

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042424\
 Data File : VY018034.D
 Acq On : 24 Apr 2024 12:50
 Operator : SY/MD
 Sample : P2247-01
 Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 PL-02-04232024

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\82Y041624S.M
 Title : SW846 8260

Signal : TIC: VY018034.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.570	121	123	124	rVB	867	486	1.32%	0.193%
2	4.101	367	374	375	rBV3	479	882	2.40%	0.350%
3	4.710	465	474	484	rBV4	1356	4012	10.92%	1.592%
4	5.741	637	643	650	rVB6	1444	4195	11.42%	1.664%
5	6.899	832	833	836	rBV	411	505	1.38%	0.200%
6	6.960	837	843	845	rBV2	1459	2491	6.78%	0.988%
7	7.088	863	864	868	rVB2	487	430	1.17%	0.171%
8	7.192	875	881	884	rVB	495	885	2.41%	0.351%
9	7.716	959	967	972	rBV2	6553	15657	42.63%	6.211%
10	7.783	972	978	987	rVB2	11419	26976	73.45%	10.702%
11	8.136	1028	1036	1047	rVB3	5397	13554	36.91%	5.377%
12	8.685	1118	1126	1135	rBV	15530	30441	82.89%	12.076%
13	9.478	1255	1256	1260	rBV	277	467	1.27%	0.185%
14	10.179	1364	1371	1378	rBV	21250	36725	100.00%	14.569%
15	10.606	1438	1441	1443	rVB2	468	451	1.23%	0.179%
16	10.636	1443	1446	1449	rBV2	333	472	1.29%	0.187%
17	11.313	1555	1557	1559	rBV2	479	436	1.19%	0.173%
18	11.398	1568	1571	1573	rBV	423	423	1.15%	0.168%
19	11.490	1581	1586	1596	rVB	15666	26193	71.32%	10.391%
20	11.715	1621	1623	1626	rBV2	592	727	1.98%	0.288%
21	11.941	1655	1660	1662	rBV	436	417	1.14%	0.165%
22	12.002	1666	1670	1672	rBV	644	697	1.90%	0.277%
23	12.032	1673	1675	1678	rVB2	520	538	1.46%	0.213%
24	12.124	1687	1690	1695	rVB3	446	535	1.46%	0.212%
25	12.245	1709	1710	1715	rVB2	745	606	1.65%	0.240%
26	12.410	1734	1737	1738	rBV	644	427	1.16%	0.169%
27	12.483	1744	1749	1760	rVB5	9383	17167	46.74%	6.810%
28	12.642	1773	1775	1777	rBV	472	474	1.29%	0.188%
29	12.758	1789	1794	1795	rBV2	534	602	1.64%	0.239%
30	12.806	1796	1802	1808	rVB8	4308	7447	20.28%	2.954%
31	12.947	1821	1825	1826	rBV2	596	763	2.08%	0.303%
32	13.038	1837	1840	1846	rVB5	1668	2732	7.44%	1.084%
33	13.172	1859	1862	1866	rBV3	656	894	2.43%	0.355%
34	13.221	1868	1870	1873	rBV3	808	1128	3.07%	0.447%
35	13.251	1873	1875	1880	rVB2	732	667	1.82%	0.265%
36	13.312	1882	1885	1891	rVV4	1872	2968	8.08%	1.177%

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37	13.355	1891	1892	1894	rVV	1058	1148	3.13%	0.455%
38	13.428	1898	1904	1913	rVV3	6523	12730	34.66%	5.050%
39	13.501	1913	1916	1919	rVB3	989	1370	3.73%	0.543%
40	13.562	1924	1926	1928	rBV2	635	537	1.46%	0.213%
41	13.629	1932	1937	1939	rVV4	1207	1647	4.48%	0.653%
42	13.672	1939	1944	1946	rVB4	1286	1793	4.88%	0.711%
43	13.751	1953	1957	1962	rBV5	4103	6152	16.75%	2.441%
44	13.971	1989	1993	1996	rVB3	1304	1678	4.57%	0.666%
45	14.087	2007	2012	2014	rBV3	1958	2266	6.17%	0.899%
46	14.154	2020	2023	2025	rVB2	688	755	2.06%	0.300%
47	14.202	2028	2031	2032	rBV2	525	548	1.49%	0.217%
48	14.257	2036	2040	2046	rVB5	1669	3062	8.34%	1.215%
49	14.300	2046	2047	2049	rBV2	566	411	1.12%	0.163%
50	14.422	2066	2067	2070	rVB2	938	655	1.78%	0.260%
51	14.568	2088	2091	2093	rBV2	829	871	2.37%	0.346%
52	14.611	2095	2098	2100	rVV3	1256	1531	4.17%	0.607%
53	14.678	2104	2109	2113	rBV5	1693	3270	8.90%	1.297%
54	14.946	2150	2153	2155	rBV3	790	838	2.28%	0.332%
55	14.983	2157	2159	2161	rBV2	1017	928	2.53%	0.368%
56	15.062	2170	2172	2175	rVB2	1375	783	2.13%	0.311%
57	15.111	2178	2180	2184	rBV4	843	1188	3.23%	0.471%
58	15.294	2209	2210	2211	rBV	665	420	1.14%	0.167%
59	15.818	2294	2296	2299	rBV3	596	745	2.03%	0.296%
60	16.159	2350	2352	2357	rBV4	618	957	2.61%	0.380%
61	16.342	2380	2382	2383	rBV2	732	495	1.35%	0.196%
62	16.483	2403	2405	2409	rBV3	982	824	2.24%	0.327%

