

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092024\
 Data File : VY019648.D
 Acq On : 20 Sep 2024 16:10
 Operator : SY/MD
 Sample : P4103-01
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WC-22A

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\82Y090924S.M
 Title : SW846 8260

Signal : TIC: VY019648.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.878	834	846	864	rBV2	38825	131256	1.05%	0.119%
2	7.628	959	969	975	rBV2	265157	638225	5.10%	0.581%
3	7.701	975	981	991	rVB	420709	961086	7.68%	0.875%
4	8.055	1026	1039	1051	rBV	247740	552452	4.42%	0.503%
5	8.609	1120	1130	1142	rBV	724636	1414847	11.31%	1.287%
6	10.103	1368	1375	1384	rBV	1120649	1895636	15.15%	1.725%
7	11.414	1582	1590	1600	rBV	1074429	1758717	14.06%	1.600%
8	11.609	1616	1622	1627	rBV3	64257	148978	1.19%	0.136%
9	11.664	1627	1631	1642	rVB5	86448	241688	1.93%	0.220%
10	11.926	1667	1674	1680	rBV4	171201	452202	3.61%	0.411%
11	12.048	1690	1694	1698	rVB	213336	309857	2.48%	0.282%
12	12.127	1698	1707	1709	rBV6	214360	464254	3.71%	0.422%
13	12.158	1709	1712	1717	rVV2	388954	630377	5.04%	0.574%
14	12.243	1717	1726	1729	rVV7	148690	447526	3.58%	0.407%
15	12.298	1729	1735	1740	rVB6	160704	424372	3.39%	0.386%
16	12.401	1746	1752	1758	rVB2	901840	1620473	12.95%	1.475%
17	12.493	1758	1767	1771	rBV9	278924	771026	6.16%	0.702%
18	12.566	1774	1779	1786	rVB2	862649	1657395	13.25%	1.508%
19	12.657	1786	1794	1799	rBV5	410170	1207756	9.65%	1.099%
20	12.731	1799	1806	1810	rBV5	644612	1569206	12.54%	1.428%
21	12.871	1825	1829	1833	rVB4	449611	588576	4.70%	0.536%
22	12.914	1833	1836	1837	rBV	186174	228572	1.83%	0.208%
23	12.987	1844	1848	1854	rVB3	401525	643628	5.14%	0.586%
24	13.054	1855	1859	1861	rBV2	288759	410647	3.28%	0.374%
25	13.090	1861	1865	1871	rBV5	600068	1182068	9.45%	1.076%
26	13.145	1871	1874	1876	rBV2	213239	264443	2.11%	0.241%
27	13.218	1881	1886	1887	rVV3	634104	995429	7.96%	0.906%
28	13.237	1887	1889	1893	rVV2	883863	1283423	10.26%	1.168%
29	13.273	1893	1895	1901	rVV6	364014	695354	5.56%	0.633%
30	13.340	1902	1906	1913	rVB2	716454	1376560	11.00%	1.253%
31	13.487	1926	1930	1933	rVV3	694306	996441	7.96%	0.907%
32	13.523	1934	1936	1940	rVB4	354555	453076	3.62%	0.412%
33	13.615	1946	1951	1952	rBV4	460319	757541	6.05%	0.689%
34	13.663	1953	1959	1964	rVV3	3310561	6190116	49.47%	5.633%
35	13.718	1965	1968	1972	rVV4	582393	997600	7.97%	0.908%
36	13.779	1974	1978	1985	rVB6	1043731	2562233	20.48%	2.332%

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

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37	13.858	1985	1991	1993	rBV5	903465	1869787	14.94%	1.701%
38	13.962	2005	2008	2009	rBV3	374754	459353	3.67%	0.418%
39	13.993	2010	2013	2017	rVV3	903635	1219745	9.75%	1.110%
40	14.066	2017	2025	2030	rVV5	1582606	3726677	29.79%	3.391%
41	14.121	2030	2034	2038	rBV4	1051673	1553456	12.42%	1.414%
42	14.176	2038	2043	2051	rBV4	3805158	9743778	77.88%	8.866%
43	14.334	2066	2069	2073	rVB2	3431492	4554396	36.40%	4.144%
44	14.462	2087	2090	2093	rBV	1002430	1435640	11.47%	1.306%
45	14.535	2098	2102	2108	rBV7	1348841	3073399	24.56%	2.797%
46	14.602	2108	2113	2117	rVV	2187601	3578535	28.60%	3.256%
47	14.651	2117	2121	2127	rVB6	2047021	3562694	28.47%	3.242%
48	14.706	2127	2130	2131	rBV2	761057	870037	6.95%	0.792%
49	14.761	2136	2139	2142	rBV3	1519384	2212066	17.68%	2.013%
50	14.852	2151	2154	2158	rVB3	2406143	3729641	29.81%	3.394%
51	14.919	2159	2165	2168	rBV3	2078234	4694037	37.52%	4.271%
52	15.120	2194	2198	2204	rBV	8634032	12511778	100.00%	11.385%
53	15.181	2204	2208	2213	rBV6	2034122	3895745	31.14%	3.545%
54	15.346	2231	2235	2242	rBV6	1297848	3419605	27.33%	3.112%
55	16.047	2345	2350	2356	rVB	2658656	4593151	36.71%	4.180%
56	16.352	2396	2400	2407	rVB5	1224216	2268405	18.13%	2.064%

