rBV	28922	46049	1.83%	0.525%
5	7.765	968	975	985	rVV3	107253	359662	14.29%	4.097%
6	7.868	985	992	1001	rVB3	32572	83714	3.33%	0.954%
7	7.996	1001	1013	1025	rBV	138430	324355	12.89%	3.695%
8	8.136	1028	1036	1047	rVB3	24818	60340	2.40%	0.687%
9	8.264	1049	1057	1063	rBV3	20160	50191	1.99%	0.572%
10	8.545	1094	1103	1112	rBV	161127	319195	12.68%	3.636%
11	8.685	1119	1126	1137	rVB	86401	172559	6.86%	1.966%
12	9.179	1195	1207	1213	rBV4	22705	59410	2.36%	0.677%
13	10.179	1363	1371	1375	rBV	119746	209838	8.34%	2.390%
14	10.240	1375	1381	1395	rVV	524228	905143	35.96%	10.311%
15	10.368	1395	1402	1409	rVB2	19704	33227	1.32%	0.379%
16	11.489	1577	1586	1591	rBV	90671	152555	6.06%	1.738%
17	11.703	1611	1621	1631	rBV3	37504	88453	3.51%	1.008%
18	12.032	1663	1675	1681	rBV6	14645	37851	1.50%	0.431%
19	12.337	1718	1725	1731	rBV	103793	175585	6.98%	2.000%
20	12.483	1744	1749	1754	rBV2	59279	92453	3.67%	1.053%
21	12.800	1793	1801	1809	rBV3	84479	153296	6.09%	1.746%
22	12.892	1812	1816	1822	rVB	23520	39952	1.59%	0.455%
23	13.038	1836	1840	1843	rBV2	33036	45132	1.79%	0.514%
24	13.172	1857	1862	1866	rBV3	15883	27915	1.11%	0.318%
25	13.337	1883	1889	1896	rVV	1714163	2517262	100.00%	28.676%
26	13.398	1896	1899	1900	rVV	24292	27463	1.09%	0.313%
27	13.428	1900	1904	1908	rVB2	103622	154006	6.12%	1.754%
28	13.495	1908	1915	1919	rBV3	70819	145088	5.76%	1.653%
29	13.751	1951	1957	1961	rBV	447855	644711	25.61%	7.344%
30	13.788	1961	1963	1967	rVV3	40639	55870	2.22%	0.636%
31	13.867	1971	1976	1980	rVV6	43952	79158	3.14%	0.902%
32	13.910	1980	1983	1988	rBV3	42811	71338	2.83%	0.813%
33	13.965	1988	1992	1996	rVB3	58635	93672	3.72%	1.067%
34	14.013	1996	2000	2006	rVB2	68422	130295	5.18%	1.484%
35	14.074	2006	2010	2013	rBV4	26089	40743	1.62%	0.464%
36	14.141	2016	2021	2026	rBV3	41147	74719	2.97%	0.851%

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37	14.196	2026	2030	2032	rBV5	22391	29389	1.17%	0.335%
38	14.251	2032	2039	2040	rBV4	81917	165743	6.58%	1.888%
39	14.312	2046	2049	2056	rVB	75223	91397	3.63%	1.041%
40	14.379	2056	2060	2063	rBV	57197	83966	3.34%	0.957%
41	14.422	2063	2067	2072	rVB3	69203	102959	4.09%	1.173%
42	14.611	2093	2098	2104	rVB	210391	283696	11.27%	3.232%
43	14.678	2105	2109	2113	rBV4	28888	46371	1.84%	0.528%
44	14.727	2113	2117	2120	rBV	56067	82986	3.30%	0.945%
45	14.849	2133	2137	2146	rVB	11390	27305	1.08%	0.311%
46	15.257	2200	2204	2210	rVV3	37581	65079	2.59%	0.741%
47	15.434	2229	2233	2240	rVB	23991	36148	1.44%	0.412%
48	15.605	2256	2261	2269	rBV2	31901	59259	2.35%	0.675%