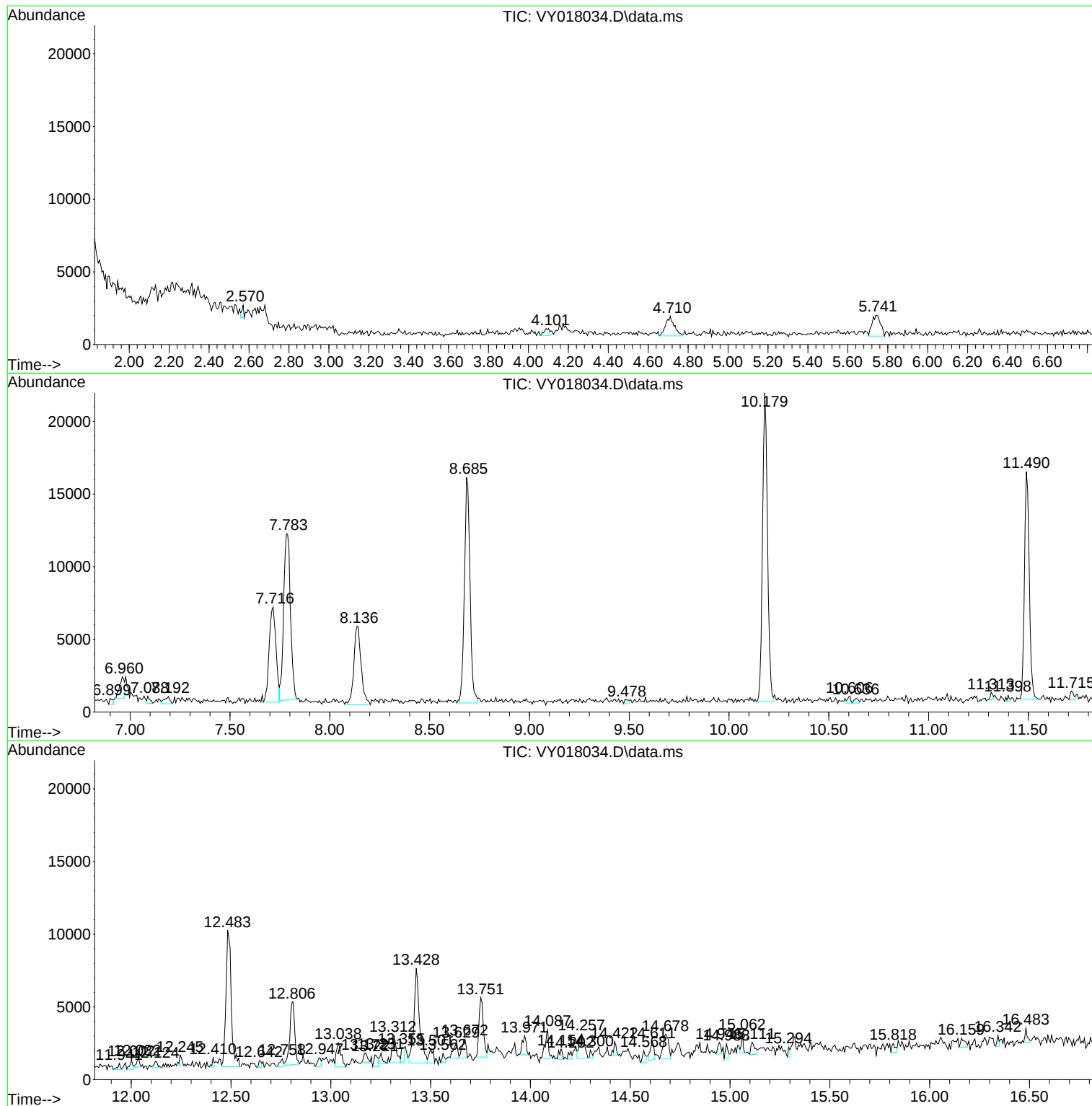
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TIC Library : C:\Database\NIST20.L
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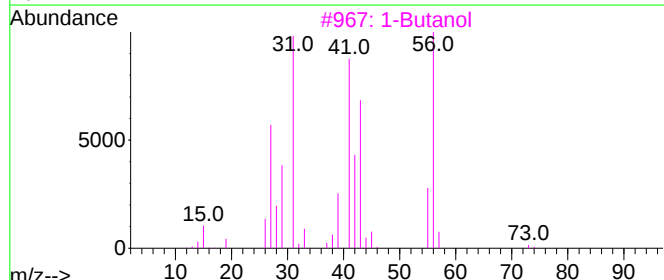
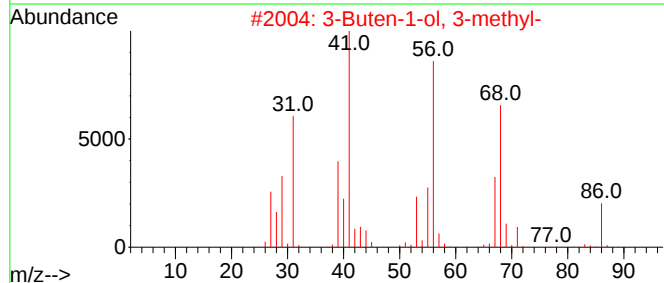
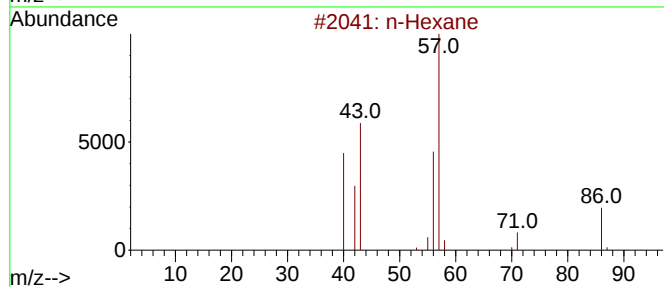
