

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011206.D
 Data File : VY011206.D
 Acq On : 31 Oct 2022 18:42
 Operator : KP/MD
 Sample : N5362-01
 Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CHRT-26516

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\82Y102822S.M
 Title : SW846 8260

Signal : TIC: VY011206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.223	61	66	76	rBV2	9359	20805	4.03%	0.517%
2	3.948	340	349	354	rBV2	2464	6232	1.21%	0.155%
3	4.710	463	474	492	rBV	28132	86676	16.78%	2.154%
4	5.740	635	643	654	rVB5	3322	10559	2.04%	0.262%
5	6.972	834	845	858	rBV	29443	90041	17.43%	2.237%
6	7.716	958	967	973	rBV2	66487	159794	30.93%	3.971%
7	7.789	973	979	988	rVB	73727	166781	32.28%	4.144%
8	8.136	1022	1036	1052	rVB2	71940	181532	35.14%	4.511%
9	8.685	1119	1126	1137	rBV	124546	247038	47.82%	6.138%
10	10.069	1347	1353	1364	rVB2	5070	9334	1.81%	0.232%
11	10.179	1364	1371	1378	rBV	169408	289251	55.99%	7.187%
12	10.240	1378	1381	1388	rVB	3930	6951	1.35%	0.173%
13	10.575	1430	1436	1442	rBV	12040	21303	4.12%	0.529%
14	10.941	1490	1496	1507	rBV	24250	41544	8.04%	1.032%
15	11.319	1553	1558	1563	rVB2	10254	17595	3.41%	0.437%
16	11.489	1579	1586	1595	rBV	127869	208850	40.43%	5.190%
17	11.593	1597	1603	1611	rVV	38642	66129	12.80%	1.643%
18	11.697	1611	1620	1630	rVV	80546	153935	29.80%	3.825%
19	12.026	1663	1674	1682	rBV	41013	69813	13.51%	1.735%
20	12.130	1682	1691	1696	rVB6	2992	7331	1.42%	0.182%
21	12.245	1705	1710	1714	rVB5	3096	5417	1.05%	0.135%
22	12.392	1727	1734	1739	rVV3	10167	23621	4.57%	0.587%
23	12.483	1739	1749	1759	rVB2	97068	184970	35.80%	4.596%
24	12.764	1782	1795	1798	rBV2	54245	99316	19.22%	2.468%
25	12.800	1798	1801	1808	rVV3	33756	63694	12.33%	1.583%
26	12.855	1808	1810	1815	rVB4	7540	10027	1.94%	0.249%
27	12.953	1822	1826	1829	rBV5	3249	5360	1.04%	0.133%
28	13.038	1836	1840	1842	rBV4	6300	8642	1.67%	0.215%
29	13.068	1842	1845	1849	rVB	12910	17236	3.34%	0.428%
30	13.117	1849	1853	1857	rVB	11943	17868	3.46%	0.444%
31	13.178	1857	1863	1868	rBV	37418	59994	11.61%	1.491%
32	13.282	1876	1880	1883	rVV2	15261	23312	4.51%	0.579%
33	13.318	1883	1886	1889	rVV5	6858	9033	1.75%	0.224%
34	13.361	1889	1893	1896	rVV2	8752	13126	2.54%	0.326%
35	13.422	1896	1903	1908	rVV	70775	123486	23.90%	3.068%
36	13.483	1908	1913	1914	rVV2	18028	32635	6.32%	0.811%

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Peak Location: TOP

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

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37	13.526	1915	1920	1928	rVV	141205	232024	44.91%	5.765%
38	13.623	1932	1936	1940	rVV3	14784	31652	6.13%	0.787%
39	13.666	1941	1943	1952	rVB4	15840	25859	5.01%	0.643%
40	13.751	1952	1957	1960	rBV	29579	42896	8.30%	1.066%
41	13.788	1960	1963	1967	rVV4	9752	15209	2.94%	0.378%
42	13.830	1967	1970	1976	rVB6	5925	11616	2.25%	0.289%
43	13.910	1981	1983	1987	rVV3	9625	14420	2.79%	0.358%
44	13.965	1987	1992	1997	rVV3	21207	38220	7.40%	0.950%
45	14.007	1997	1999	2004	rVB5	6049	8685	1.68%	0.216%
46	14.074	2005	2010	2016	rBV5	10922	19863	3.84%	0.494%
47	14.251	2033	2039	2046	rBV10	9852	28075	5.43%	0.698%
48	14.306	2046	2048	2056	rVB5	6642	14178	2.74%	0.352%
49	14.397	2056	2063	2071	rBV	336575	516633	100.00%	12.837%
50	14.477	2072	2076	2079	rBV5	5214	7000	1.35%	0.174%
51	14.574	2087	2092	2095	rBV5	8410	14526	2.81%	0.361%
52	14.605	2095	2097	2101	rVV2	14349	19237	3.72%	0.478%
53	14.660	2101	2106	2113	rVV3	23027	52680	10.20%	1.309%
54	14.727	2113	2117	2125	rVB5	13875	24484	4.74%	0.608%
55	14.836	2132	2135	2142	rVB8	4581	5789	1.12%	0.144%
56	14.995	2156	2161	2164	rBV7	3389	6316	1.22%	0.157%
57	15.044	2165	2169	2173	rVB6	3227	6240	1.21%	0.155%
58	15.135	2180	2184	2191	rVB9	5732	12066	2.34%	0.300%
59	15.208	2191	2196	2200	rBV5	6347	12406	2.40%	0.308%
60	15.312	2207	2213	2221	rVB	12179	23703	4.59%	0.589%
61	15.434	2229	2233	2241	rVB8	3780	7343	1.42%	0.182%
62	15.720	2277	2280	2286	rVB7	3073	5240	1.01%	0.130%
63	16.007	2320	2327	2336	rBV	142592	268820	52.03%	6.680%