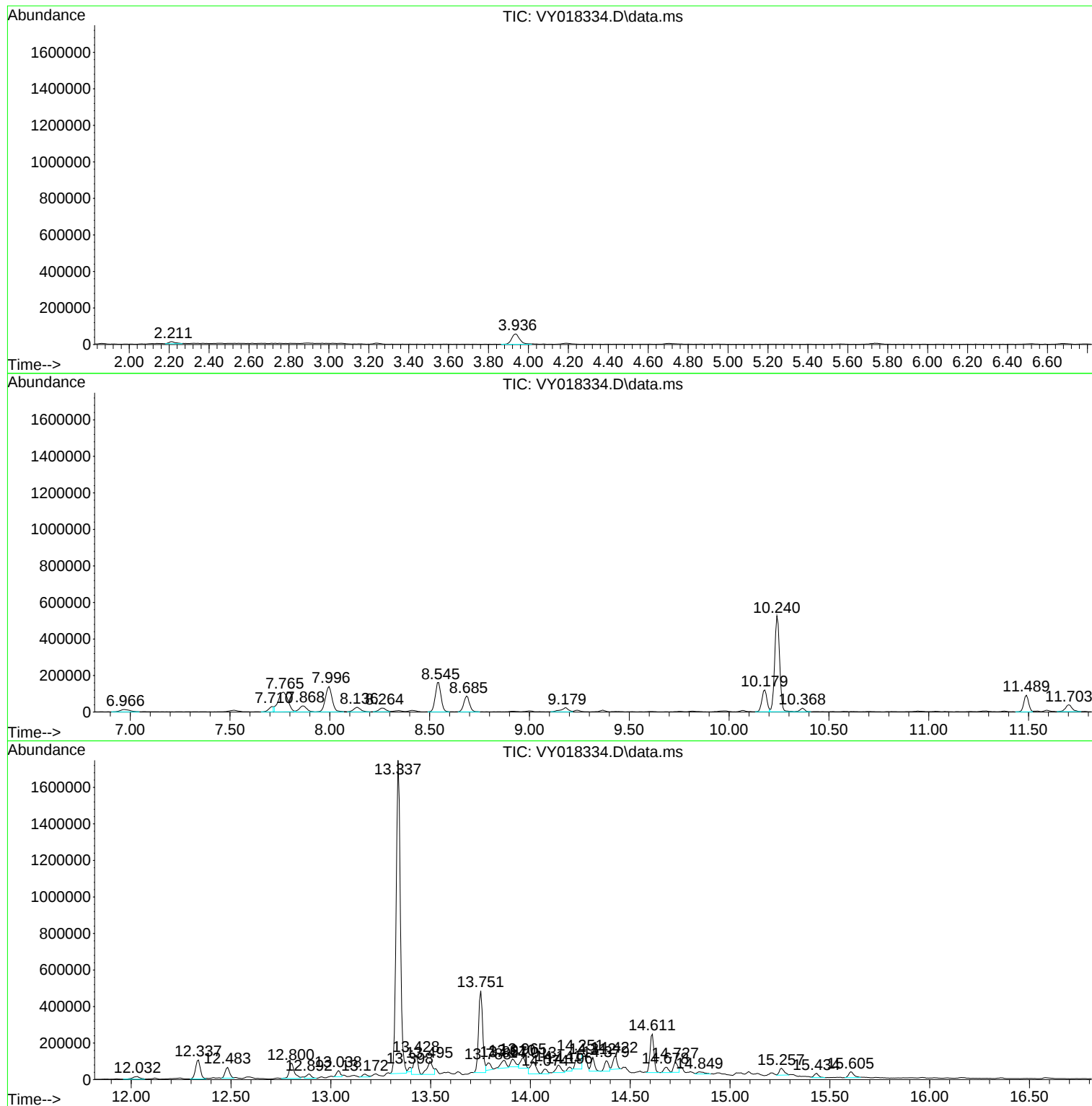
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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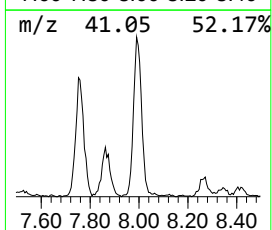
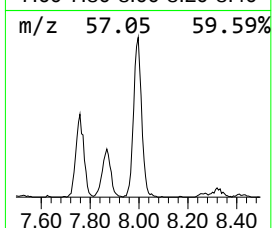
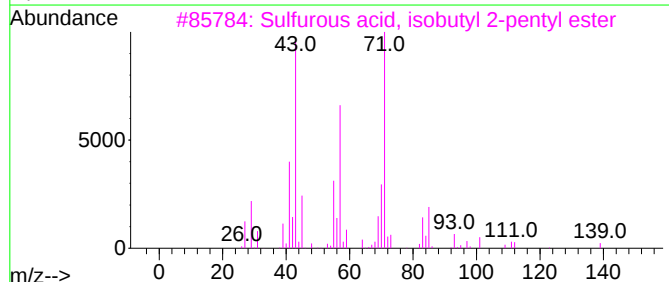
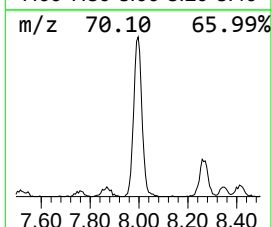
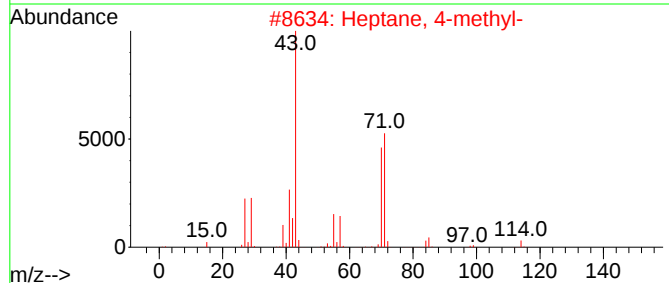
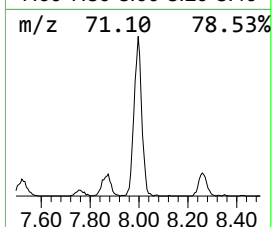
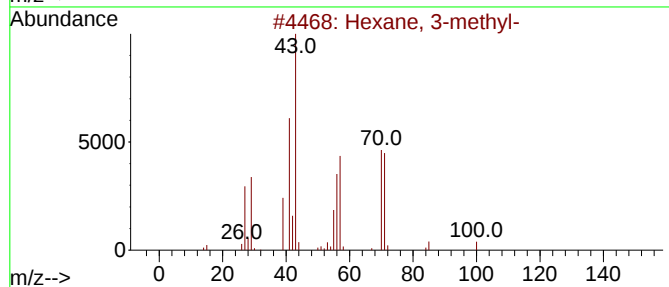
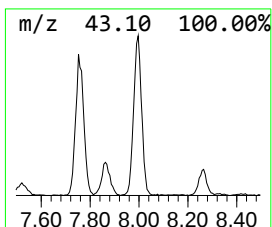
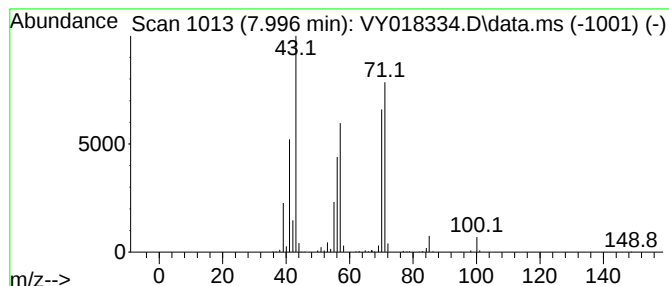
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.996	45.09 ug/l	324355	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Sulfurous acid, isobutyl 2-penty...	208	C9H20O3S	1000309-15-2	59
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59



