

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091124\
 Data File : VY019515.D
 Acq On : 11 Sep 2024 17:39
 Operator : SY/MD
 Sample : P3911-05
 Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SP-3

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: VY019515.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.824	13	17	26	rVB3	34995	64408	1.31%	0.187%
2	2.172	68	74	83	rBV	106525	179753	3.64%	0.522%
3	4.610	463	474	494	rBV6	31232	129999	2.63%	0.377%
4	5.640	630	643	656	rBV3	32321	103004	2.09%	0.299%
5	6.683	807	814	827	rVB3	29563	98965	2.01%	0.287%
6	7.634	959	970	975	rBV	311177	765338	15.51%	2.222%
7	7.701	975	981	991	rVB	513737	1213145	24.59%	3.522%
8	7.914	1007	1016	1025	rBV2	21974	54332	1.10%	0.158%
9	8.067	1031	1041	1053	rBV2	459548	1247305	25.28%	3.621%
10	8.469	1098	1107	1117	rVB	67530	137928	2.80%	0.400%
11	8.609	1119	1130	1145	rBV	842504	1691028	34.27%	4.909%
12	9.103	1200	1211	1218	rBV	99819	222901	4.52%	0.647%
13	9.286	1235	1241	1248	rBV	36761	69942	1.42%	0.203%
14	9.749	1311	1317	1327	rVB2	42873	95865	1.94%	0.278%
15	9.884	1331	1339	1350	rVB2	37946	88642	1.80%	0.257%
16	10.103	1368	1375	1381	rVV	1342800	2336661	47.36%	6.784%
17	10.170	1381	1386	1398	rVV	1003122	1713138	34.72%	4.973%
18	10.298	1398	1407	1414	rVB	116414	207220	4.20%	0.602%
19	11.206	1548	1556	1566	rVB3	48279	98799	2.00%	0.287%
20	11.310	1566	1573	1582	rVB	31168	56655	1.15%	0.164%
21	11.414	1582	1590	1602	rBV	1220558	1995543	40.44%	5.793%
22	11.517	1602	1607	1615	rVB	185777	293301	5.94%	0.851%
23	11.621	1615	1624	1635	rBV	813774	1569248	31.80%	4.556%
24	11.956	1667	1679	1690	rBV	546488	1003715	20.34%	2.914%
25	12.133	1702	1708	1711	rBV5	29694	52410	1.06%	0.152%
26	12.407	1747	1753	1758	rBV	860697	1316608	26.68%	3.822%
27	12.596	1780	1784	1788	rVB	41013	68387	1.39%	0.199%
28	12.657	1788	1794	1797	rBV	165975	270183	5.48%	0.784%
29	12.688	1797	1799	1802	rVV2	91343	121894	2.47%	0.354%
30	12.731	1802	1806	1812	rVB2	262686	413226	8.37%	1.200%
31	12.895	1827	1833	1841	rBV2	82866	171853	3.48%	0.499%
32	13.042	1851	1857	1862	rBV	418780	650065	13.17%	1.887%
33	13.090	1862	1865	1870	rVB3	42031	64592	1.31%	0.188%
34	13.285	1886	1897	1900	rBV6	73702	200455	4.06%	0.582%
35	13.346	1900	1907	1916	rVB2	1076263	2118331	42.93%	6.150%
36	13.426	1916	1920	1921	rBV	79732	97062	1.97%	0.282%

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Integrator: RTE

Smoothing : ON

Sampling : 1

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Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

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Title : SW846 8260

37	13.548	1935	1940	1943	rBV3	117121	174823	3.54%	0.508%
38	13.584	1943	1946	1952	rVB2	93767	141170	2.86%	0.410%
39	13.676	1957	1961	1964	rBV	139673	181219	3.67%	0.526%
40	13.724	1964	1969	1974	rBV	276591	425416	8.62%	1.235%
41	13.791	1977	1980	1985	rVV2	48662	68443	1.39%	0.199%
42	13.889	1992	1996	2002	rVB2	67494	109768	2.22%	0.319%
43	13.999	2009	2014	2018	rBV4	44822	67118	1.36%	0.195%
44	14.163	2037	2041	2051	rVV3	116626	290023	5.88%	0.842%
45	14.255	2053	2056	2060	rVV	51778	80493	1.63%	0.234%
46	14.303	2060	2064	2073	rVB3	49987	124229	2.52%	0.361%
47	14.529	2097	2101	2105	rVB	198065	253843	5.14%	0.737%
48	14.590	2105	2111	2117	rBV2	82589	185120	3.75%	0.537%
49	14.651	2117	2121	2128	rVB4	59033	113726	2.30%	0.330%
50	14.962	2166	2172	2176	rBV5	36775	74544	1.51%	0.216%
51	15.047	2182	2186	2191	rVB3	60684	101056	2.05%	0.293%
52	15.139	2192	2201	2211	rBV	2892670	4934137	100.00%	14.324%
53	15.236	2212	2217	2222	rVB	75288	131735	2.67%	0.382%
54	15.340	2224	2234	2241	rVB	477445	729740	14.79%	2.119%
55	15.444	2243	2251	2255	rBV8	42728	105740	2.14%	0.307%
56	15.626	2277	2281	2289	rVB2	39027	69085	1.40%	0.201%
57	15.773	2300	2305	2309	rBV3	92369	177568	3.60%	0.516%
58	15.858	2314	2319	2322	rVV	71948	112888	2.29%	0.328%
59	15.901	2322	2326	2333	rVV2	144431	259324	5.26%	0.753%
60	15.980	2334	2339	2345	rVB3	103011	189875	3.85%	0.551%
61	16.041	2345	2349	2356	rBV	118188	198483	4.02%	0.576%
62	16.175	2363	2371	2377	rBV	606194	1161501	23.54%	3.372%
63	16.242	2377	2382	2394	rVB	900134	1617766	32.79%	4.697%
64	16.364	2394	2402	2408	rBV	440952	1023834	20.75%	2.972%
65	16.577	2432	2437	2442	rBV5	37760	90643	1.84%	0.263%
66	16.742	2458	2464	2468	rBV3	111494	270467	5.48%	0.785%