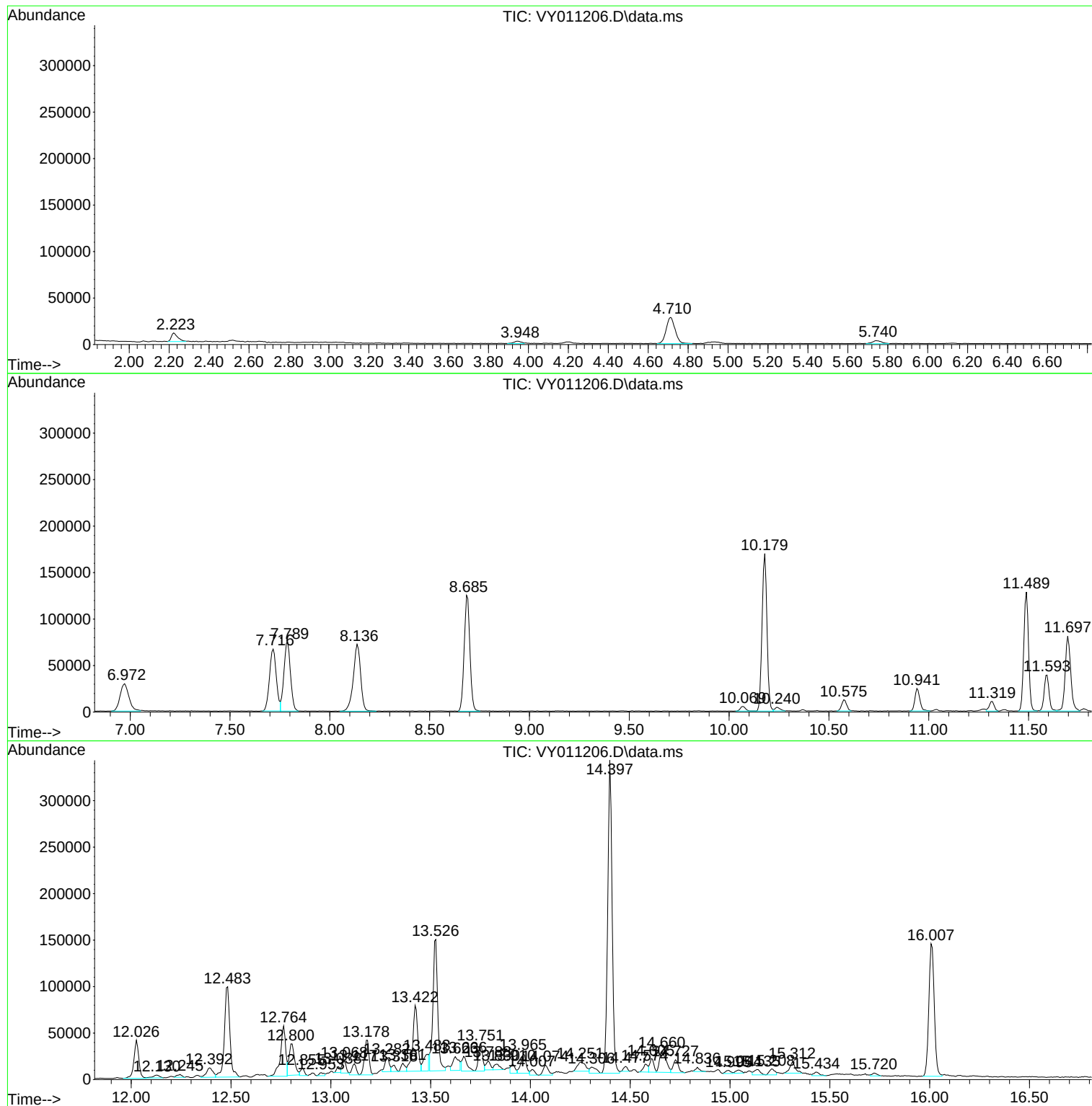
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Quant Title : SW846 8260

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



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ClientSampleId :
CHRT-26516

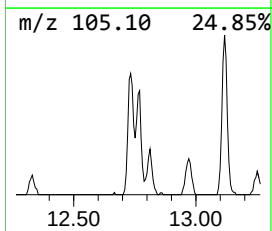
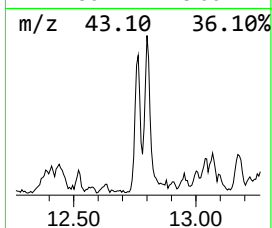
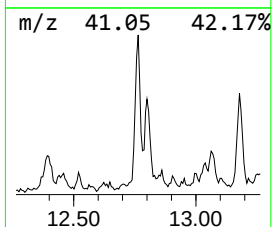
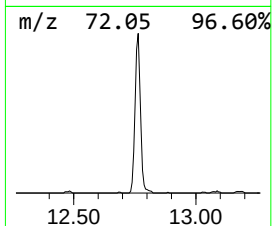
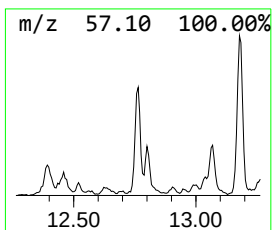
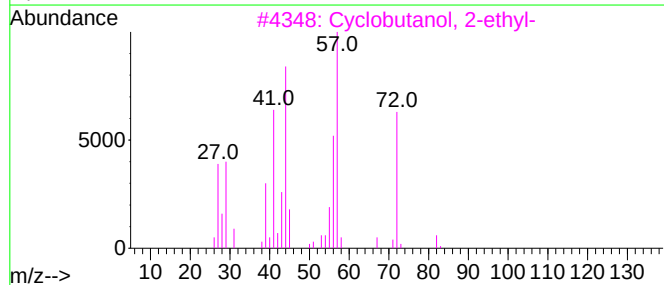
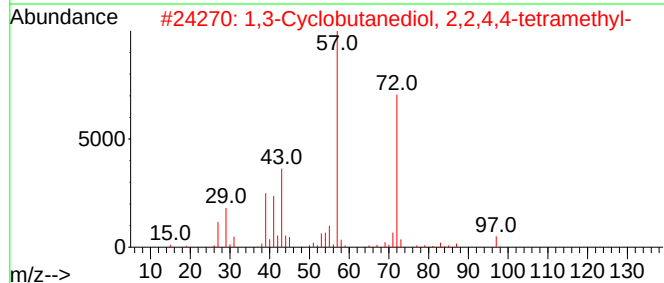
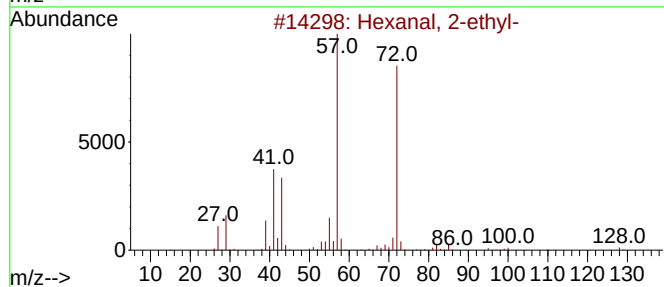
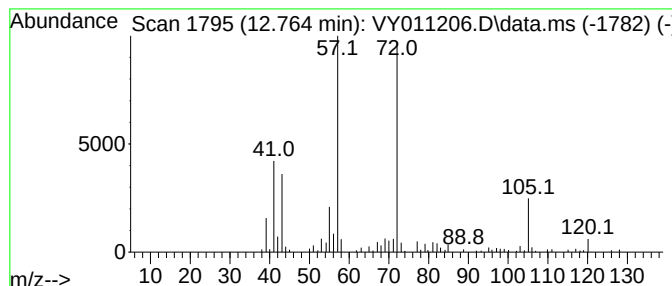
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102822S.M
Quant Title : SW846 8260