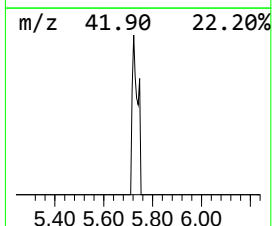
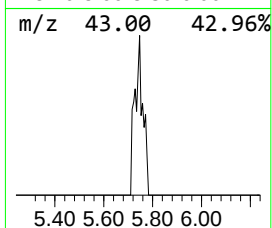
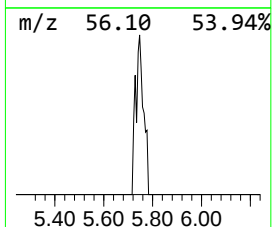
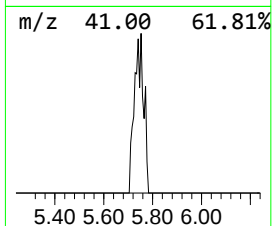
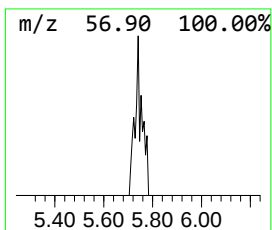
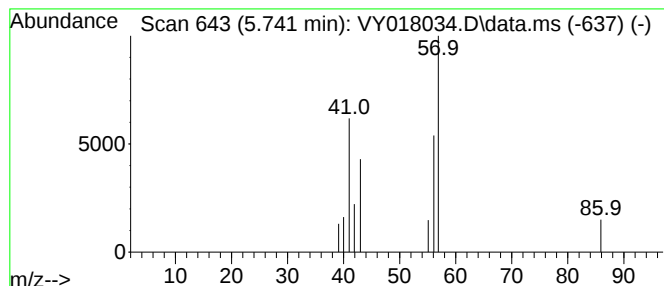
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.M
Quant Title : SW846 8260