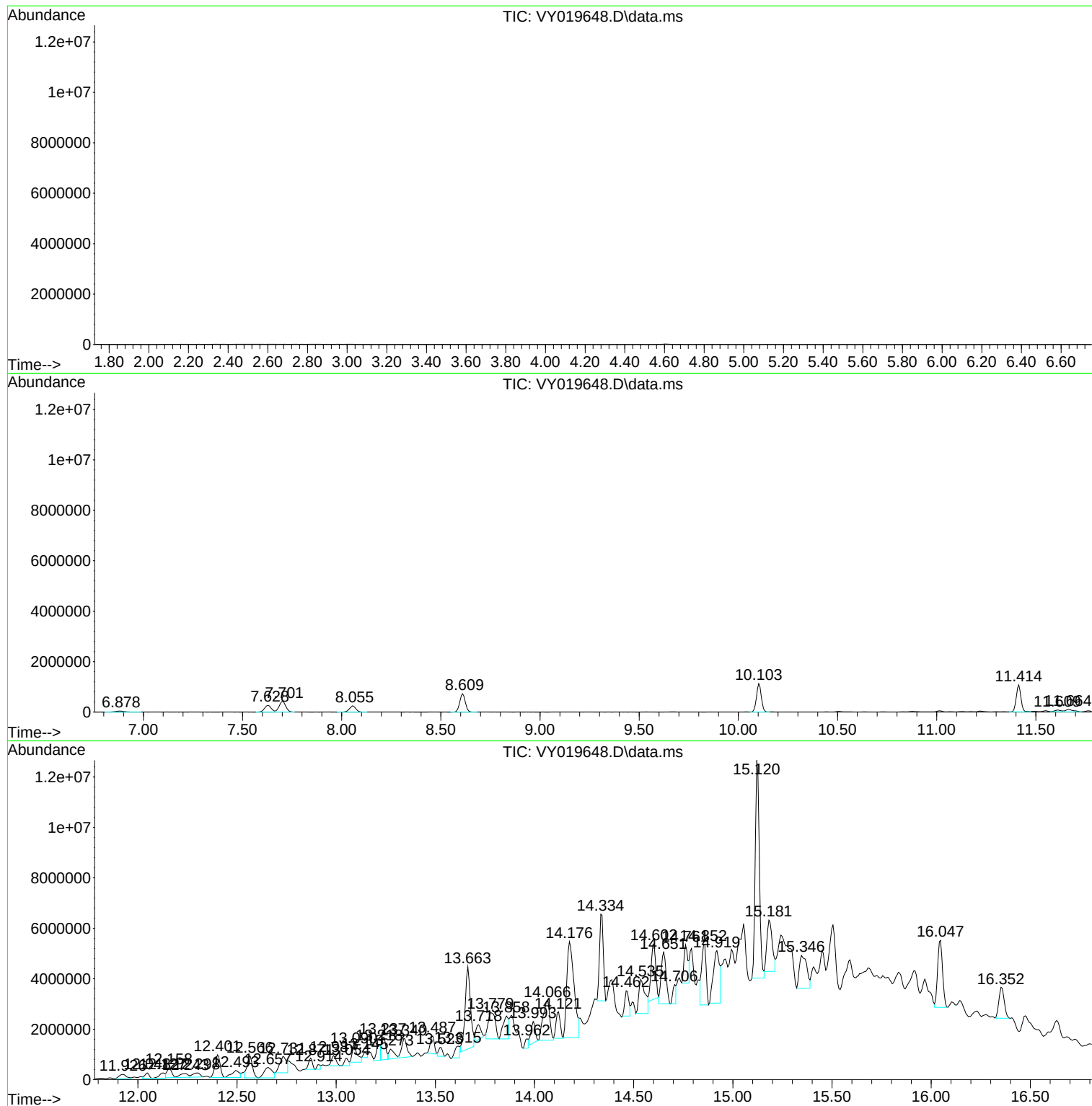
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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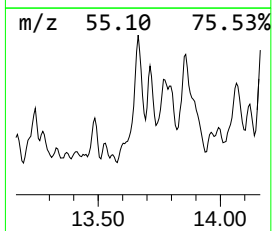
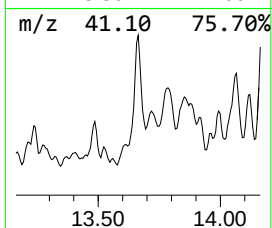
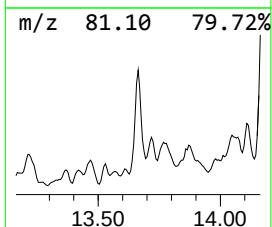
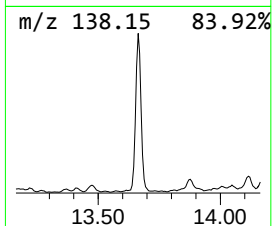
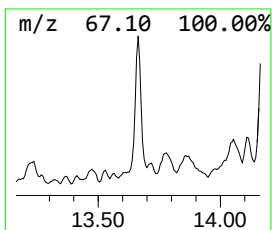
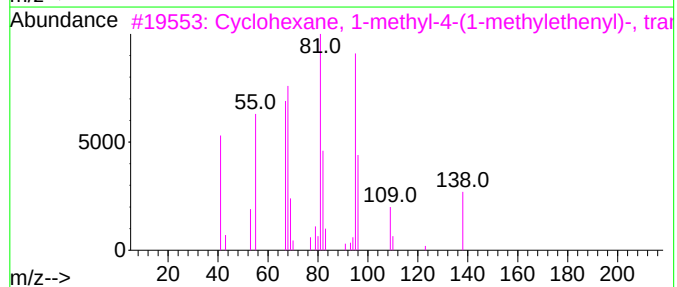
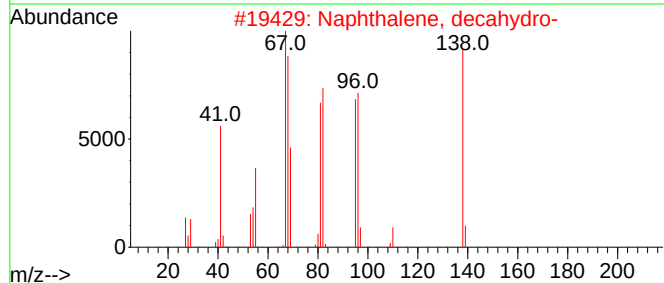
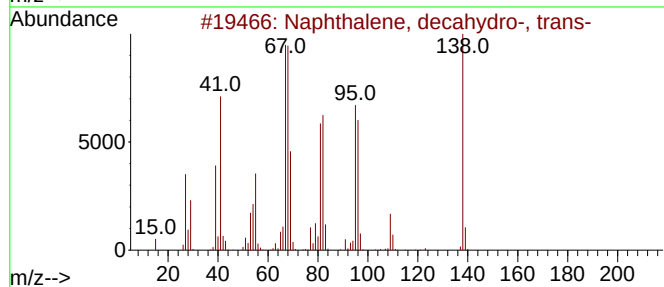
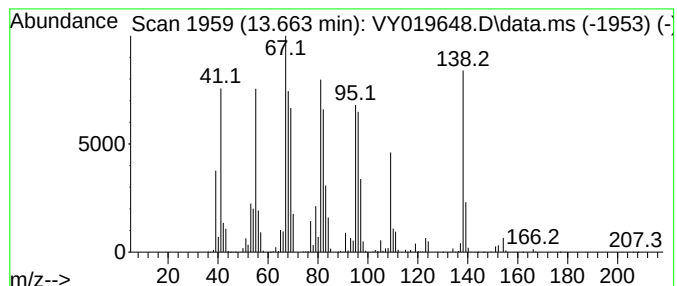
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