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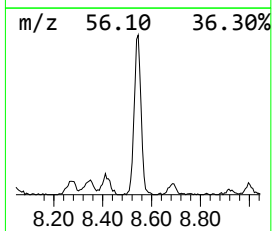
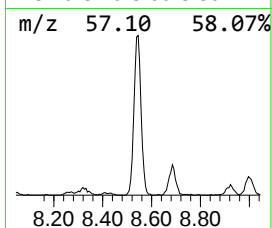
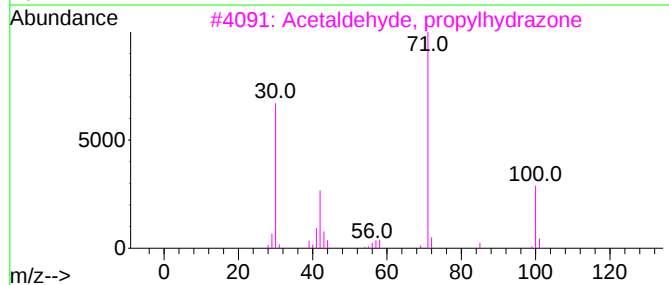
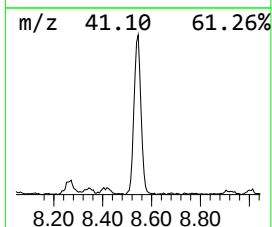
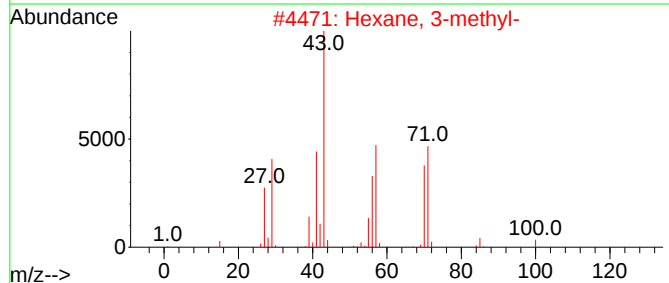
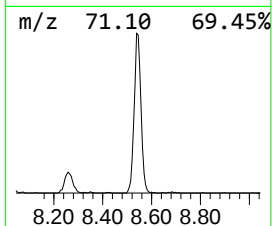
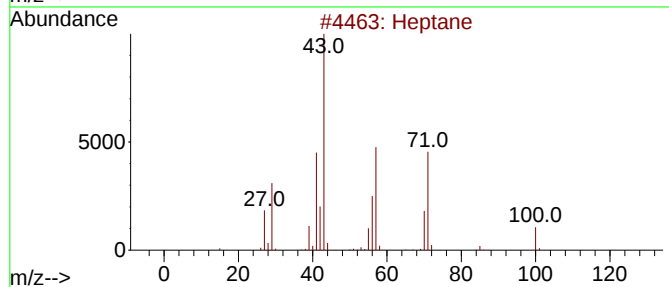
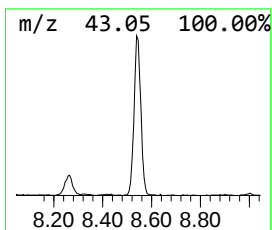
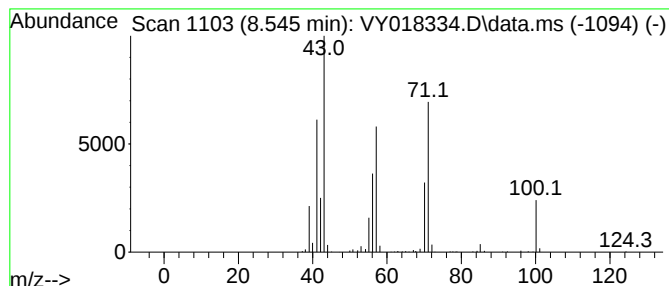
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	92.49 ug/l	319195	1,4-Difluorobenzene	8.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	50
3			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	49
4			3-Hexanone	100	C6H12O	000589-38-8	46
5			Pentane, 2-methyl-	86	C6H14	000107-83-5	43



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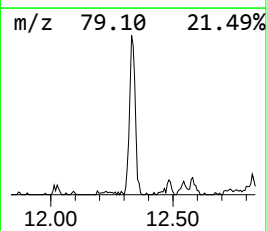
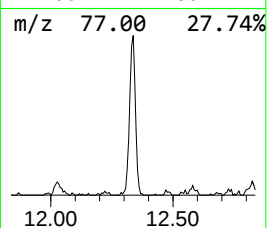
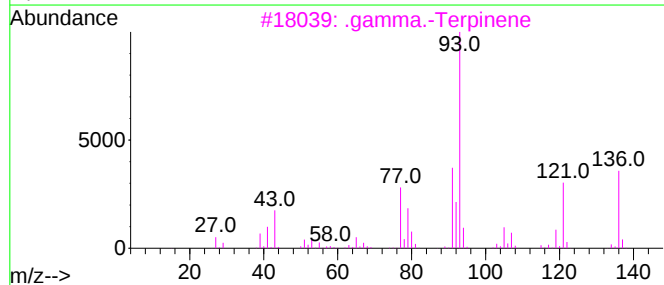
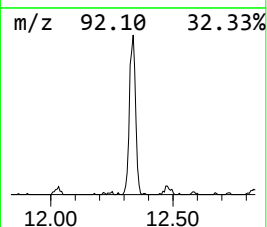
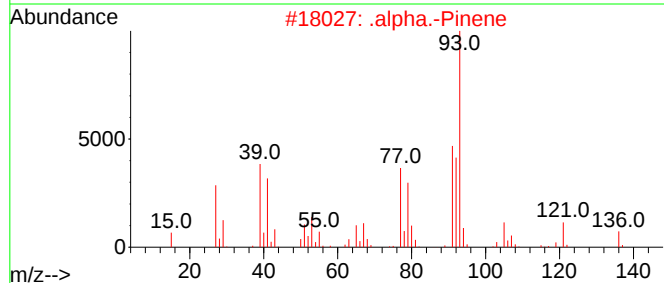
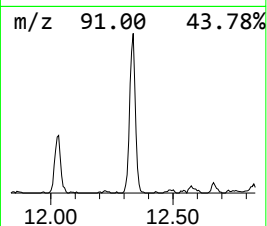
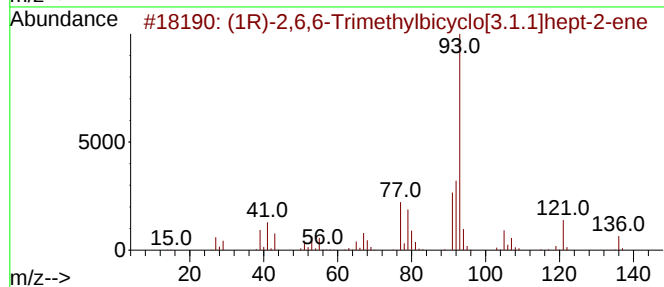
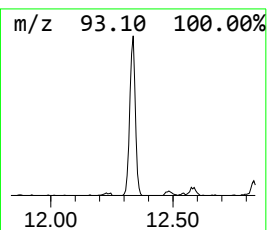
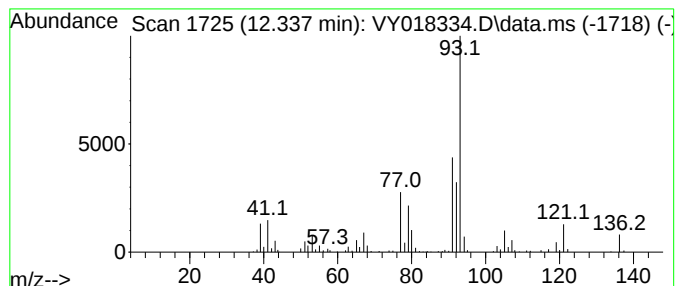
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Peak Number 3 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	57.55 ug/l	175585	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	94
2			.alpha.-Pinene	136	C10H16	000080-56-8	94
3			.gamma.-Terpinene	136	C10H16	000099-85-4	91
4			(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	91
5			Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91