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

Peak Number 1 Hexanal, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.764	40.21 ug/l	99316	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	76
2			1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	42
3			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	42
4			N-tert-Butylmethylaniline	87	C5H13N	014610-37-8	40
5			1-Phenylpentan-2-amine	163	C11H17N	063951-01-9	38



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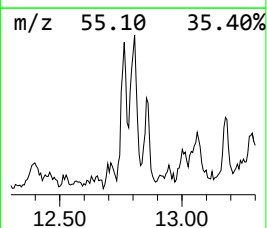
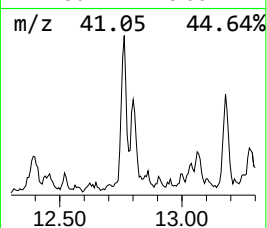
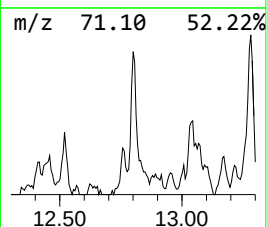
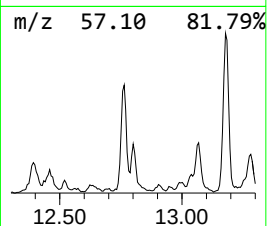
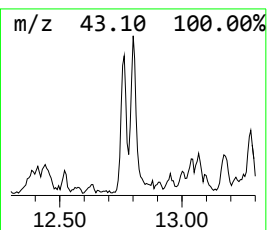
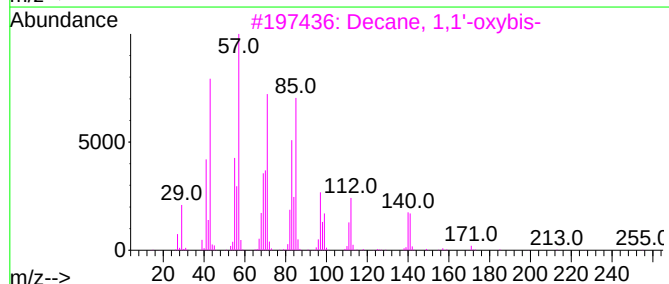
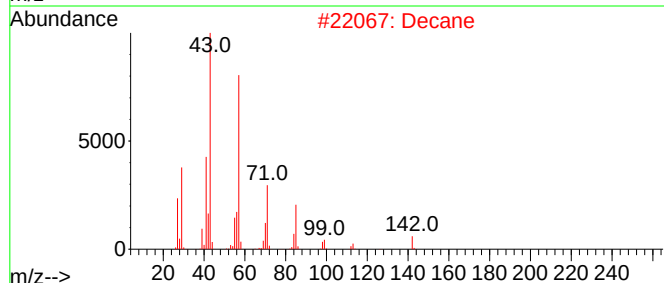
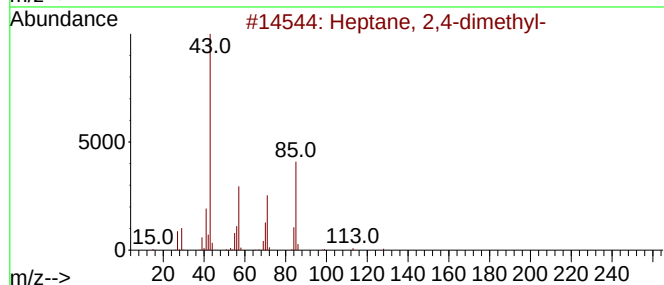
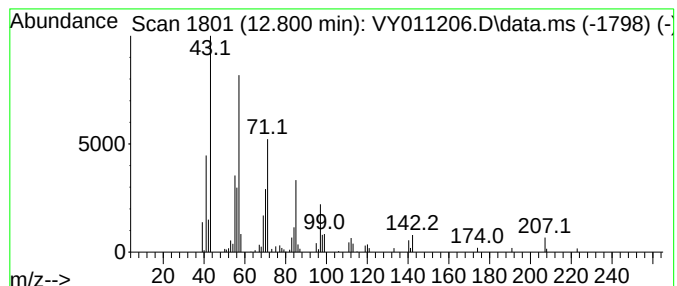
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102822S.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.800	25.79 ug/l	63694	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
2			Decane	142	C10H22	000124-18-5	70
3			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	64
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	64
5			Tridecane	184	C13H28	000629-50-5	50