Peak Number 1 Naphthalene, decahydro-, tr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.663	224.84 ug/l	6190120	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	95
2			Naphthalene, decahydro-	138	C10H18	000091-17-8	94
3			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	70
4			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	68
5			2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	68



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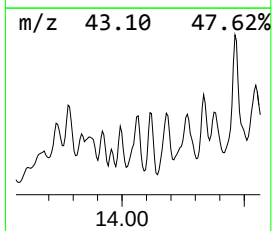
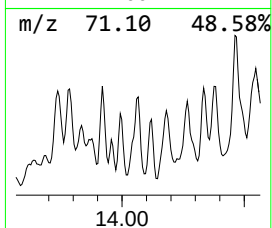
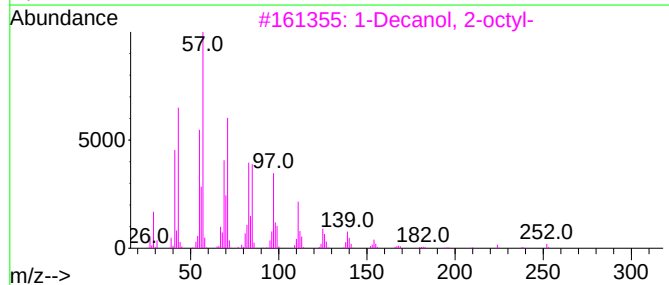
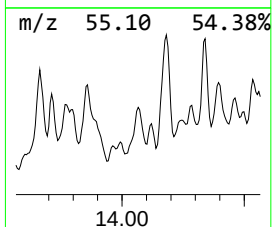
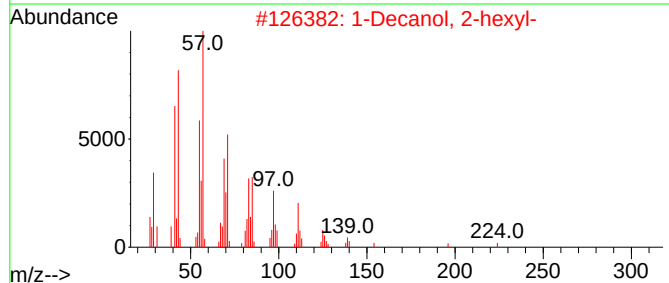
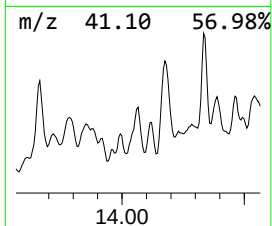
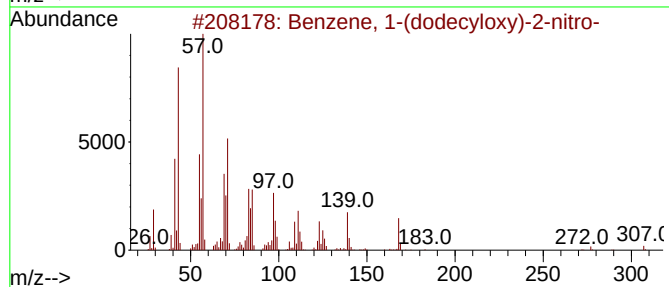
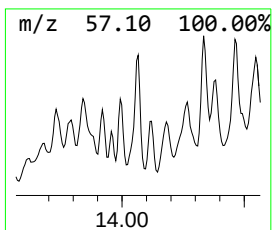
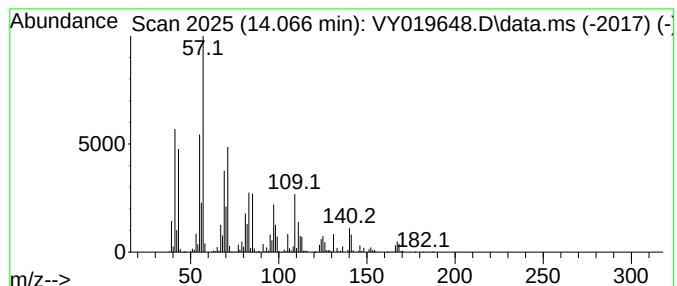
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-(dodecyloxy)-2-n... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.066	135.36 ug/l	3726680	1,4-Dichlorobenzene-d4	13.346

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-(dodecyloxy)-2-nitro-	307	C18H29NO3	083027-71-8	86
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83
3		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	74
4		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	72
5		Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	64



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ALS Vial : 15 Sample Multiplier: 1