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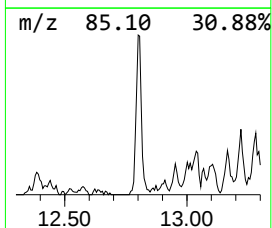
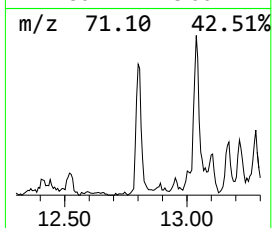
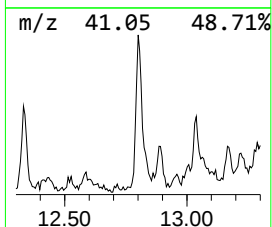
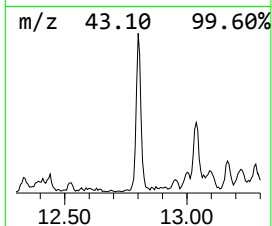
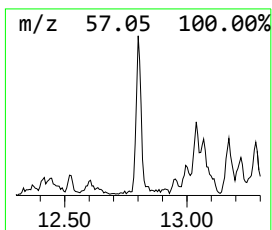
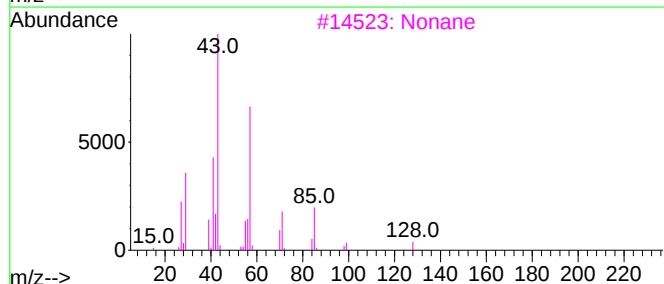
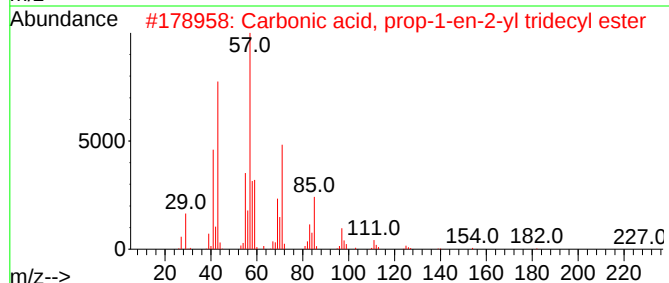
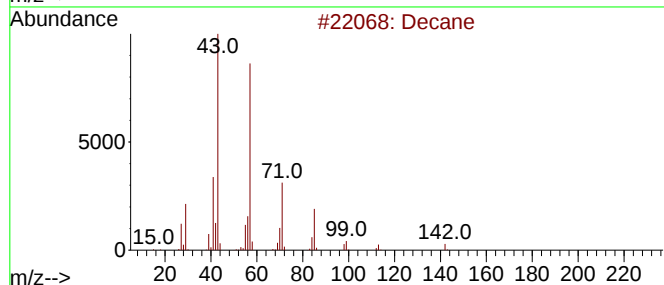
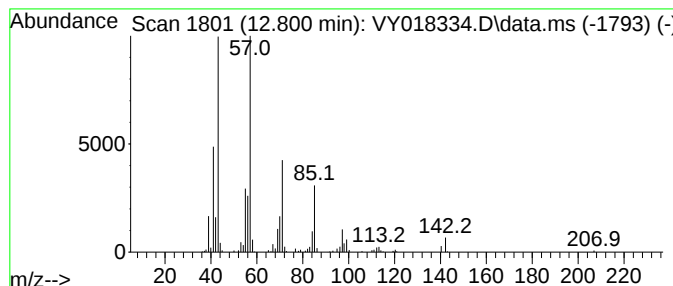
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.800	49.77 ug/l	153296	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	90
2			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	80
3			Nonane	128	C9H20	000111-84-2	78
4			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	72
5			Tridecane	184	C13H28	000629-50-5	64