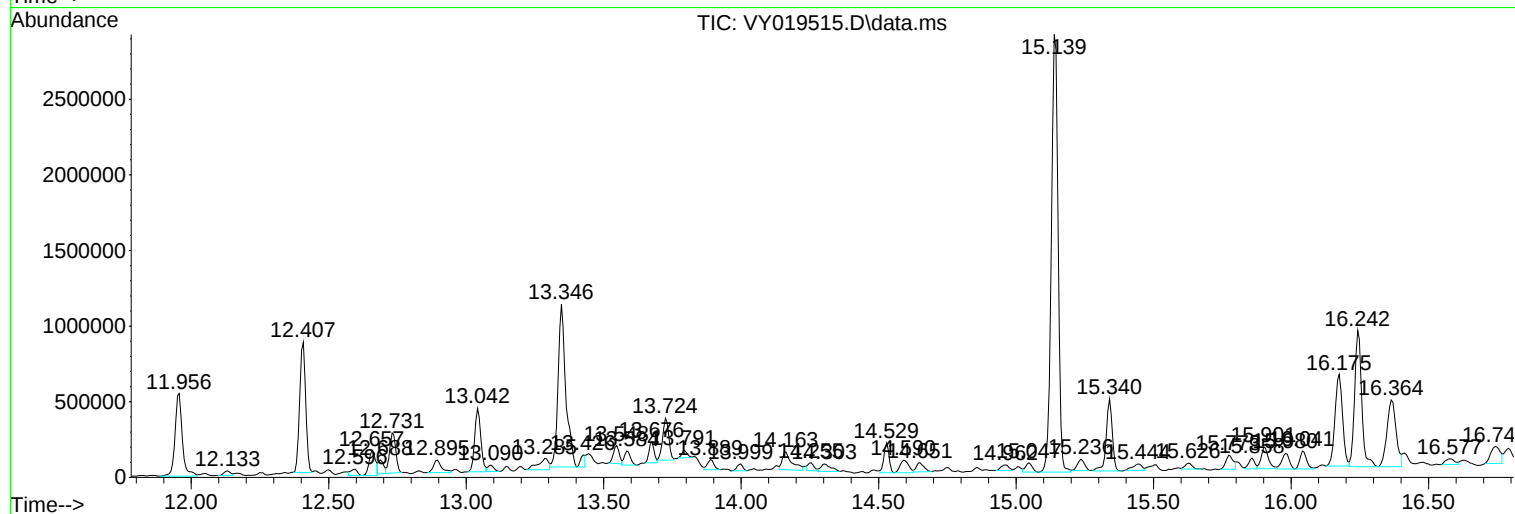
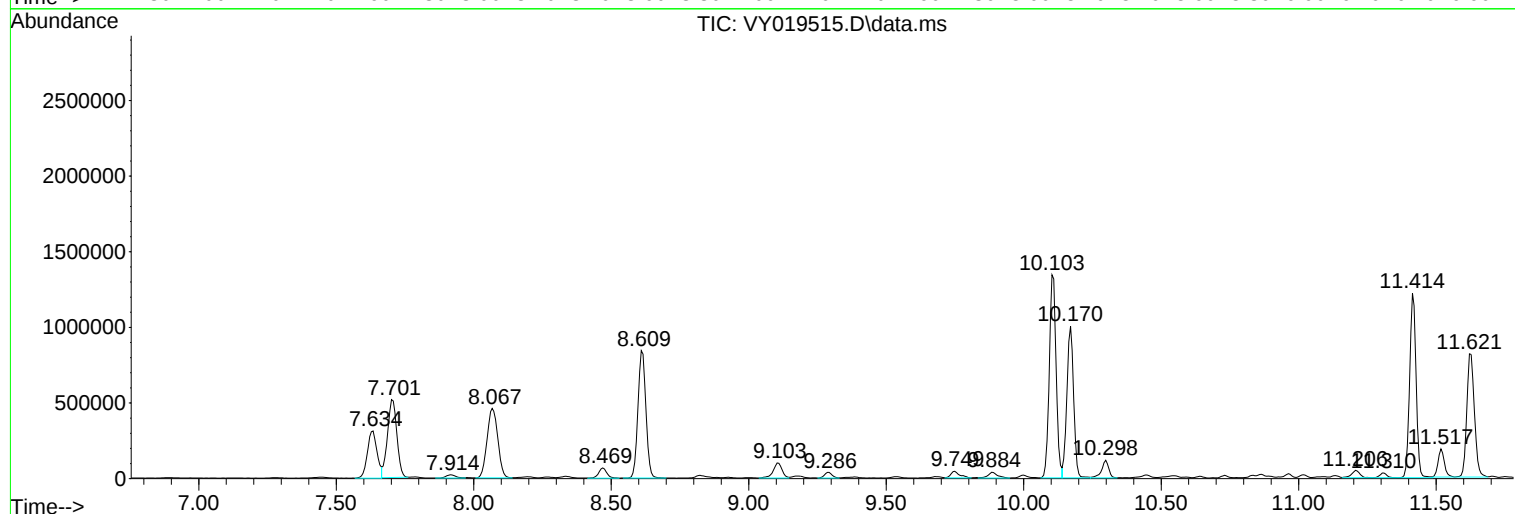