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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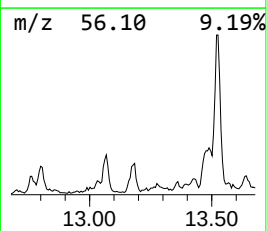
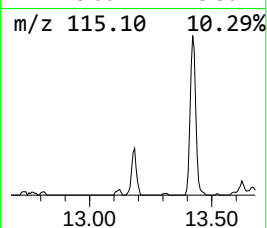
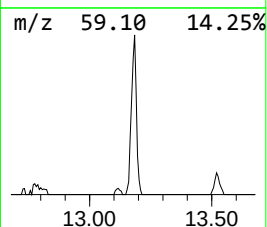
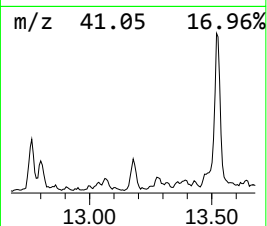
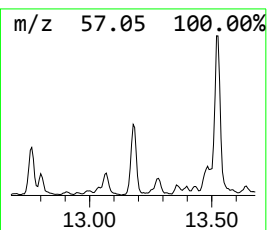
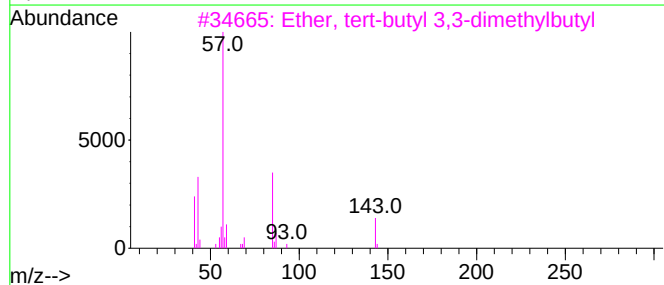
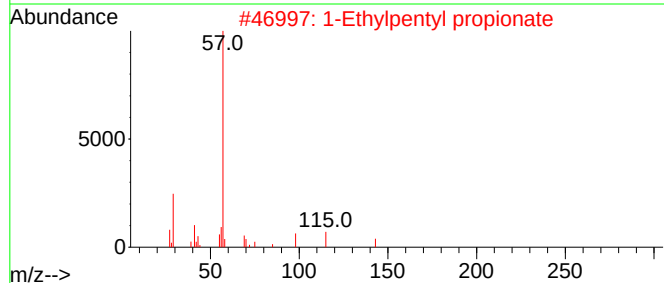
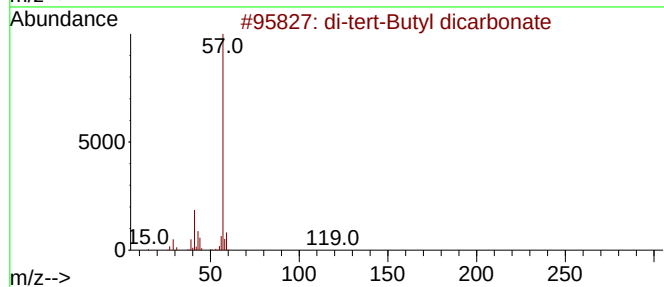
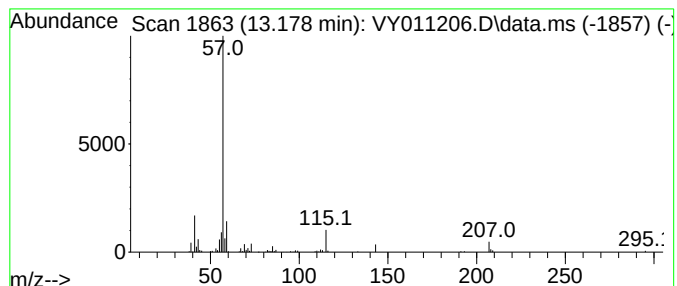
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102822S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown13.178 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	24.29 ug/l	59994	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	43
2			1-Ethylpentyl propionate	172	C10H20O2	1000430-89-7	38
3			Ether, tert-butyl 3,3-dimethylbutyl	158	C10H22O	004419-58-3	38
4			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	27
5			Hexanoic acid, 2-ethyl-, 1,1-dim...	200	C12H24O2	071648-27-6	25



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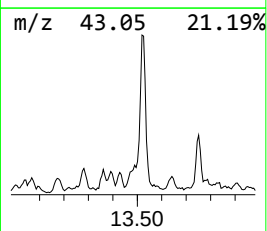
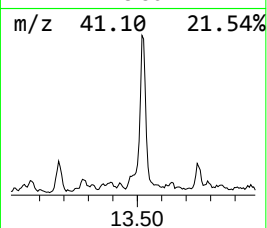
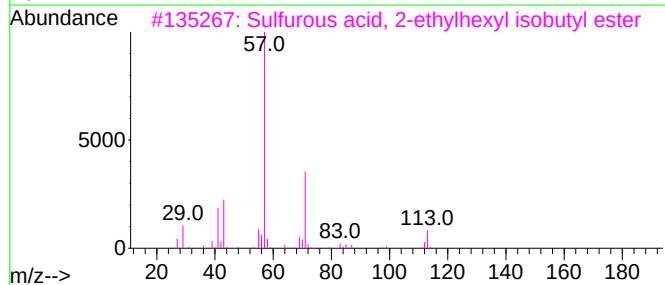
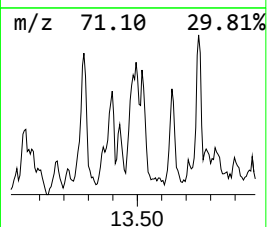
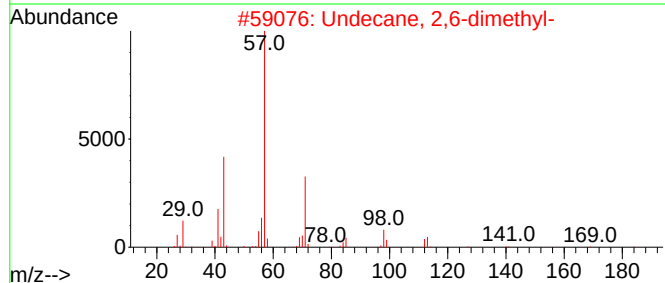
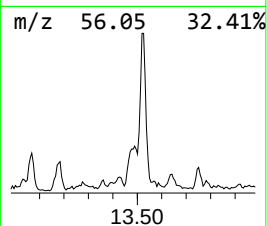
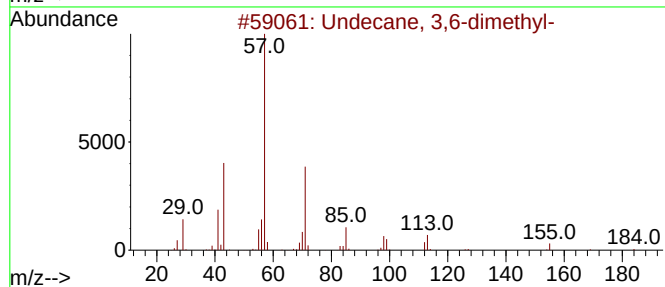
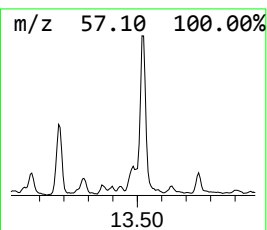
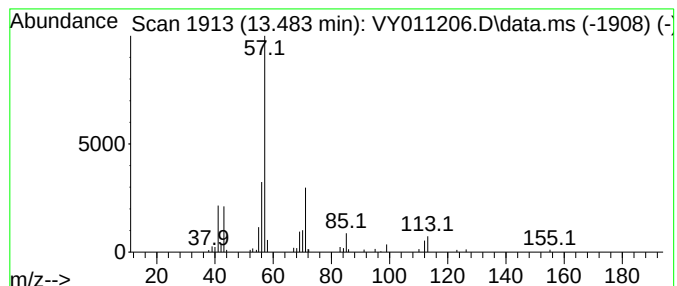
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Quant Title : SW846 8260

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

Peak Number 4 Undecane, 3,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.483	13.21 ug/l	32635	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59
3			Sulfurous acid, 2-ethylhexyl iso...	250	C12H26O3S	1000309-18-7	50
4			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	50
5			Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	50