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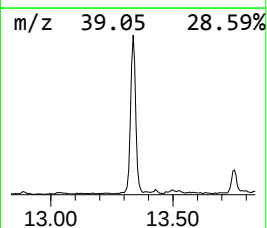
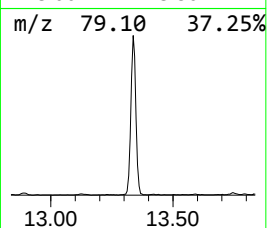
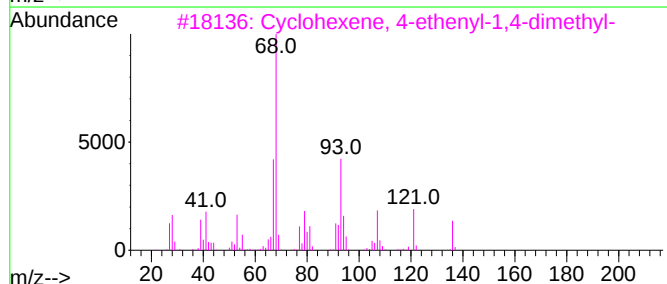
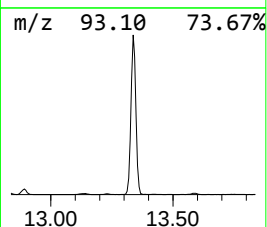
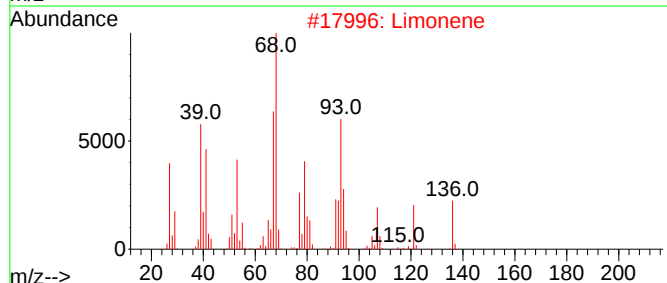
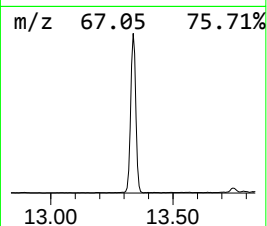
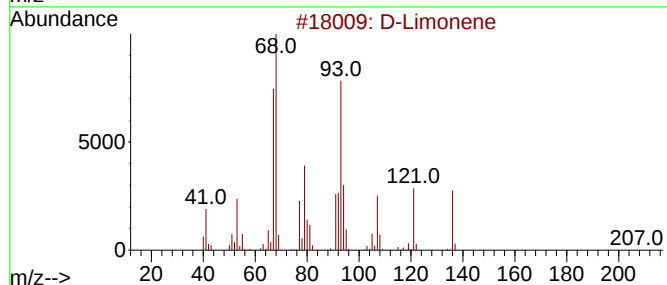
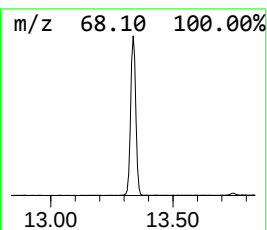
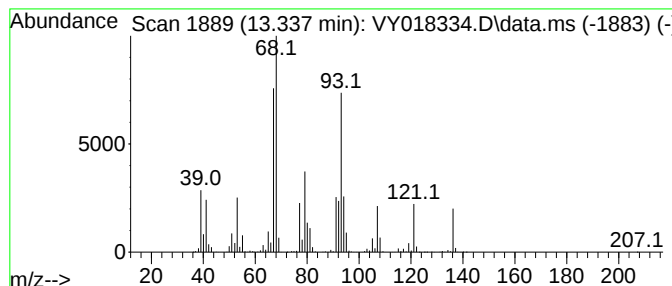
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Quant Title : SW846 8260

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

Peak Number 5 D-Limonene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.337	817.26 ug/l	2517260	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	98
2			Limonene	136	C10H16	000138-86-3	93
3			Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	86
4			Cyclohexanol, 1-methyl-4-(1-meth...	196	C12H20O2	010198-23-9	72
5			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052024\
Data File : VY018334.D
Acq On : 20 May 2024 14:51
Operator : SY/MD
Sample : P2511-02
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
510-D

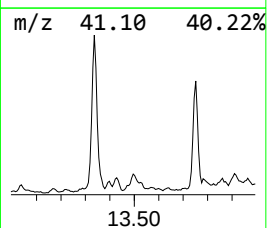
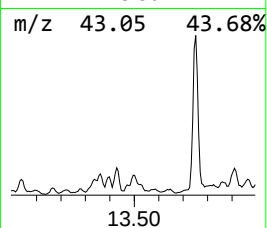
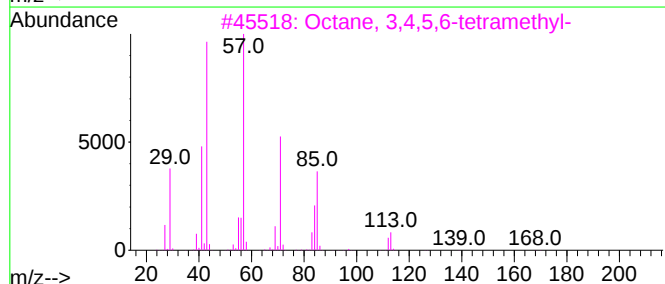
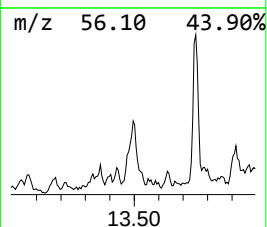
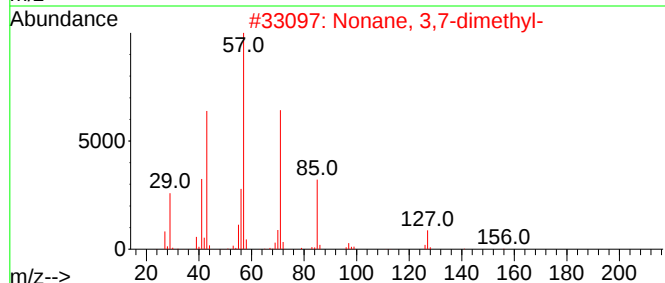
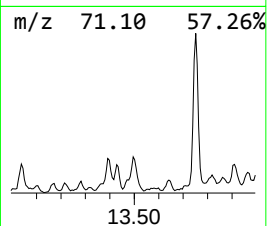
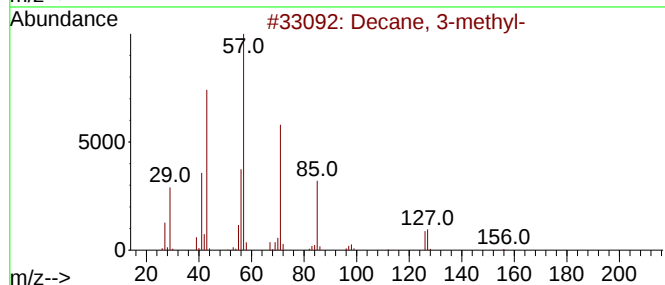
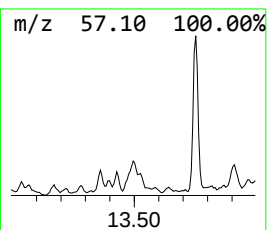
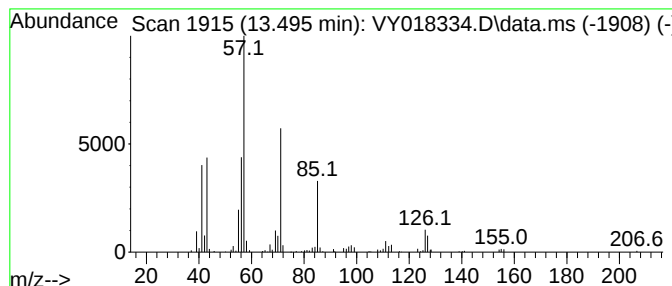
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Quant Title : SW846 8260