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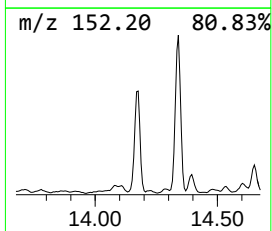
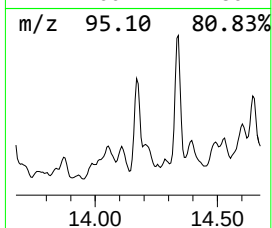
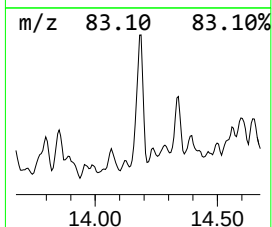
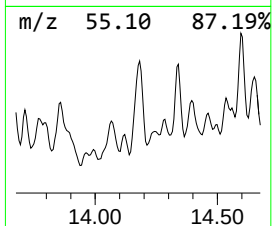
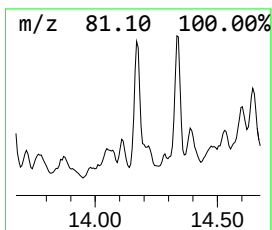
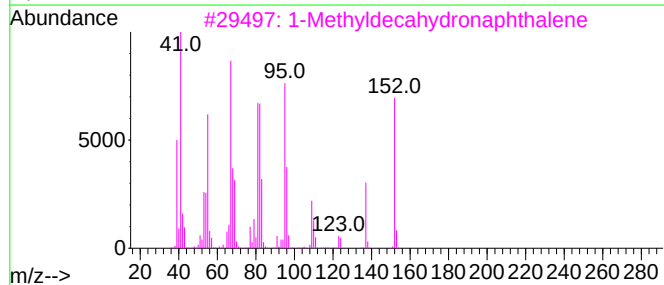
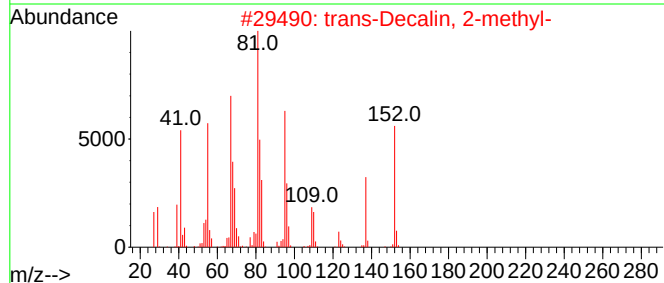
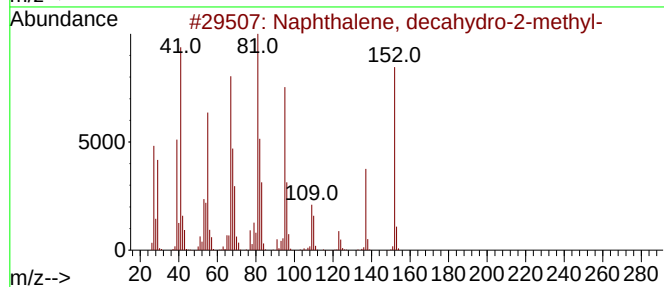
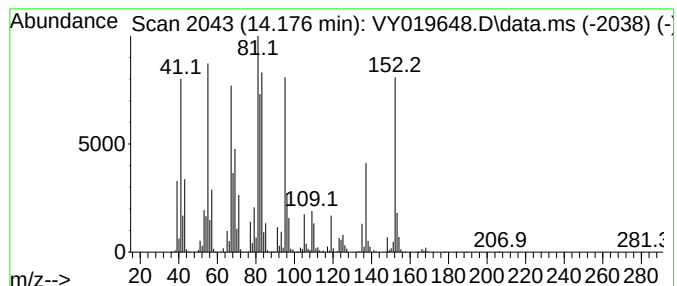
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, decahydro-2-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	353.92 ug/l	9743780	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	83
3			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	64
4			Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	62
5			Pulegone	152	C10H16O	000089-82-7	58



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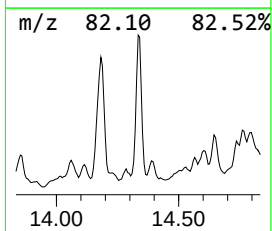
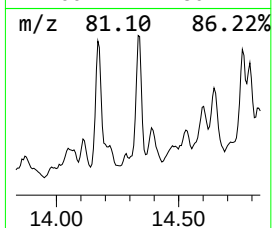
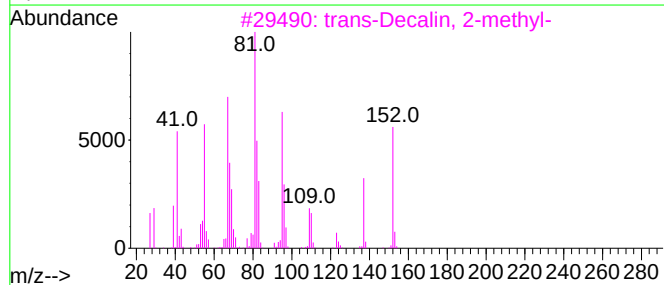
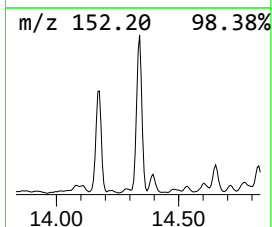
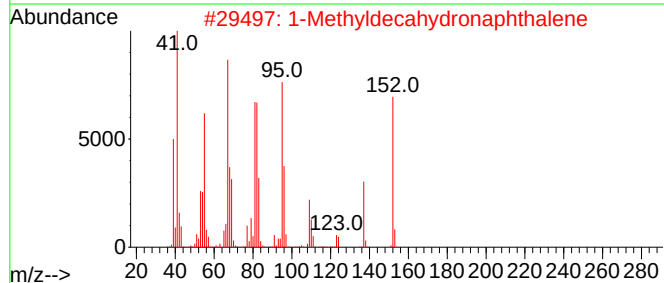
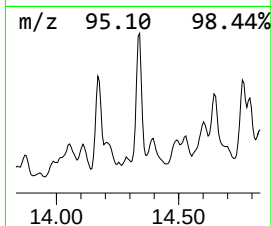
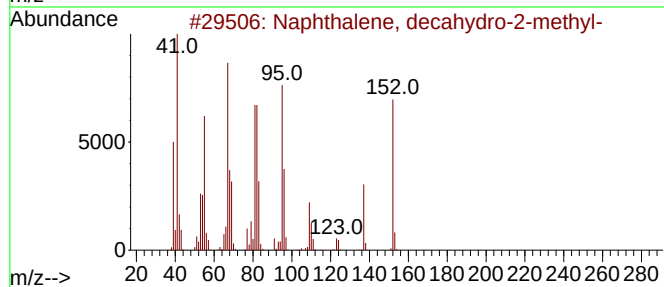
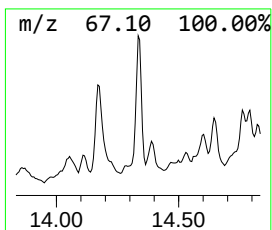
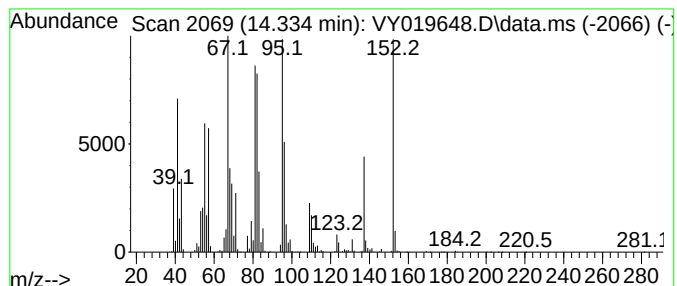
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Quant Title : SW846 8260

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

Peak Number 4 1-Methyldecahydronaphthalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.334	165.43 ug/l	4554400	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	97
2			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	97
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	89
4			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	58
5			Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	58