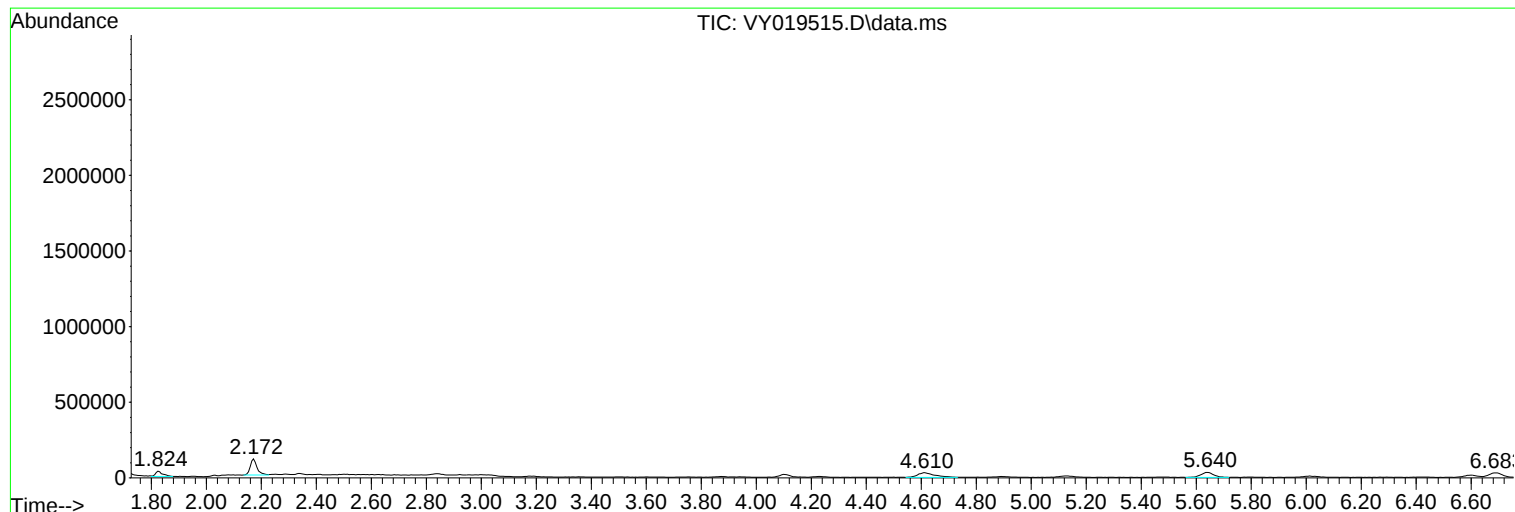
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ClientSampleId :
SP-3