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CHRT-26516

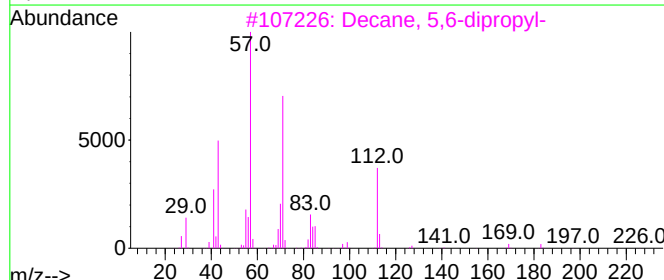
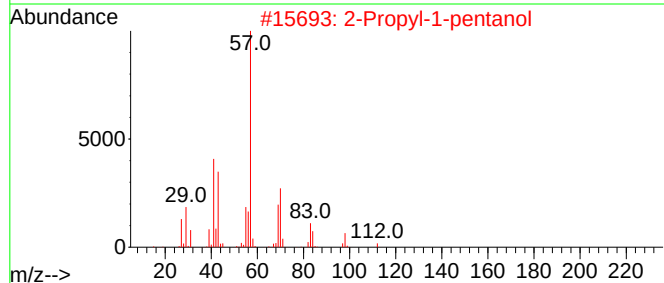
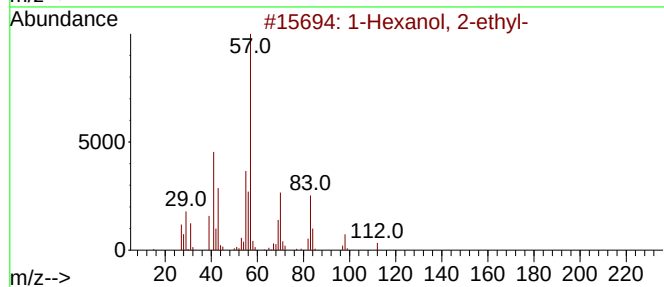
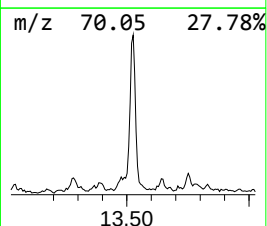
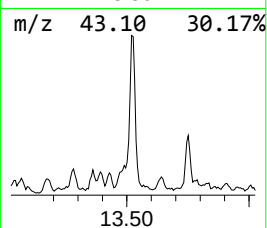
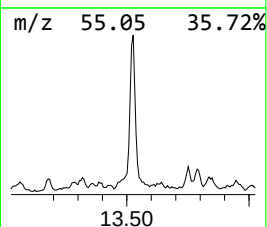
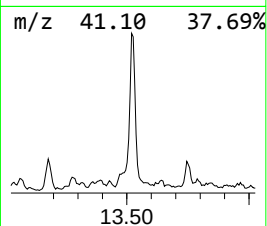
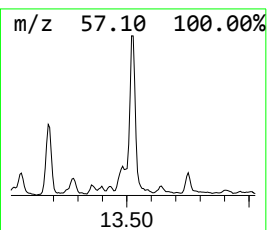
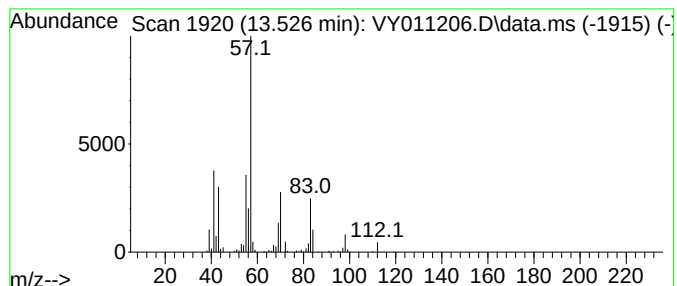
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.526	93.95 ug/l	232024	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY103122\
Data File : VY011206.D
Acq On : 31 Oct 2022 18:42
Operator : KP/MD
Sample : N5362-01
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26516

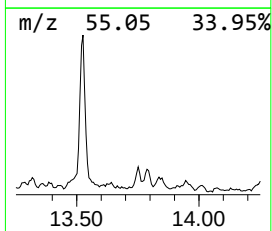
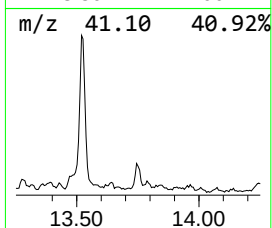
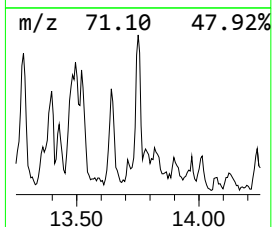
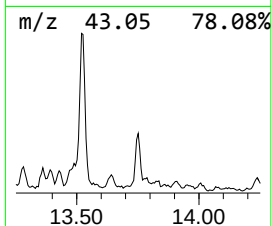
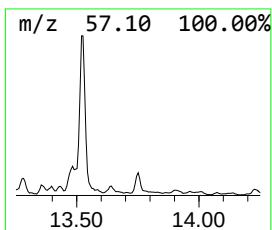
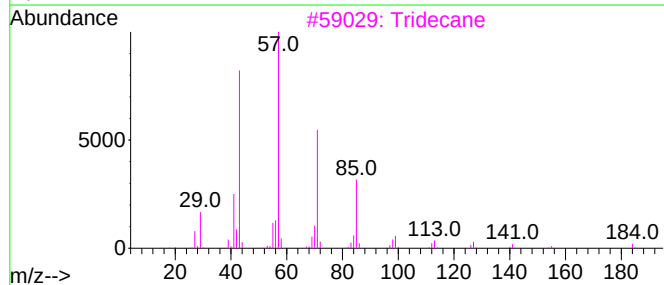
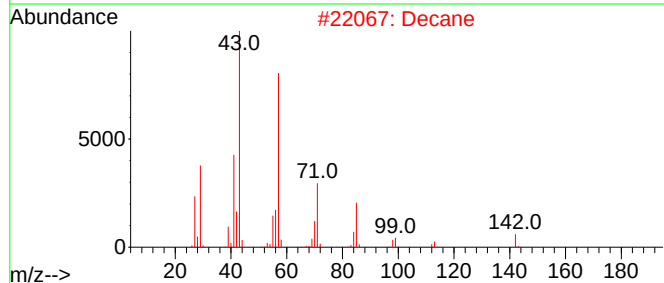
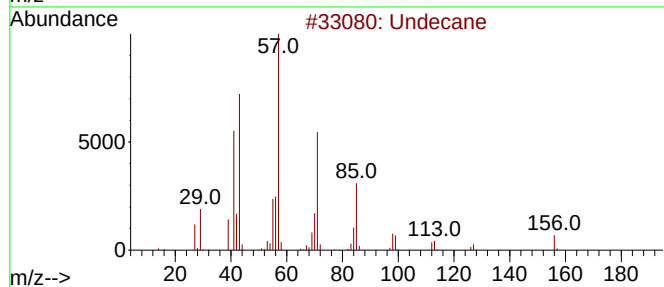
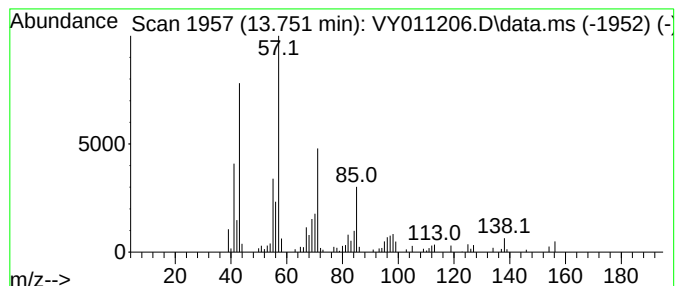
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Quant Title : SW846 8260