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

Peak Number 6 Decane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.495	47.10 ug/l	145088	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3-methyl-	156	C11H24	013151-34-3	72
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	50
3			Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	47
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052024\
Data File : VY018334.D
Acq On : 20 May 2024 14:51
Operator : SY/MD
Sample : P2511-02
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

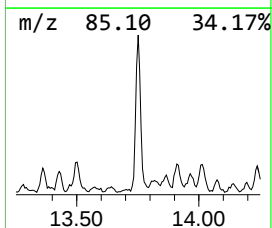
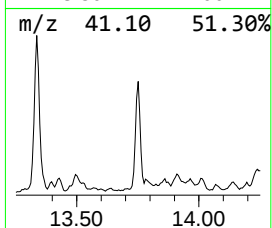
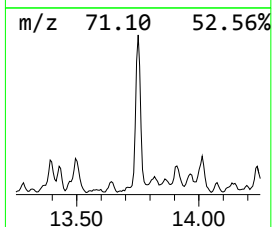
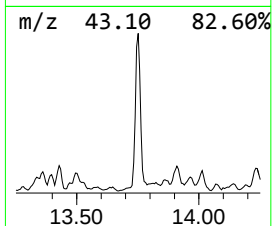
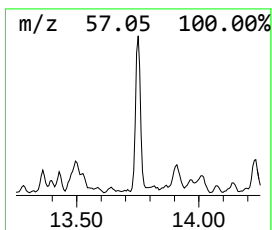
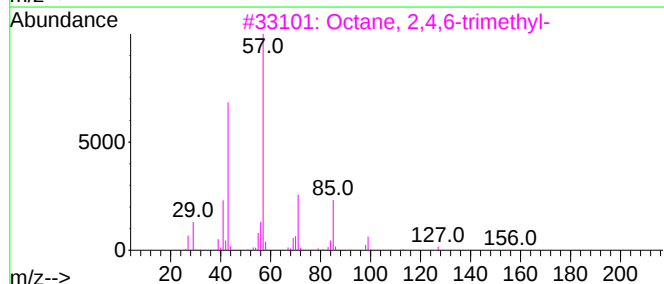
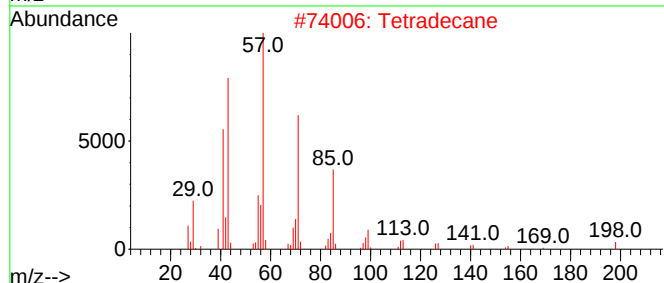
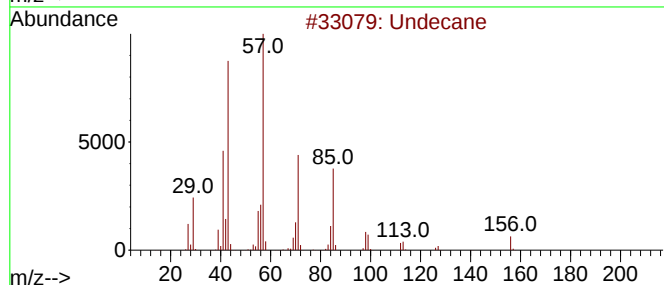
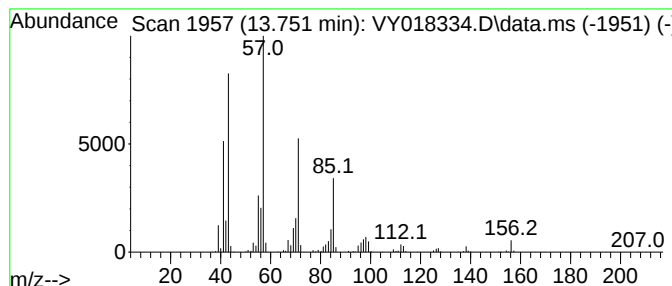
Instrument :
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ClientSampleId :
510-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.M
Quant Title : SW846 8260

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

Peak Number 7 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.751	209.31 ug/l	644711	1,4-Dichlorobenzene-d4	13.428	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	94
2	Tetradecane	198	C14H30	000629-59-4	80
3	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72
4	Heneicosane	296	C21H44	000629-94-7	64
5	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052024\
Data File : VY018334.D
Acq On : 20 May 2024 14:51
Operator : SY/MD
Sample : P2511-02
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
510-D