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



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Acq On : 11 Sep 2024 17:39
Operator : SY/MD
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Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SP-3

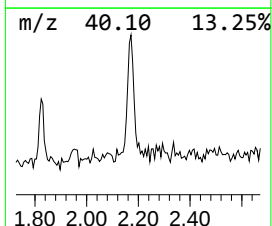
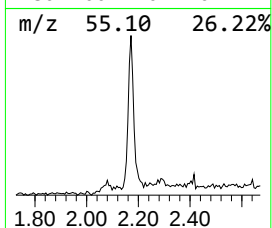
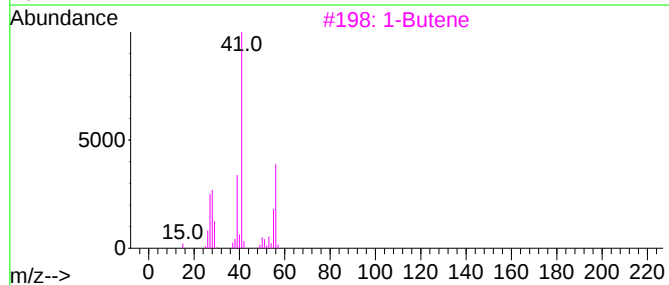
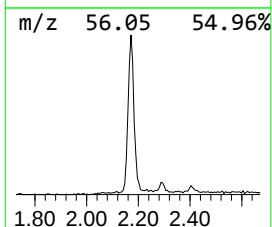
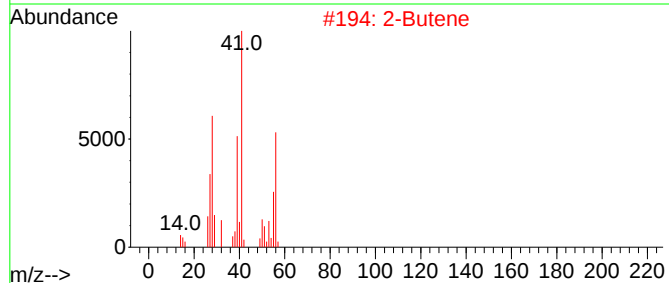
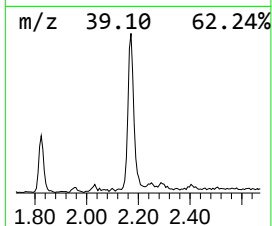
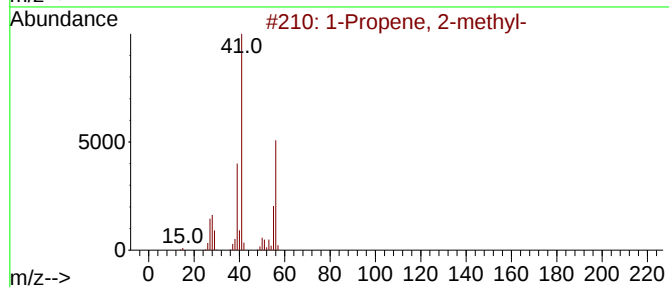
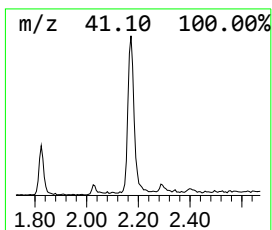
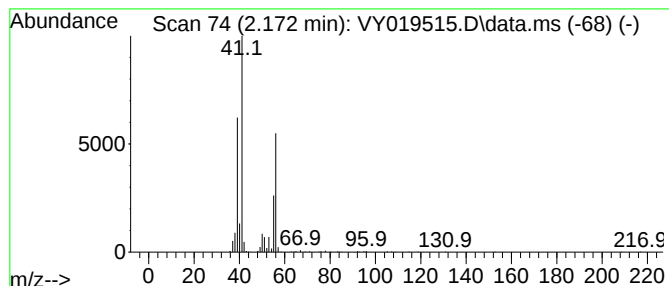
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

Peak Number 1 1-Propene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.172	7.41 ug/l	179753	Pentafluorobenzene	7.707

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-			56	C4H8	000115-11-7	87
2	2-Butene			56	C4H8	000107-01-7	80
3	1-Butene			56	C4H8	000106-98-9	49
4	2-Butene, (Z)-			56	C4H8	000590-18-1	49
5	Cyclobutane			56	C4H8	000287-23-0	43