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

Peak Number 6 Undecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	17.37 ug/l	42896	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	96
2	Decane			142	C10H22	000124-18-5	72
3	Tridecane			184	C13H28	000629-50-5	64
4	Decane, 1,1'-oxybis-			298	C20H42O	002456-28-2	59
5	Octane, 2,7-dimethyl-			142	C10H22	001072-16-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY103122\
Data File : VY011206.D
Acq On : 31 Oct 2022 18:42
Operator : KP/MD
Sample : N5362-01
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26516

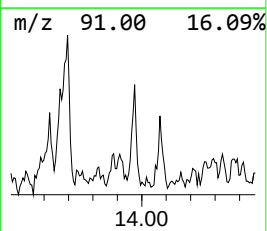
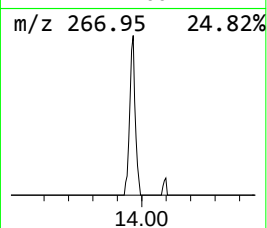
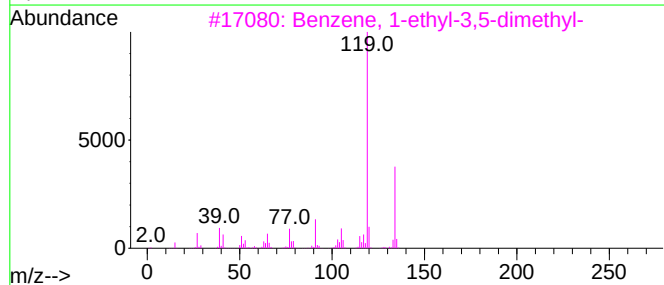
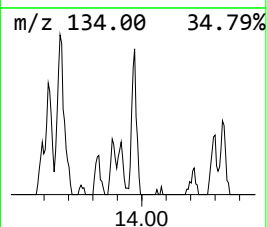
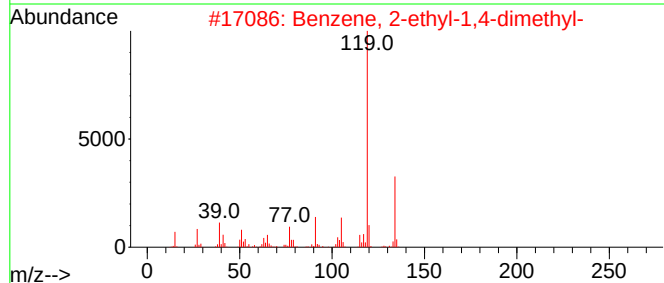
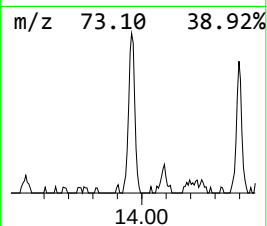
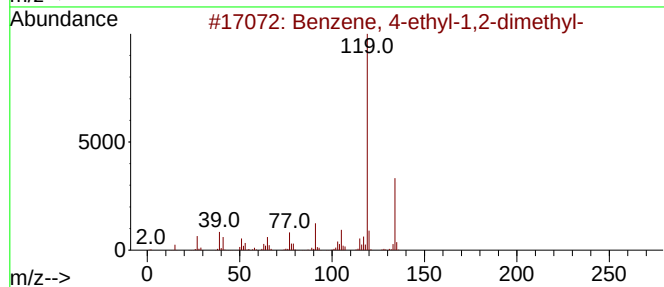
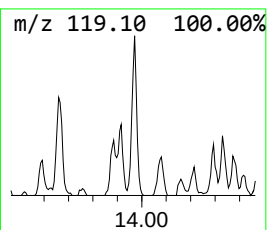
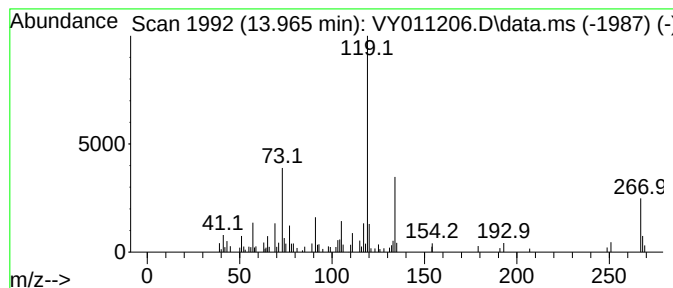
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.964	15.48 ug/l	38220	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	92
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	92
3			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	86
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY103122\
Data File : VY011206.D
Acq On : 31 Oct 2022 18:42
Operator : KP/MD
Sample : N5362-01
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26516