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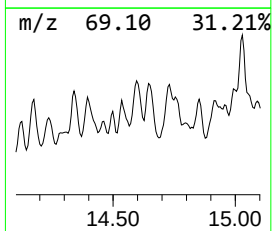
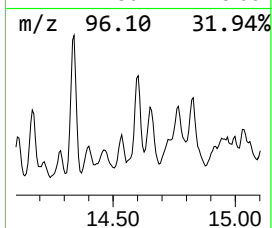
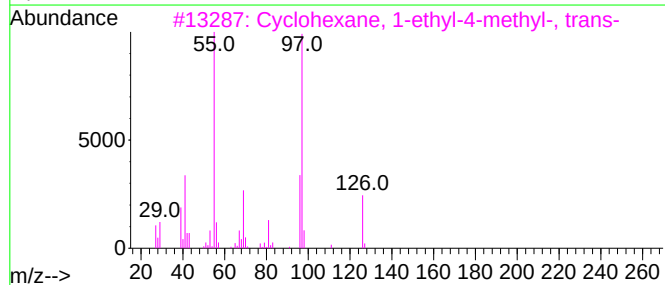
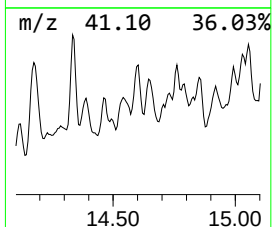
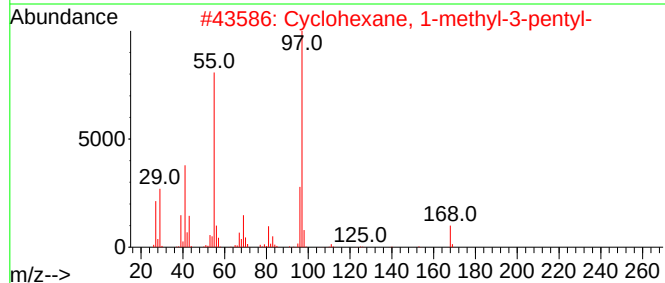
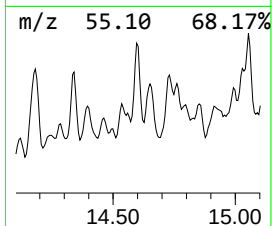
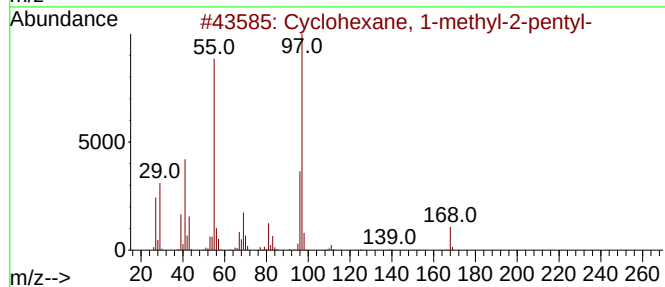
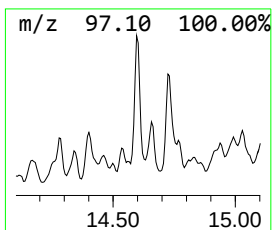
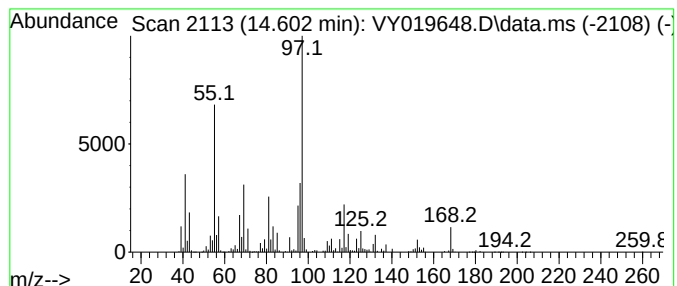
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Quant Title : SW846 8260

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

Peak Number 5 unknown14.602 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.602	129.98 ug/l	3578540	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	49
2			Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	49
3			Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	46
4			Pyrollidine, 2,5-bis(imino)-	97	C4H7N3	000503-84-4	46
5			Oxalic acid, di(cyclohexylmethyl-...	282	C16H26O4	1000309-68-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092024\
Data File : VY019648.D
Acq On : 20 Sep 2024 16:10
Operator : SY/MD
Sample : P4103-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-22A

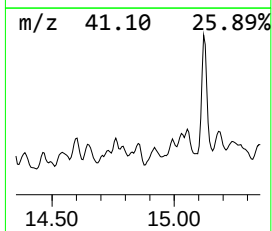
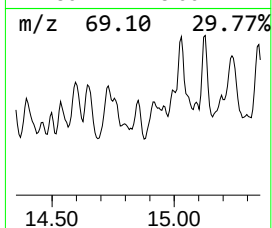
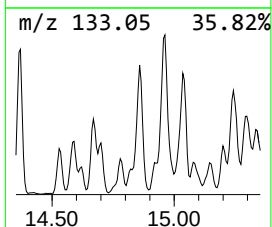
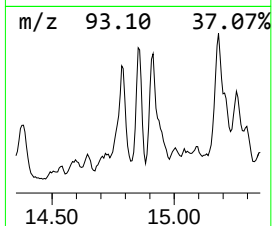
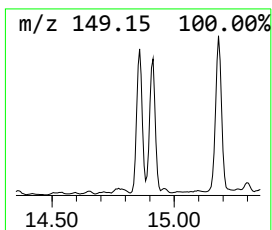
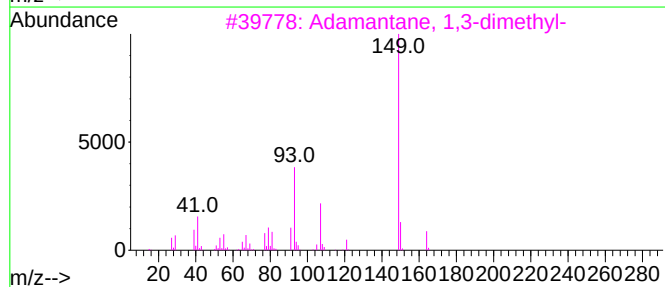
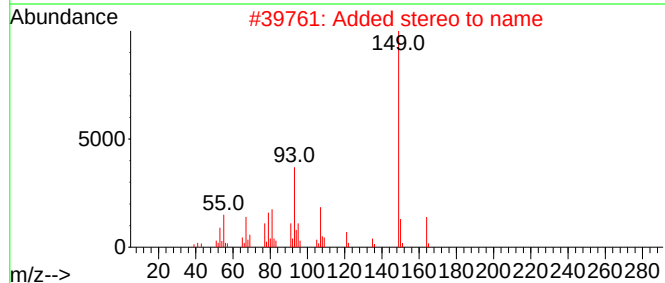
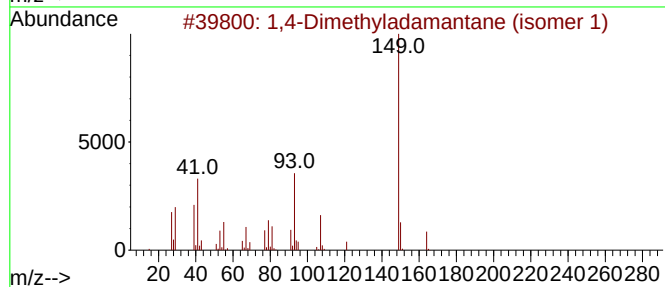
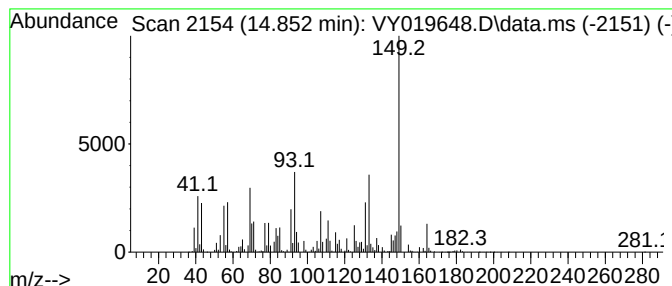
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Quant Title : SW846 8260