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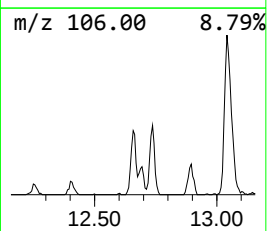
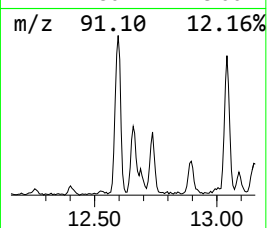
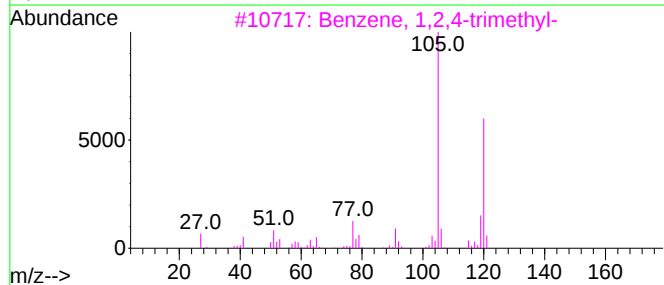
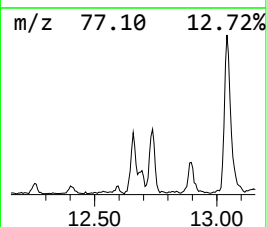
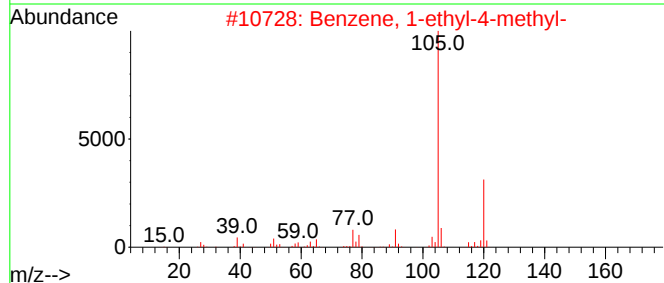
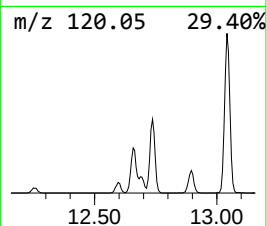
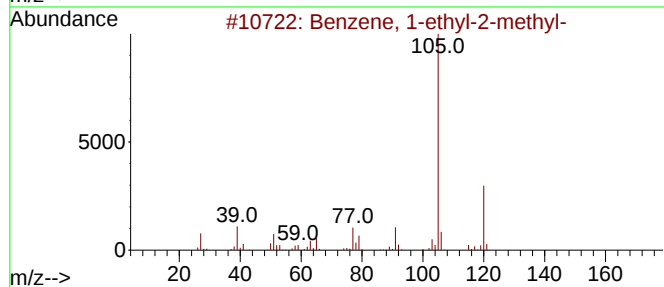
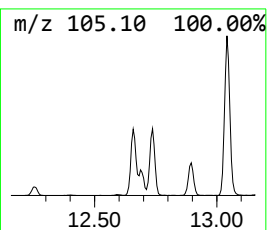
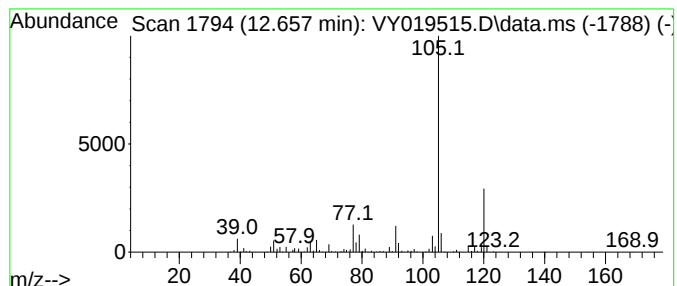
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	6.38 ug/l	270183	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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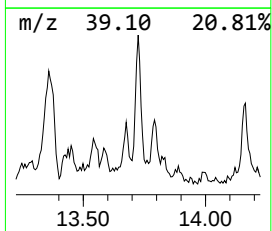
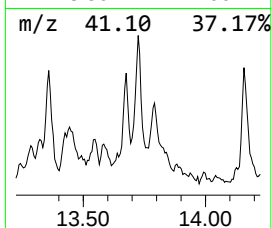
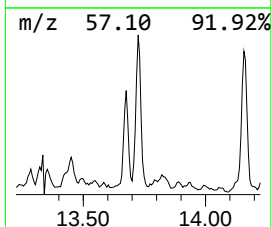
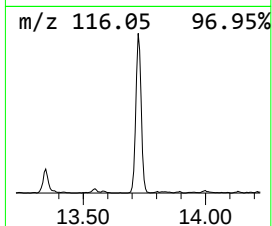
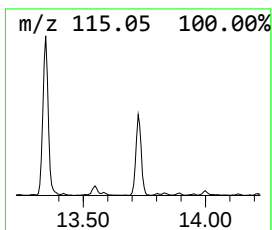
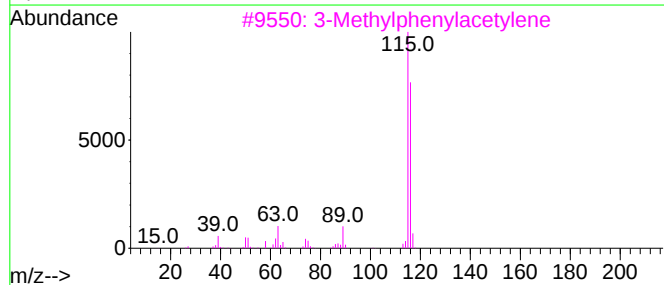
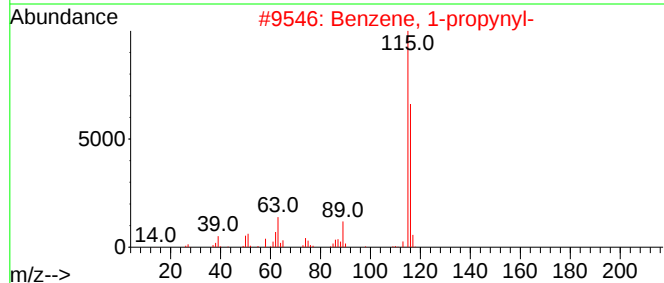
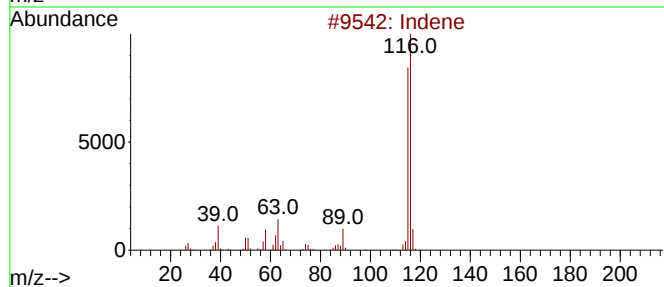
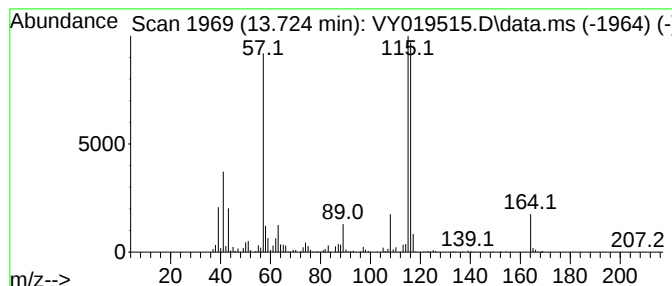
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Quant Title : SW846 8260