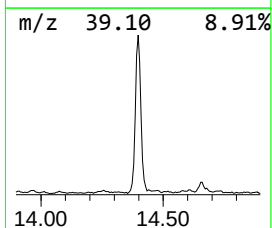
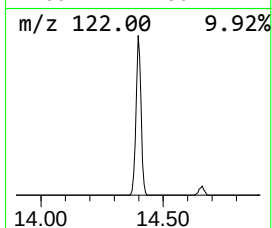
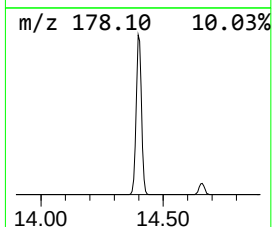
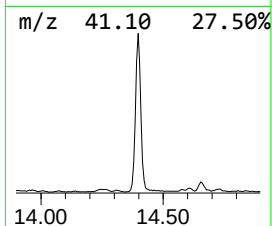
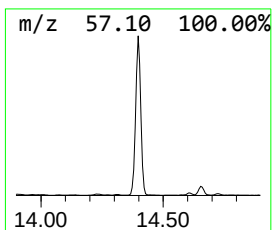
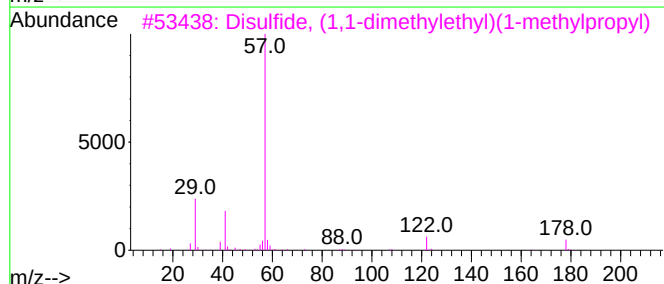
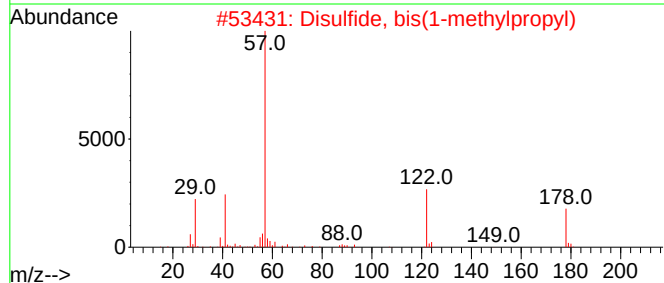
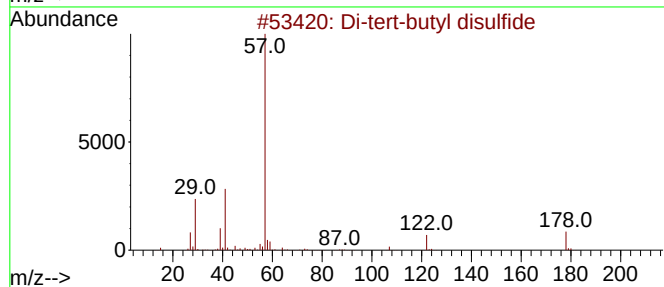
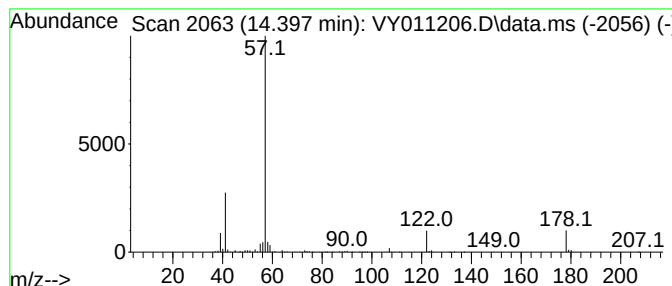
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Quant Title : SW846 8260

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

Peak Number 8 Di-tert-butyl disulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.397	209.19 ug/l	516633	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	87
2			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	64
3			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	53
4			Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	53
5			Disulfide, dibutyl	178	C8H18S2	000629-45-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY103122\
Data File : VY011206.D
Acq On : 31 Oct 2022 18:42
Operator : KP/MD
Sample : N5362-01
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

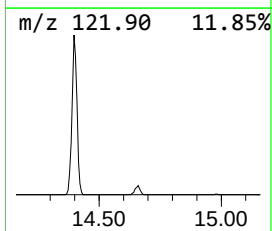
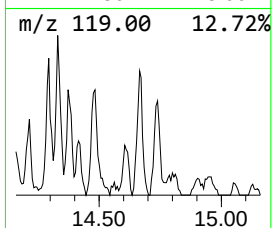
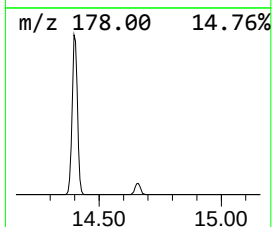
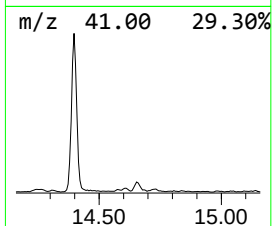
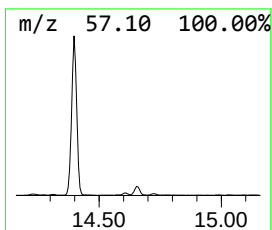
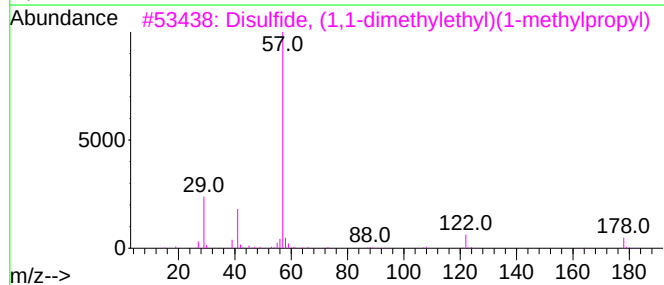
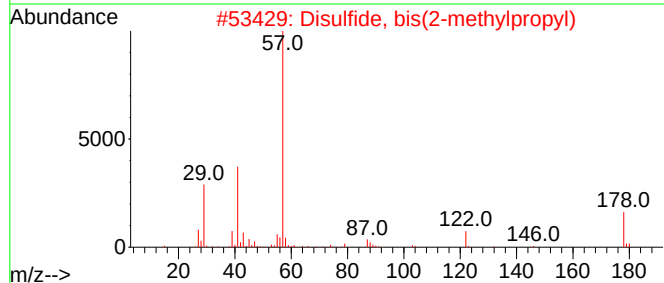
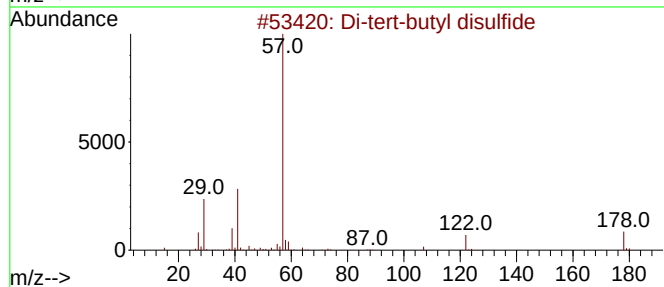
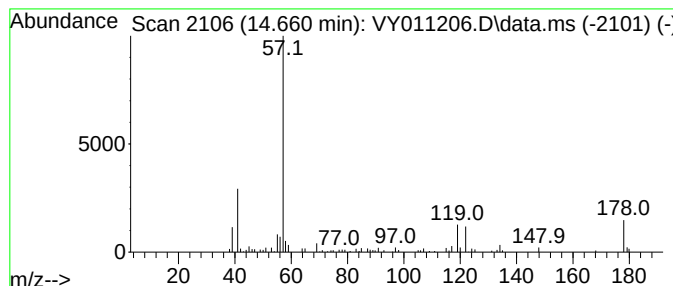
Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26516