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

Peak Number 2 n-Hexane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.741	7.78 ug/l	4195	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	64
2			3-Buten-1-ol, 3-methyl-	86	C5H10O	000763-32-6	47
3			1-Butanol	74	C4H10O	000071-36-3	45
4			Cyclobutane	56	C4H8	000287-23-0	9
5			Butyl aldoxime, 2-methyl-, anti-	101	C5H11NO	049805-55-2	9



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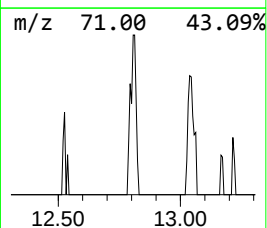
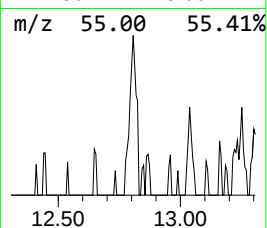
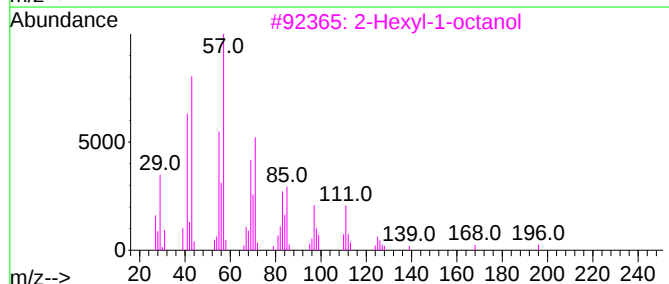
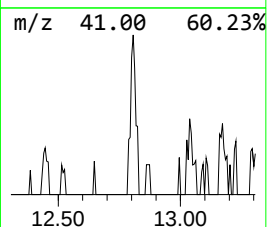
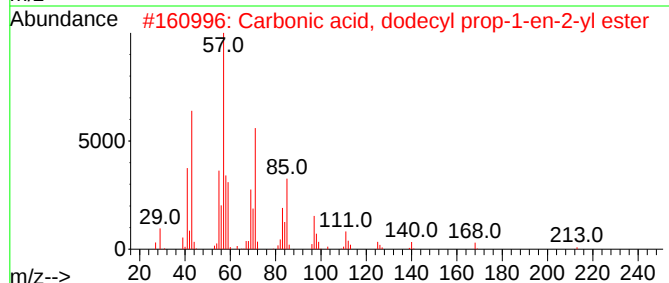
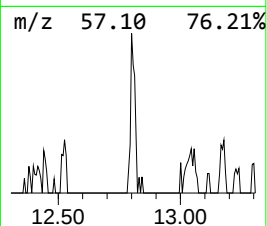
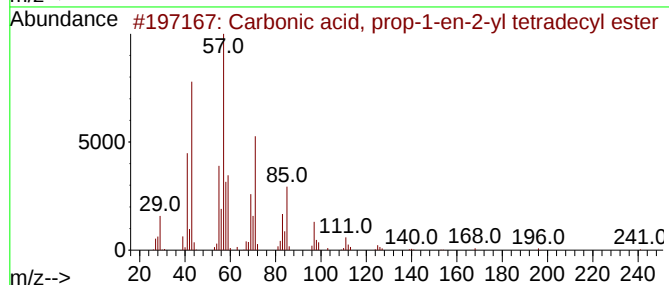
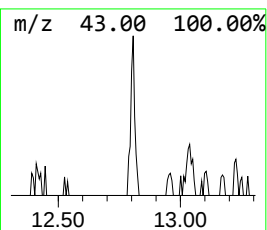
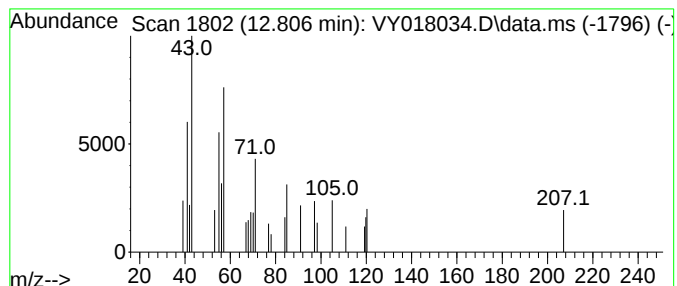
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown12.806 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.806	29.25 ug/l	7447	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	43
2			Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	43
3			2-Hexyl-1-octanol	214	C14H30O	019780-79-1	38
4			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	38
5			Octacosyl acetate	452	C30H60O2	018206-97-8	38