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

Peak Number 3 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.724	10.04 ug/l	425416	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	81
3			3-Methylphenylacetylene	116	C9H8	000766-82-5	81
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	74
5			2-Methylphenylacetylene	116	C9H8	000766-47-2	74



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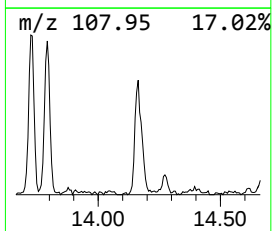
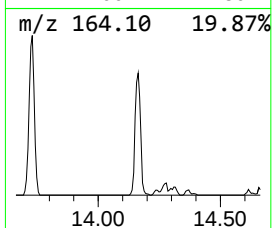
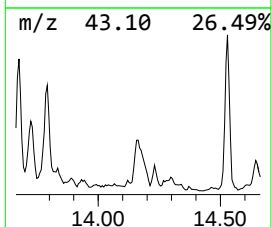
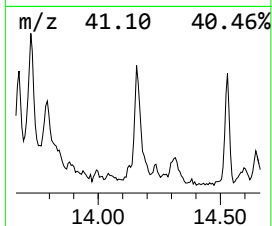
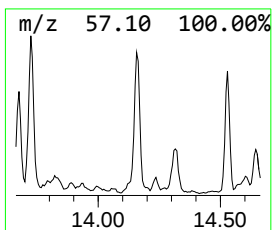
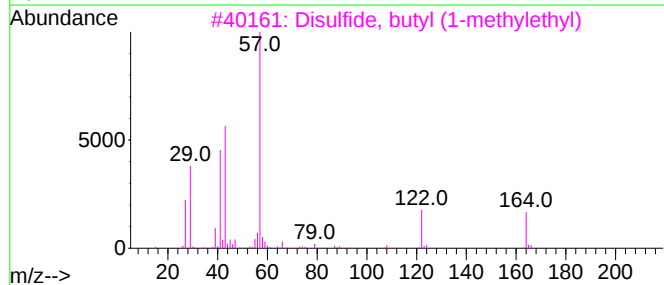
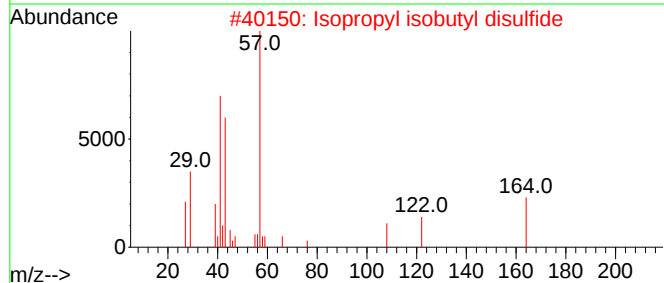
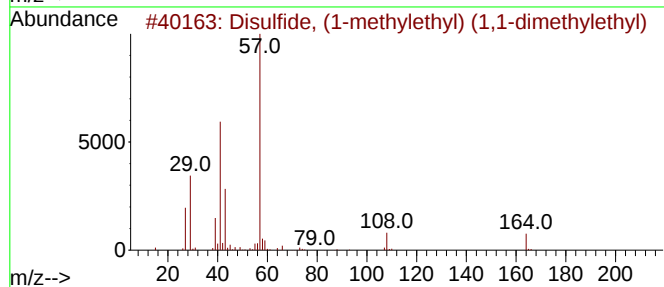
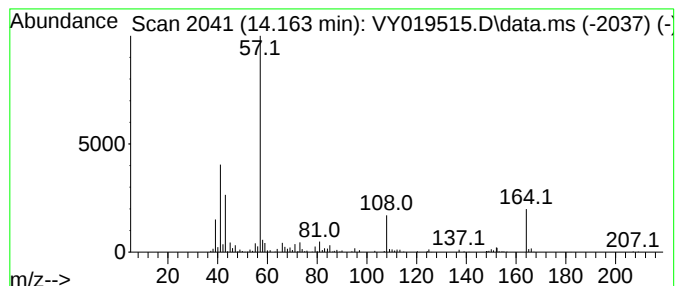
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y090924S.M
Quant Title : SW846 8260