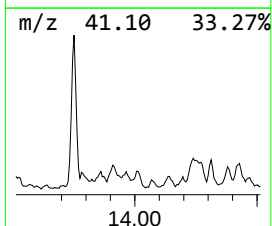
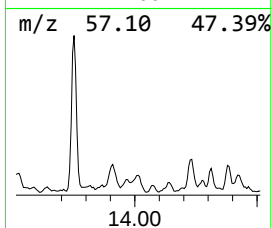
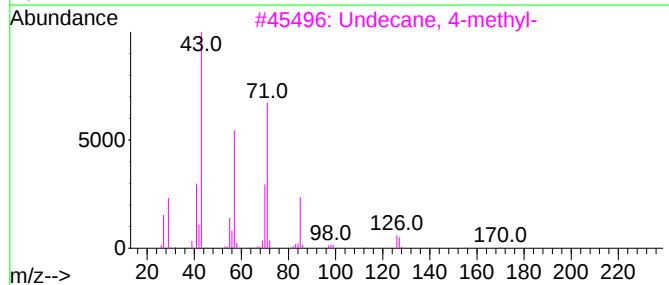
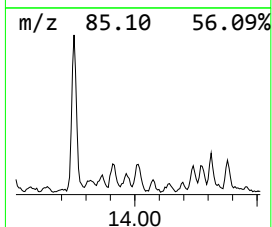
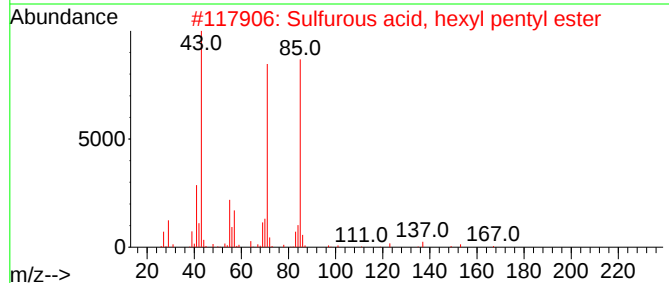
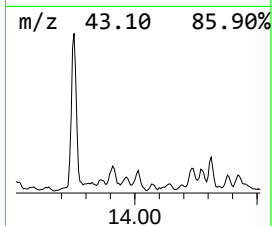
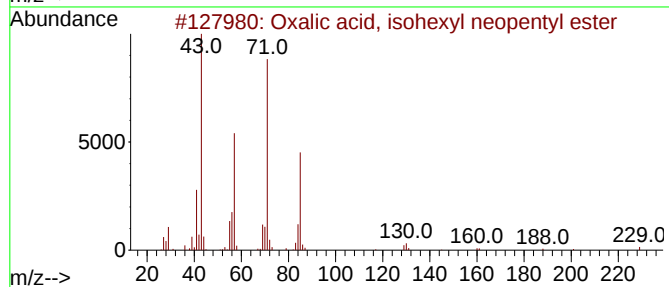
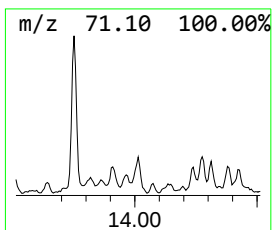
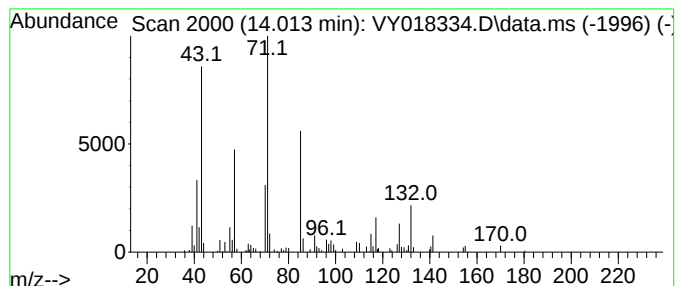
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Quant Title : SW846 8260

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

Peak Number 8 Oxalic acid, isohexyl neope... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.013	42.30 ug/l	130295	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	50
2			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	50
3			Undecane, 4-methyl-	170	C12H26	002980-69-0	50
4			Octane, 2,6,6-trimethyl-	156	C11H24	054166-32-4	47
5			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052024\
Data File : VY018334.D
Acq On : 20 May 2024 14:51
Operator : SY/MD
Sample : P2511-02
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
510-D

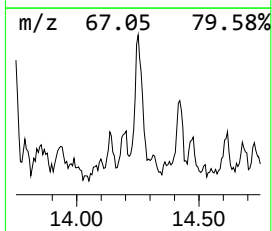
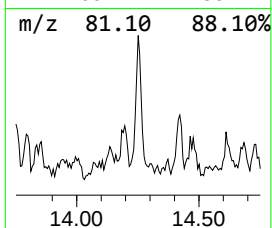
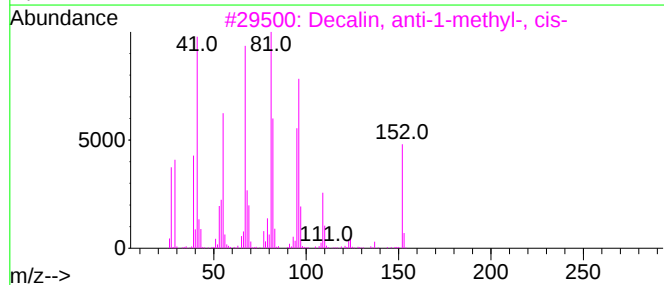
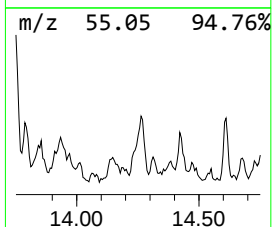
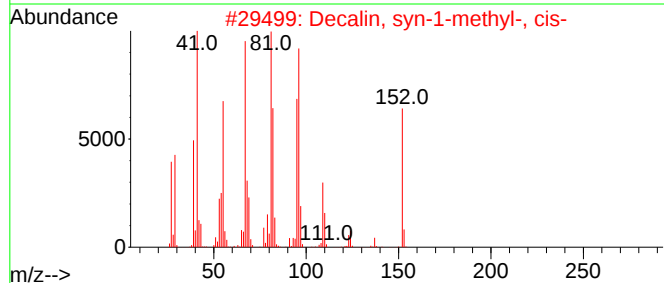
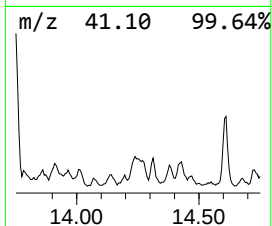
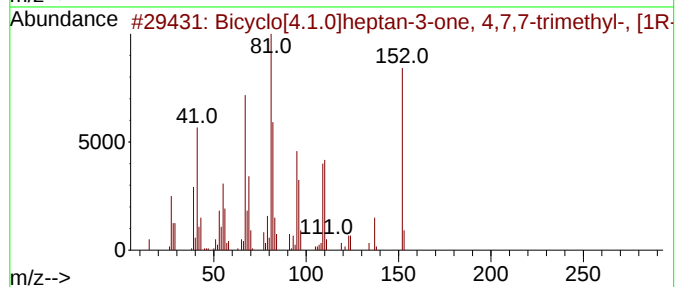
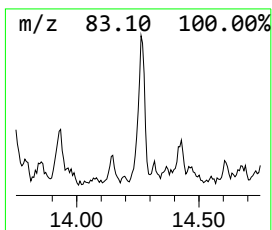
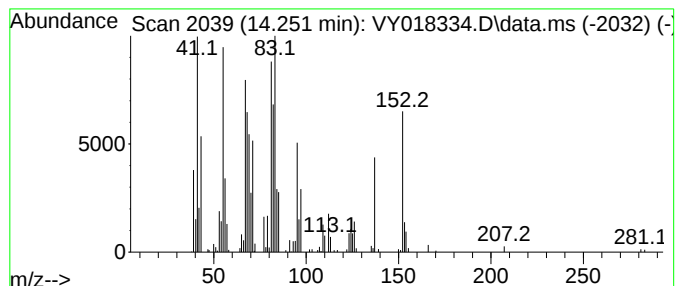
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Quant Title : SW846 8260