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102822S.M
Quant Title : SW846 8260

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

Peak Number 9 Disulfide, bis(2-methylpropyl) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.660	21.33 ug/l	52680	1,4-Dichlorobenzene-d4			13.422
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Di-tert-butyl disulfide		178	C8H18S2	000110-06-5	62
2	Disulfide, bis(2-methylpropyl)		178	C8H18S2	001518-72-5	58
3	Disulfide, (1,1-dimethylethyl)(1...		178	C8H18S2	072437-46-8	50
4	Disulfide, dibutyl		178	C8H18S2	000629-45-8	43
5	Disulfide, bis(1-methylpropyl)		178	C8H18S2	005943-30-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY103122\
Data File : VY011206.D
Acq On : 31 Oct 2022 18:42
Operator : KP/MD
Sample : N5362-01
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26516

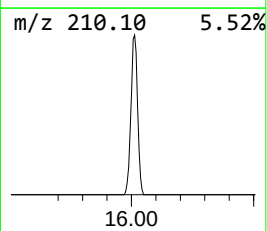
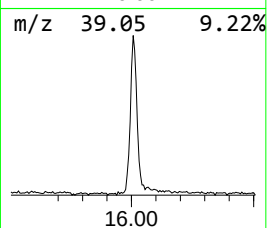
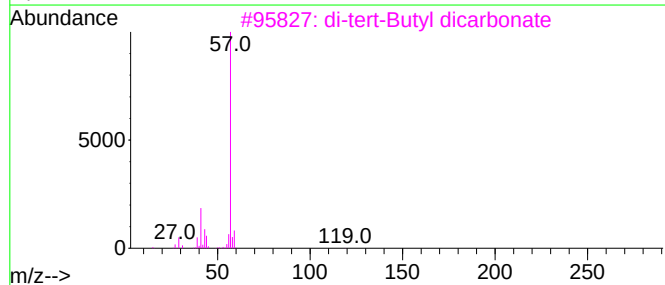
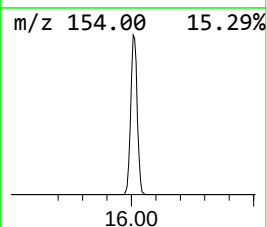
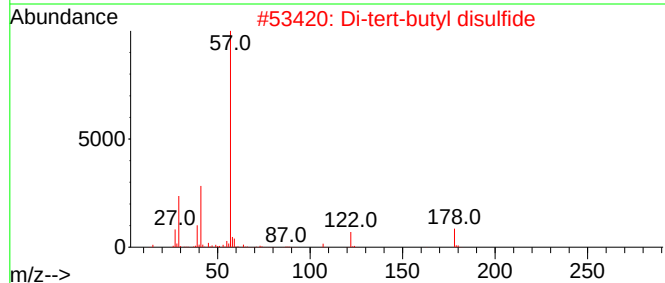
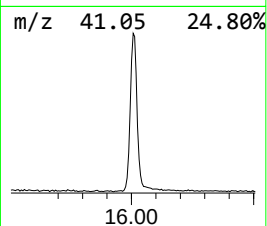
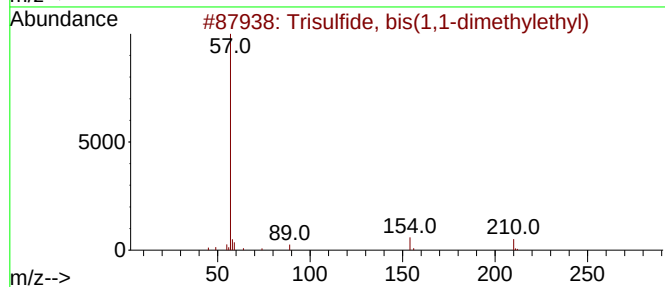
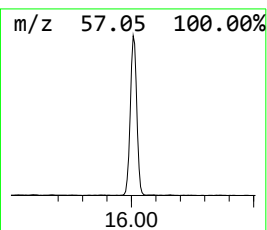
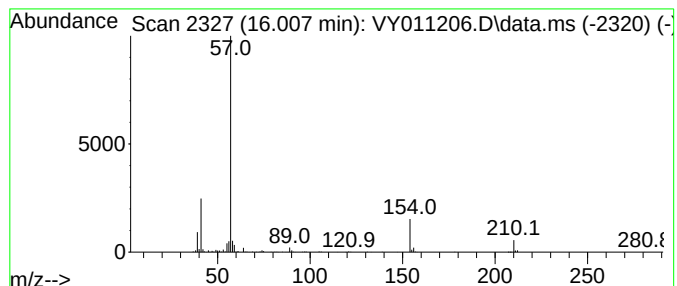
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Quant Title : SW846 8260

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

Peak Number 10 Trisulfide, bis(1,1-dimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	108.85 ug/l	268820	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	86
2			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	35
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	22
4			Isobutyl ether	130	C8H18O	000628-55-7	16
5			Phosphinous chloride, (chloromet...	172	C5H11Cl2P	078055-63-7	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY103122\
Data File : VY011206.D
Acq On : 31 Oct 2022 18:42
Operator : KP/MD
Sample : N5362-01
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHRT-26516

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102822S.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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Heptane, 2,4-di...	12.800	25.8	ug/l	63694	4	13.422	123486	50.0
unknown13.178	13.178	24.3	ug/l	59994	4	13.422	123486	50.0
Undecane, 3,6-d...	13.483	13.2	ug/l	32635	4	13.422	123486	50.0
1-Hexanol, 2-et...	13.526	94.0	ug/l	232024	4	13.422	123486	50.0
Undecane	13.751	17.4	ug/l	42896	4	13.422	123486	50.0
Benzene, 4-ethy...	13.964	15.5	ug/l	38220	4	13.422	123486	50.0
Di-tert-butyl d...	14.397	209.2	ug/l	516633	4	13.422	123486	50.0
Disulfide, bis(...	14.660	21.3	ug/l	52680	4	13.422	123486	50.0
Trisulfide, bis...	16.007	108.8	ug/l	268820	4	13.422	123486	50.0