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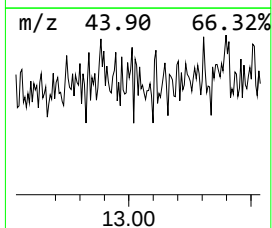
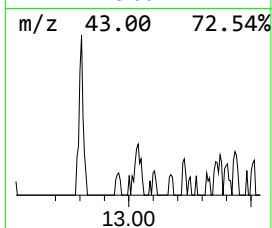
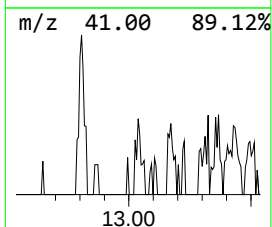
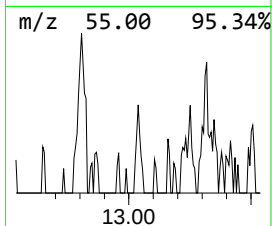
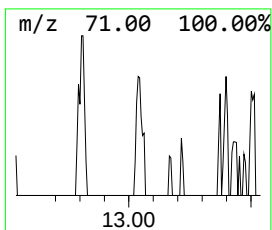
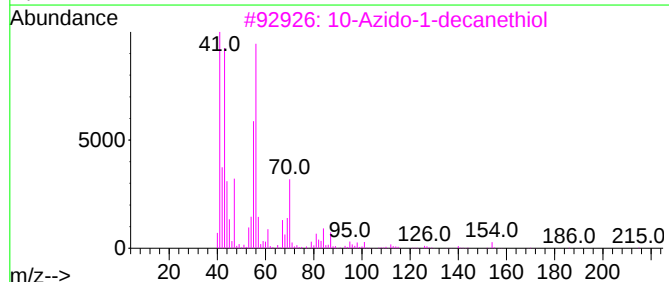
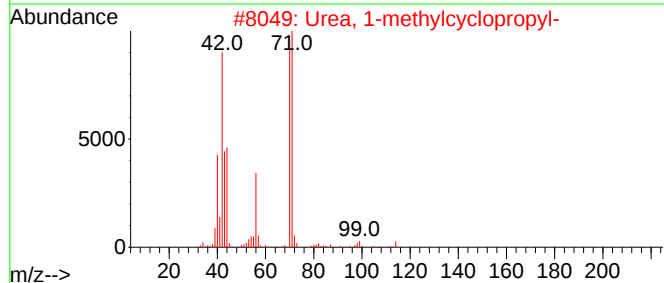
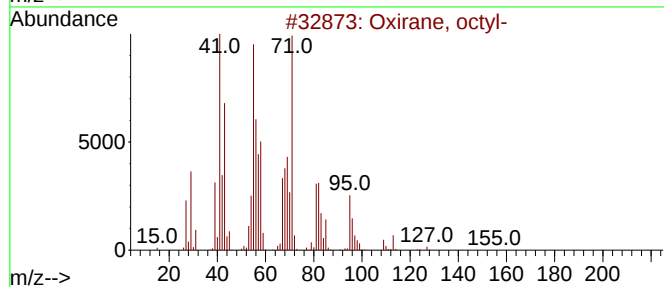
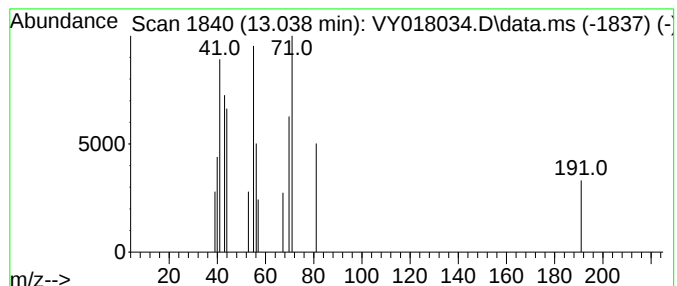
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Quant Title : SW846 8260

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

Peak Number 4 unknown13.038 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.038	10.73 ug/l	2732	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, octyl-	156	C10H20O	002404-44-6	38
2			Urea, 1-methylcyclopropyl-	114	C5H10N2O	058102-14-0	25
3			10-Azido-1-decanethiol	215	C10H21N3S	1152113-44-4	17
4			3-Dodecene, (Z)-	168	C12H24	007239-23-8	16
5			Cyclobutanone, 2,3,3-trimethyl-	112	C7H12O	028290-01-9	10