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

Peak Number 9 Bicyclo[4.1.0]heptan-3-one,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	53.81 ug/l	165743	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	52
2			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	49
3			Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	49
4			1,5-Hexadiene, 2,5-dipropyl-	166	C12H22	1000158-33-4	43
5			3-Isopropylidene-5-methyl-hex-4-...	152	C10H16O	064149-32-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052024\
Data File : VY018334.D
Acq On : 20 May 2024 14:51
Operator : SY/MD
Sample : P2511-02
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
510-D

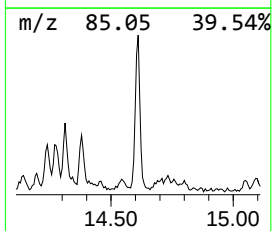
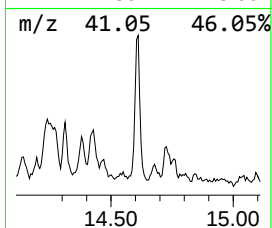
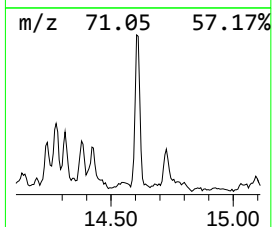
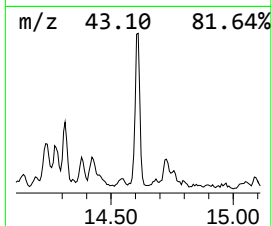
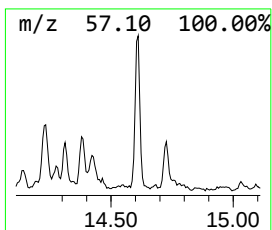
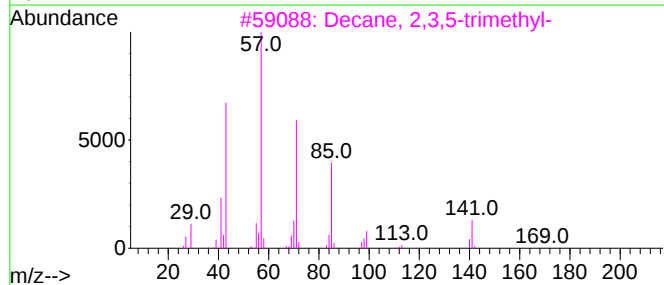
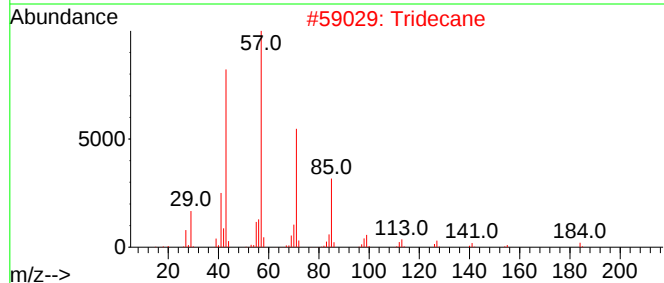
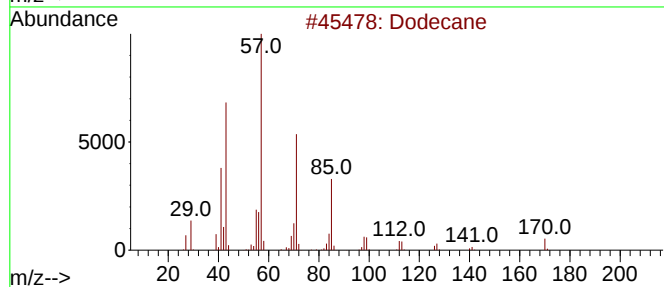
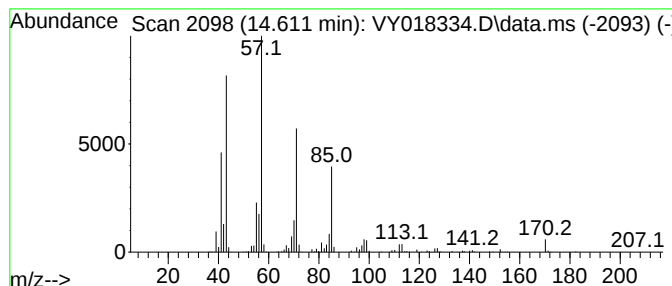
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Quant Title : SW846 8260

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

Peak Number 10 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.611	92.11 ug/l	283696	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	87
2			Tridecane	184	C13H28	000629-50-5	86
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	86
4			Hexadecane	226	C16H34	000544-76-3	86
5			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052024\
Data File : VY018334.D
Acq On : 20 May 2024 14:51
Operator : SY/MD
Sample : P2511-02
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
510-D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y050724S.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
Hexane, 3-methyl-	7.996	45.1	ug/l	324355	1	7.783	359662	50.0
Heptane	8.545	92.5	ug/l	319195	2	8.685	172559	50.0
(1R)-2,6,6-Trim...	12.337	57.5	ug/l	175585	3	11.490	152555	50.0
Decane	12.800	49.8	ug/l	153296	4	13.428	154006	50.0
D-Limonene	13.337	817.3	ug/l	2517260	4	13.428	154006	50.0
Decane, 3-methyl-	13.495	47.1	ug/l	145088	4	13.428	154006	50.0
Undecane	13.751	209.3	ug/l	644711	4	13.428	154006	50.0
Oxalic acid, is...	14.013	42.3	ug/l	130295	4	13.428	154006	50.0
Bicyclo[4.1.0]h...	14.251	53.8	ug/l	165743	4	13.428	154006	50.0
Dodecane	14.611	92.1	ug/l	283696	4	13.428	154006	50.0