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

Peak Number 6 1,4-Dimethyladamantane (iso... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.852	135.47 ug/l	3729640	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	60
2			Added stereo to name	164	C12H20	024145-89-9	60
3			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	60
4			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	53
5			1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092024\
Data File : VY019648.D
Acq On : 20 Sep 2024 16:10
Operator : SY/MD
Sample : P4103-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-22A

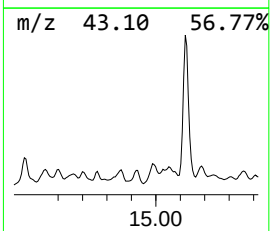
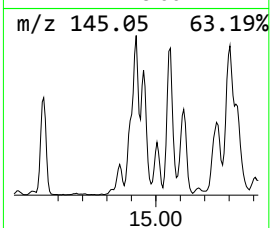
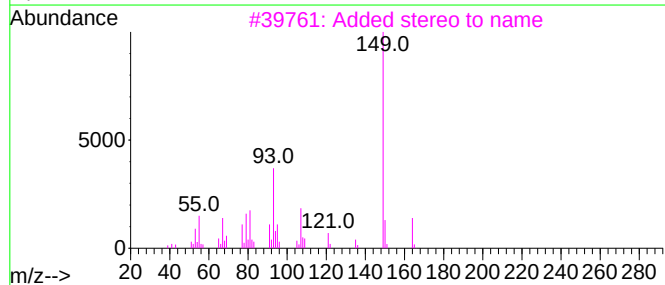
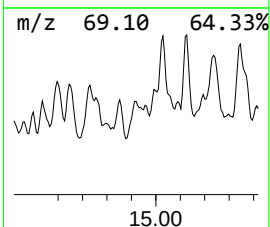
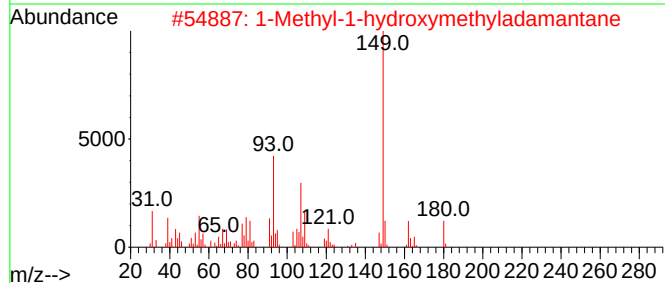
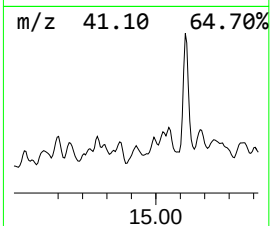
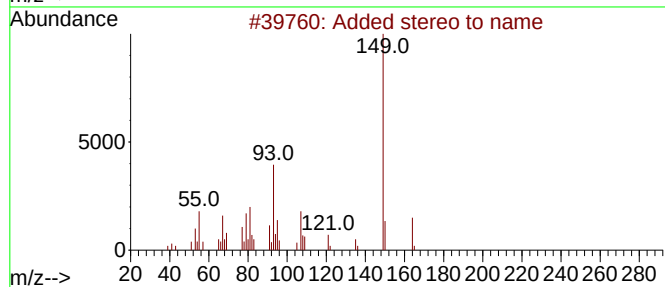
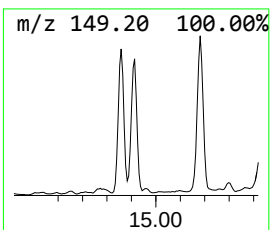
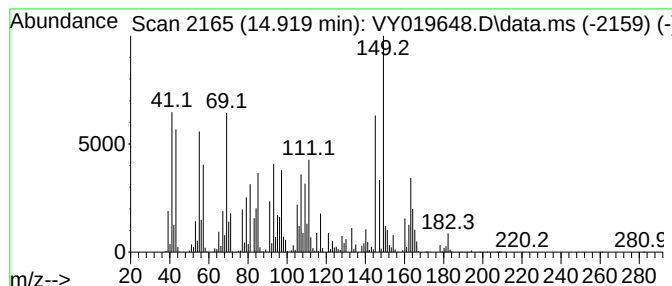
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.919 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.919	170.50 ug/l	4694040	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-88-8	41
2	1-Methyl-1-hydroxymethyladamantane			180	C12H20O	001200-78-8	38
3	Added stereo to name			164	C12H20	024145-89-9	35
4	3-Methyl-1-adamantanecarboxylic ...			194	C12H18O2	1000504-38-9	27
5	Phenol, 4-(1,1-dimethylethyl)-2-...			164	C11H16O	000098-27-1	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092024\
Data File : VY019648.D
Acq On : 20 Sep 2024 16:10
Operator : SY/MD
Sample : P4103-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-22A