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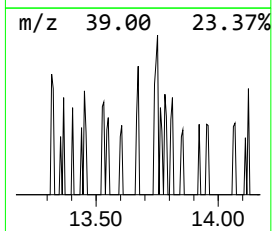
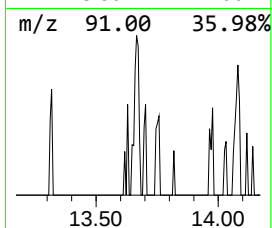
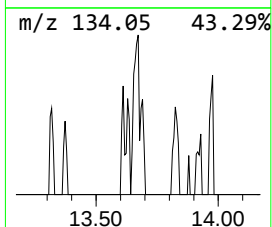
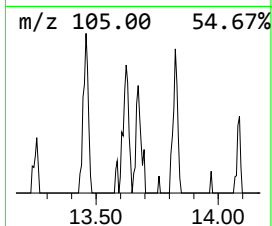
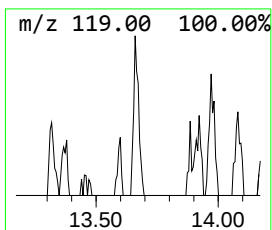
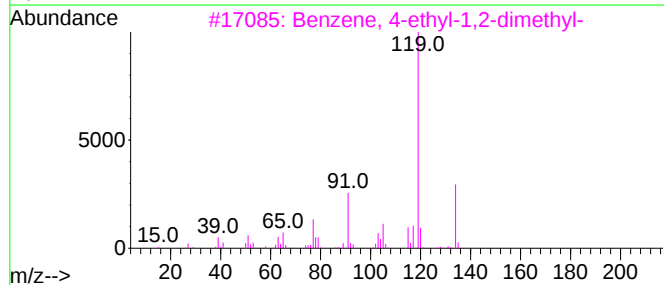
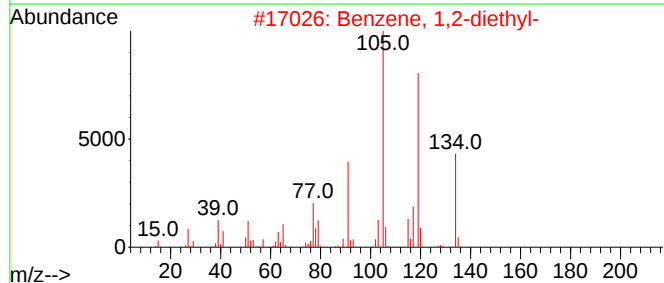
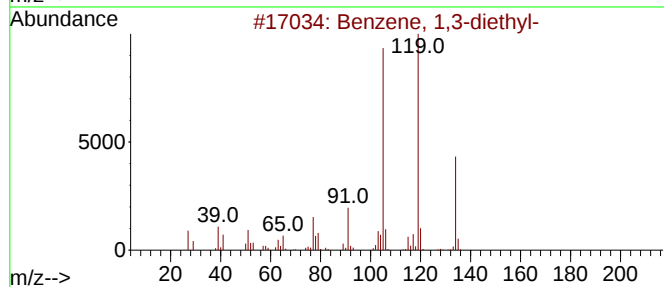
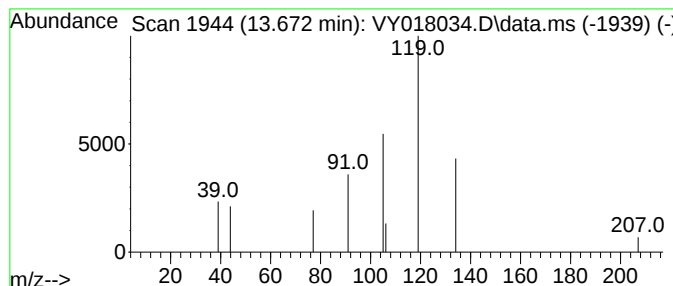
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,3-diethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.672	7.04 ug/l	1793	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	72
2			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	56
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	50
4			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	9
5			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	7