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

Peak Number 4 Disulfide, (1-methylethyl) ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	6.85 ug/l	290023	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	64
2			Isopropyl isobutyl disulfide	164	C7H16S2	067421-82-3	50
3			Disulfide, butyl (1-methylethyl)	164	C7H16S2	072437-53-7	38
4			t-Butylthiothioacetic acid, S-t-...	220	C10H20OS2	1000189-14-7	36
5			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091124\
Data File : VY019515.D
Acq On : 11 Sep 2024 17:39
Operator : SY/MD
Sample : P3911-05
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SP-3

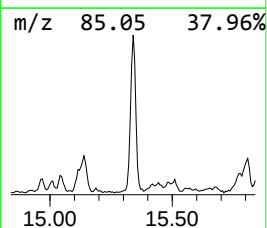
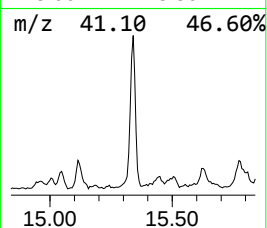
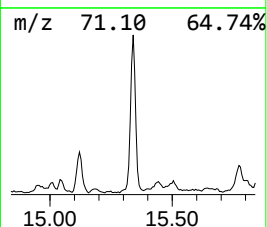
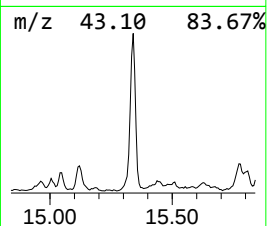
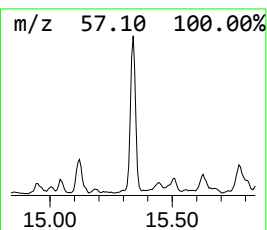
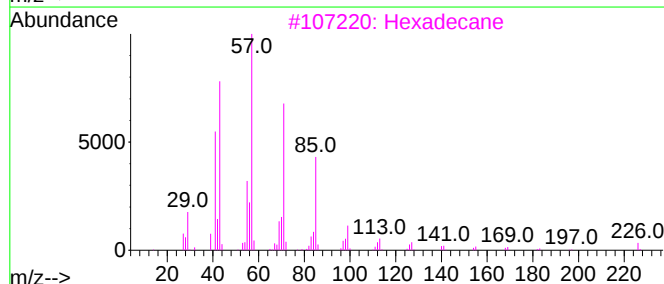
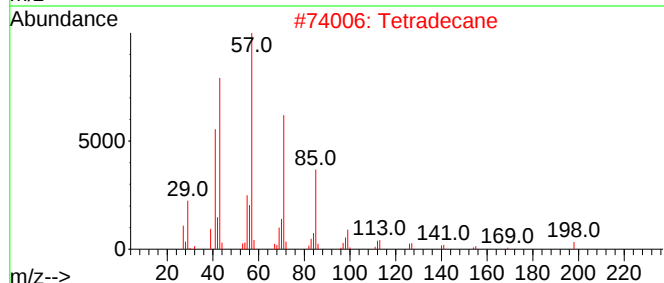
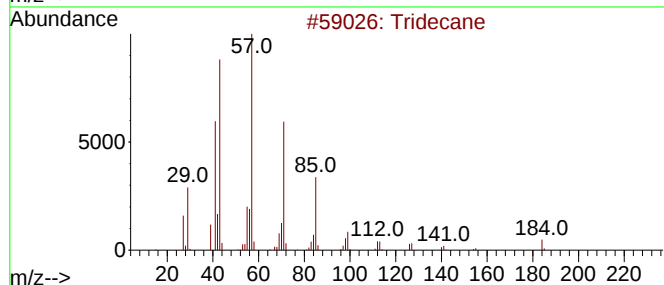
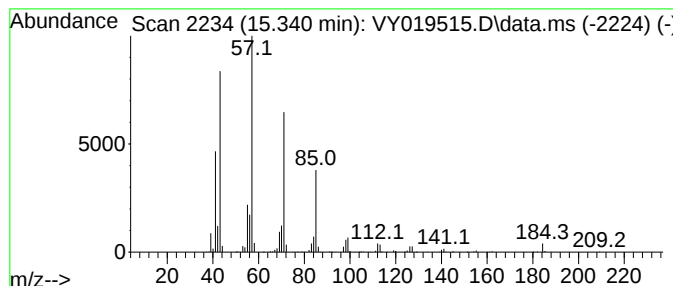
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Quant Title : SW846 8260

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

Peak Number 5 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.340	17.22 ug/l	729740	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	95
2			Tetradecane	198	C14H30	000629-59-4	91
3			Hexadecane	226	C16H34	000544-76-3	91
4			Dodecane	170	C12H26	000112-40-3	86
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091124\
Data File : VY019515.D
Acq On : 11 Sep 2024 17:39
Operator : SY/MD
Sample : P3911-05
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SP-3