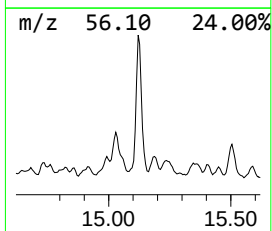
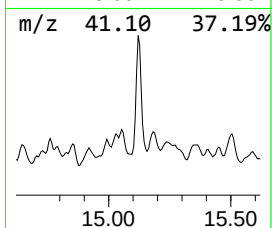
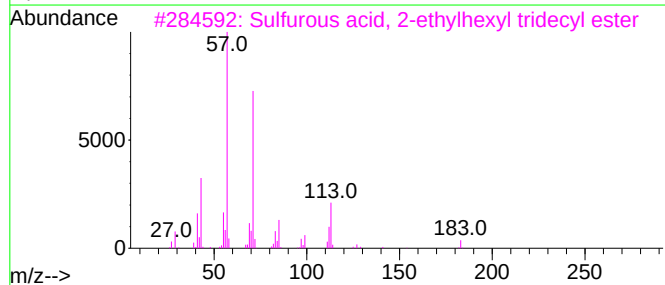
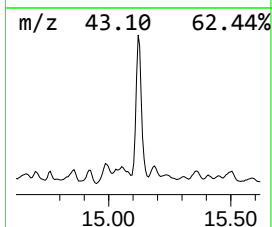
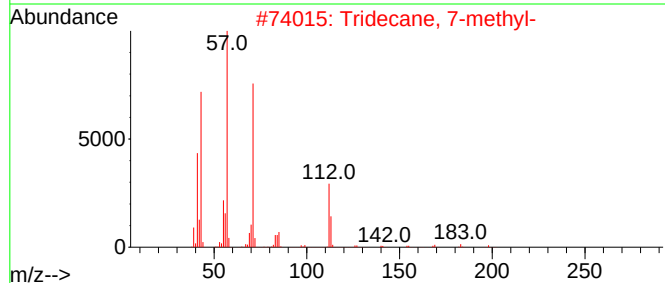
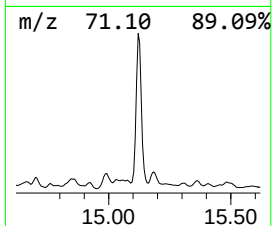
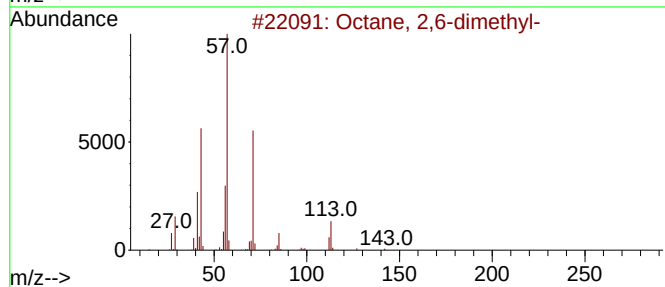
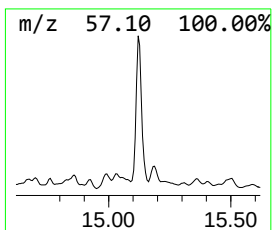
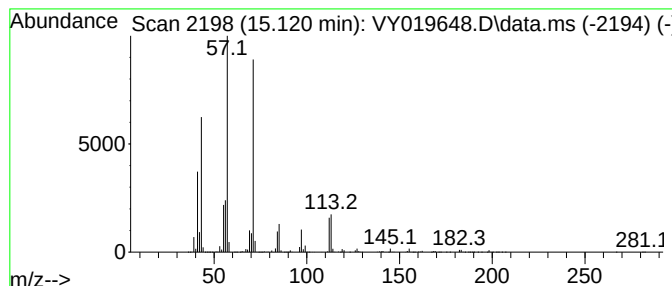
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	454.46 ug/l	12511800	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	86
2			Tridecane, 7-methyl-	198	C14H30	026730-14-3	74
3			Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	72
4			Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	72
5			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092024\
Data File : VY019648.D
Acq On : 20 Sep 2024 16:10
Operator : SY/MD
Sample : P4103-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-22A

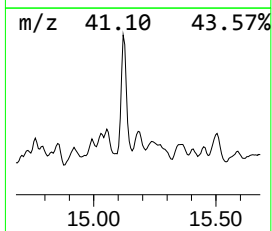
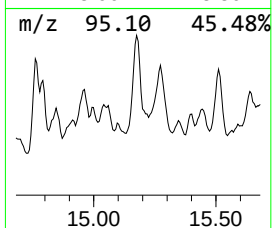
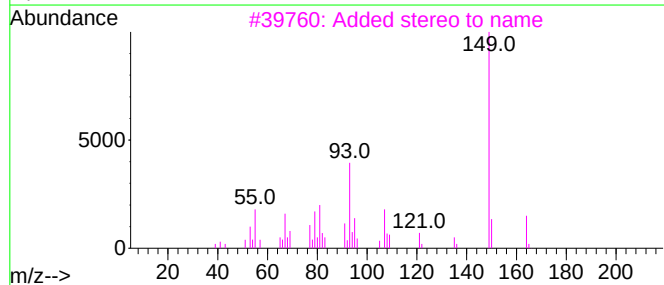
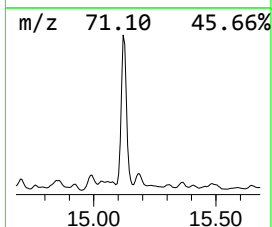
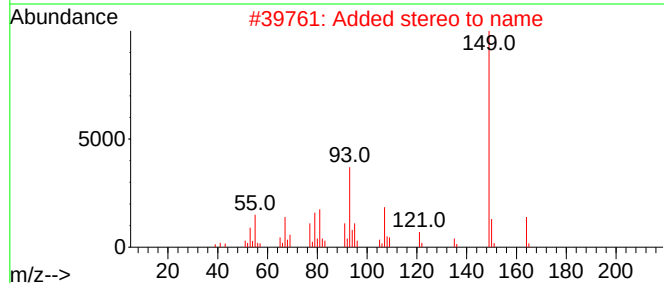
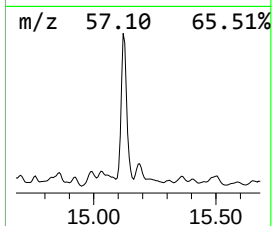
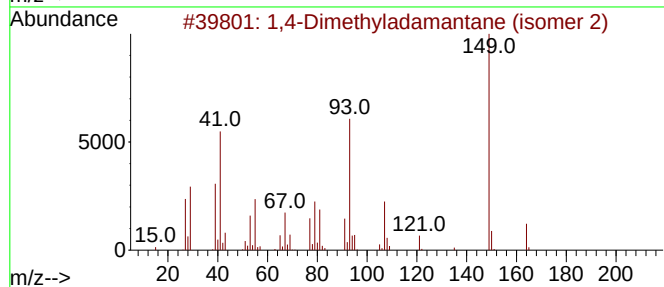
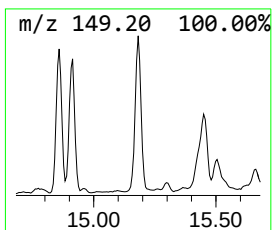
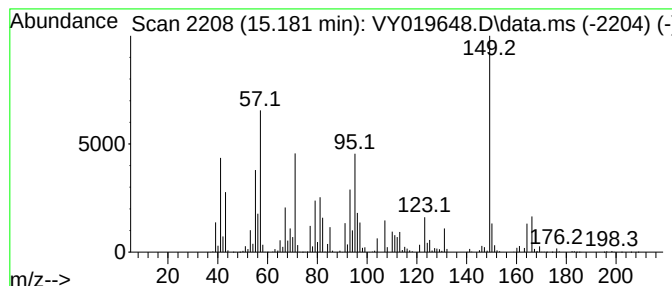
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown15.181 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.181	141.50 ug/l	3895750	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	41
2			Added stereo to name	164	C12H20	024145-89-9	41
3			Added stereo to name	164	C12H20	024145-88-8	41
4			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	41
5			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092024\
Data File : VY019648.D
Acq On : 20 Sep 2024 16:10
Operator : SY/MD
Sample : P4103-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-22A