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PL-02-04232024

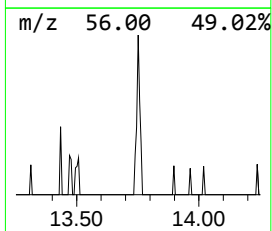
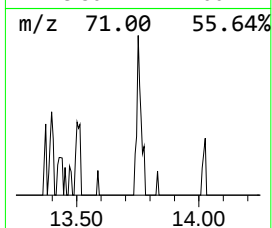
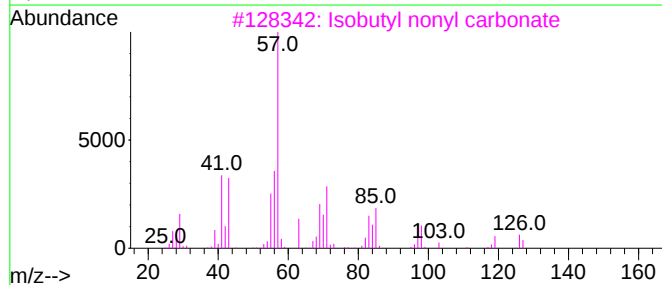
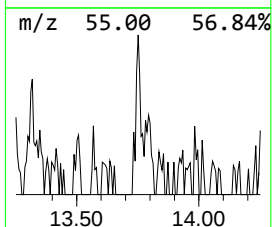
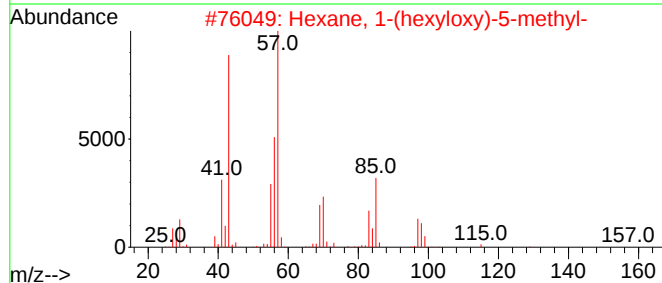
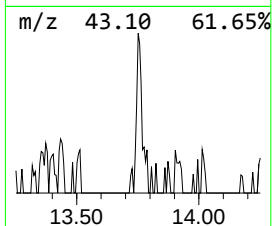
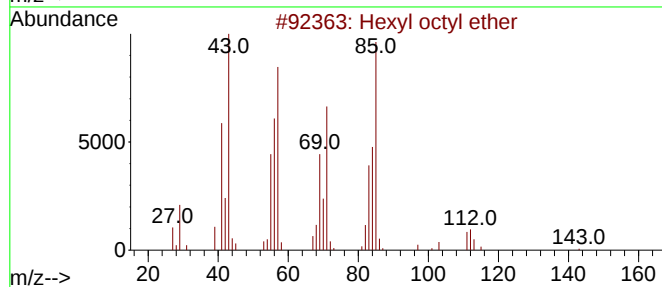
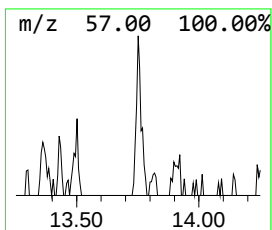
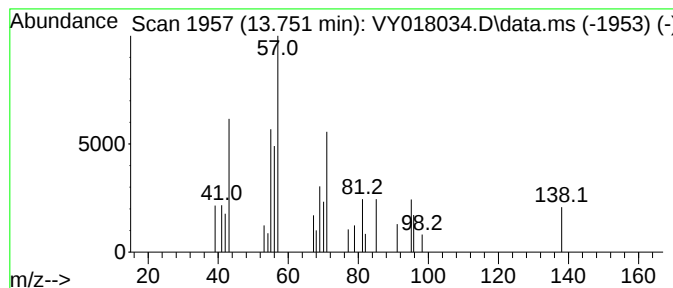
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.751 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	24.16 ug/l	6152	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexyl octyl ether	214	C14H30O	017071-54-4	49
2			Hexane, 1-(hexyloxy)-5-methyl-	200	C13H28O	074421-19-5	38
3			Isobutyl nonyl carbonate	244	C14H28O3	959311-27-4	38
4			Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	38
5			Decyl octyl ether	270	C18H38O	1000406-38-3	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042424\
Data File : VY018034.D
Acq On : 24 Apr 2024 12:50
Operator : SY/MD
Sample : P2247-01
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
PL-02-04232024

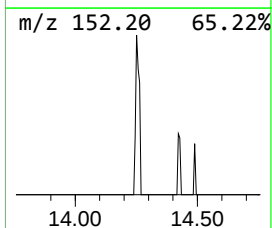
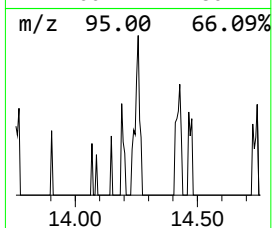
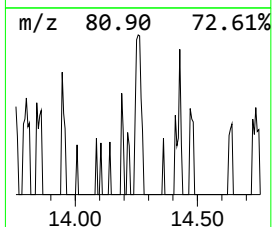
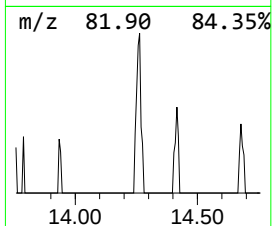
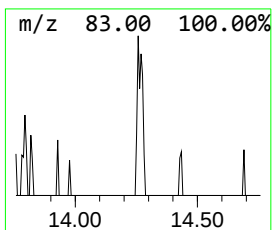
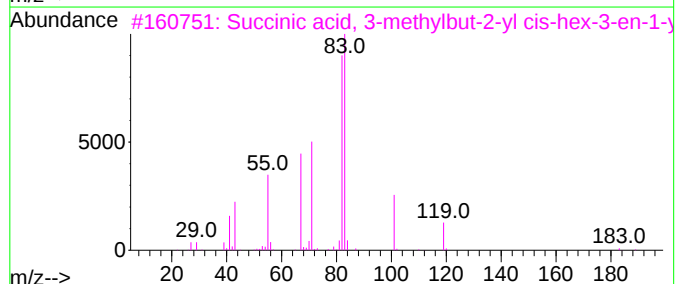
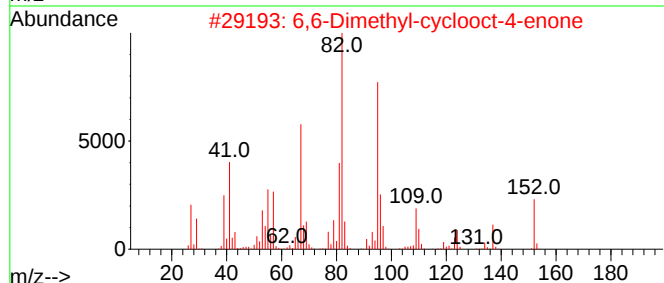
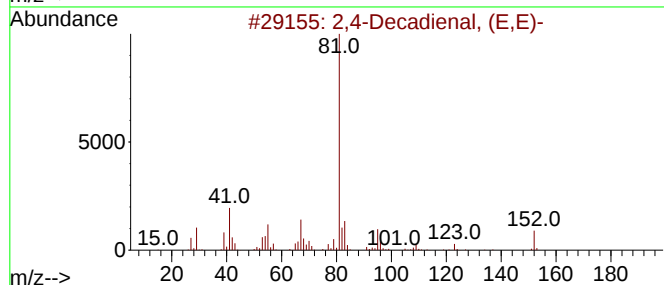
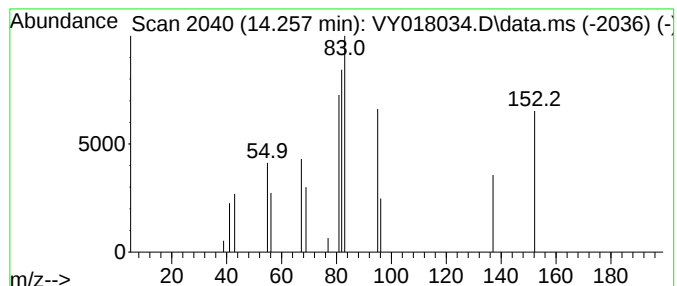
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.M
Quant Title : SW846 8260

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

Peak Number 9 2,4-Decadienal, (E,E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	12.03 ug/l	3062	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	53
2			6,6-Dimethyl-cyclooct-4-enone	152	C10H16O	1000194-10-0	50
3			Succinic acid, 3-methylbut-2-yl ...	270	C15H26O4	1000391-08-2	38
4			(+)-2-Bornanone	152	C10H16O	000464-49-3	35
5			2(1H)-Pyridinone, 1-propyl-	137	C8H11NO	019006-63-4	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042424\
Data File : VY018034.D
Acq On : 24 Apr 2024 12:50
Operator : SY/MD
Sample : P2247-01
Misc : 5.02g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
PL-02-04232024

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041624S.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
n-Hexane	5.741	7.8	ug/l	4195	1	7.783	26976	50.0
unknown12.806	12.806	29.3	ug/l	7447	4	13.428	12730	50.0
unknown13.038	13.038	10.7	ug/l	2732	4	13.428	12730	50.0
Benzene, 1,3-di...	13.672	7.0	ug/l	1793	4	13.428	12730	50.0
unknown13.751	13.751	24.2	ug/l	6152	4	13.428	12730	50.0
2,4-Decadienal,...	14.257	12.0	ug/l	3062	4	13.428	12730	50.0