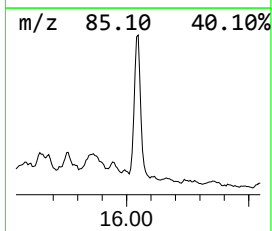
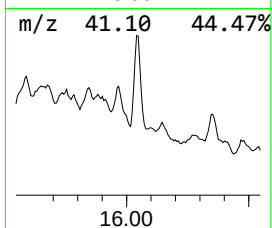
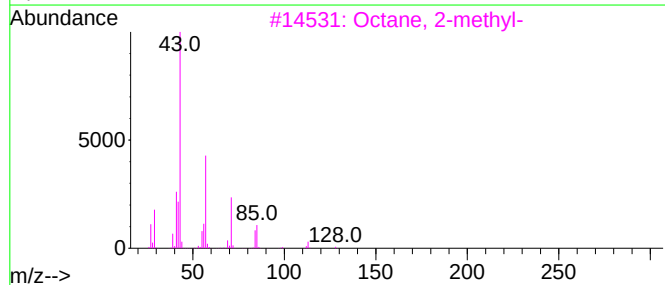
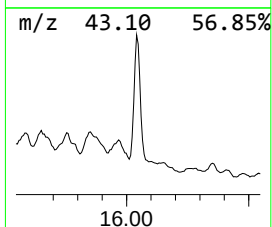
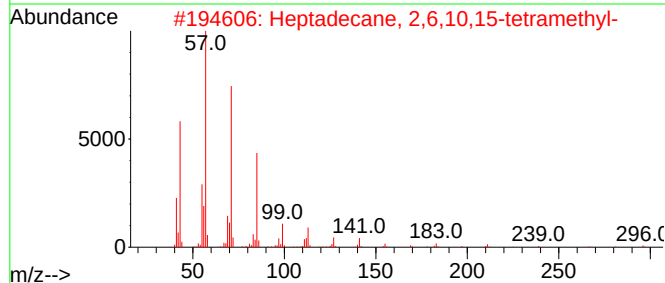
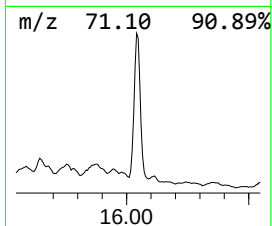
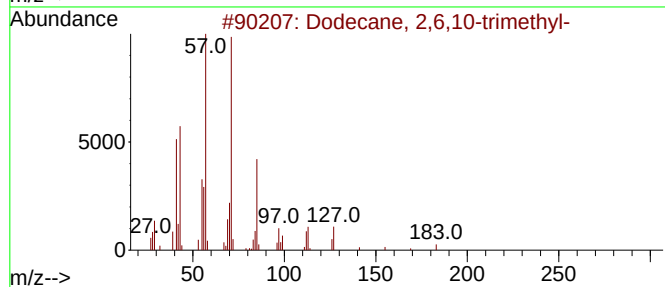
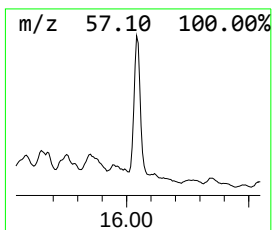
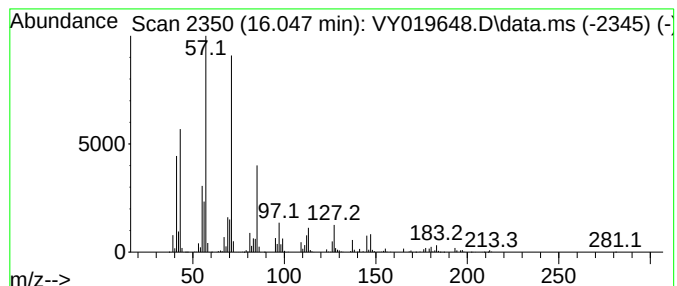
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

Peak Number 10 Dodecane, 2,6,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.047	166.83 ug/l	4593150	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	90
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
3			Octane, 2-methyl-	128	C9H20	003221-61-2	74
4			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	72
5			Decane, 3-methyl-	156	C11H24	013151-34-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY092024\
Data File : VY019648.D
Acq On : 20 Sep 2024 16:10
Operator : SY/MD
Sample : P4103-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-22A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.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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Benzene, 1-(dod...	14.066	135.4	ug/l	3726680	4	13.346	1376560	50.0
Naphthalene, de...	14.176	353.9	ug/l	9743780	4	13.346	1376560	50.0
1-Methyldecahyd...	14.334	165.4	ug/l	4554400	4	13.346	1376560	50.0
unknown14.602	14.602	130.0	ug/l	3578540	4	13.346	1376560	50.0
1,4-Dimethylada...	14.852	135.5	ug/l	3729640	4	13.346	1376560	50.0
unknown14.919	14.919	170.5	ug/l	4694040	4	13.346	1376560	50.0
Octane, 2,6-dim...	15.121	454.5	ug/l	12511800	4	13.346	1376560	50.0
unknown15.181	15.181	141.5	ug/l	3895750	4	13.346	1376560	50.0
Dodecane, 2,6,1...	16.047	166.8	ug/l	4593150	4	13.346	1376560	50.0