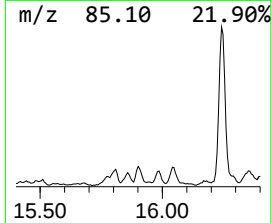
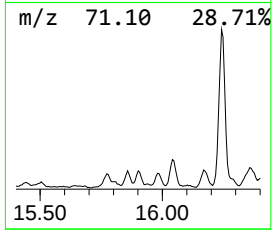
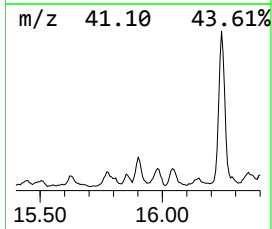
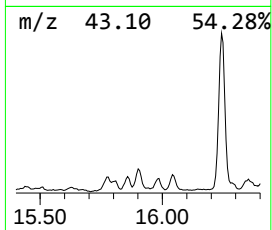
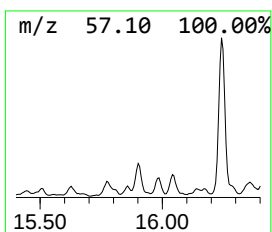
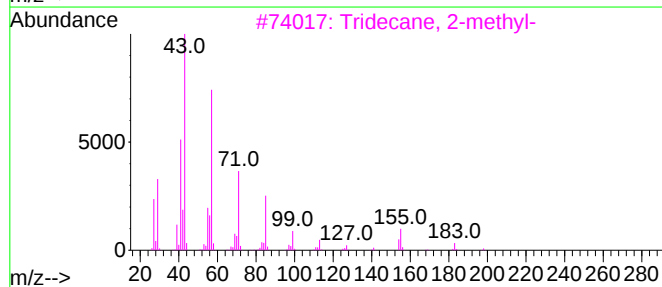
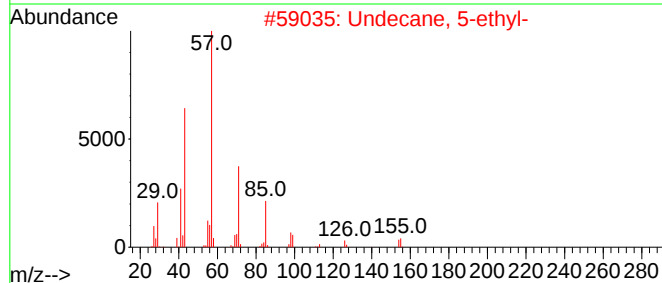
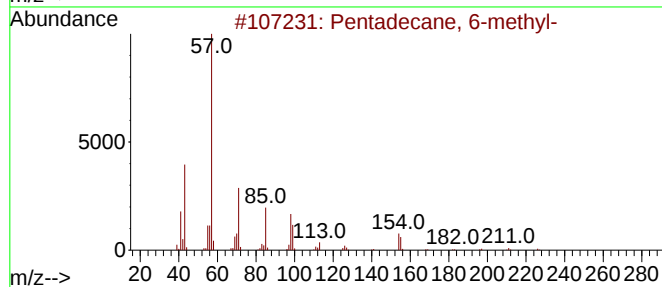
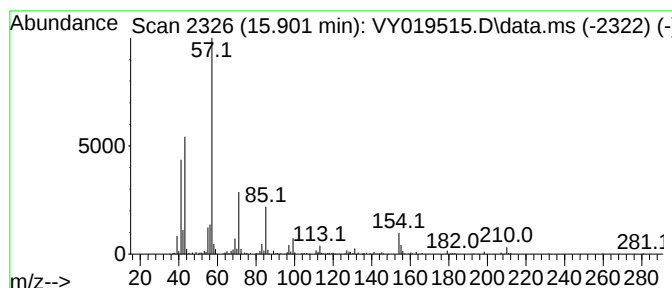
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Quant Title : SW846 8260

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

Peak Number 6 Pentadecane, 6-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.901	6.12 ug/l	259324	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 6-methyl-	226	C16H34	010105-38-1	64
2			Undecane, 5-ethyl-	184	C13H28	017453-94-0	64
3			Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
4			Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	52
5			Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091124\
Data File : VY019515.D
Acq On : 11 Sep 2024 17:39
Operator : SY/MD
Sample : P3911-05
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SP-3

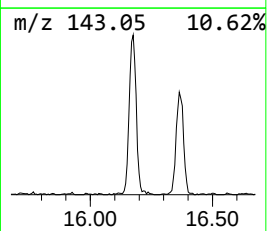
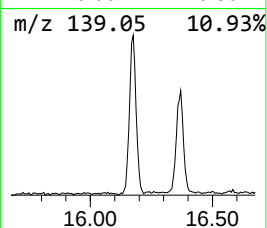
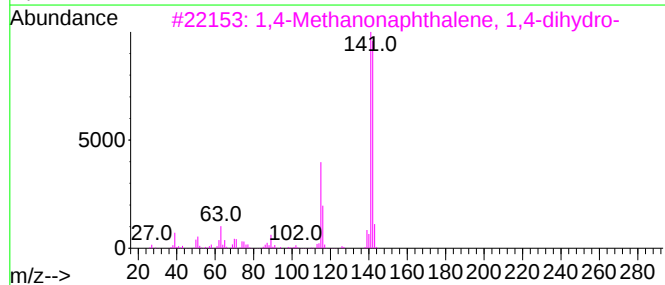
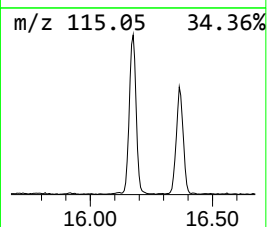
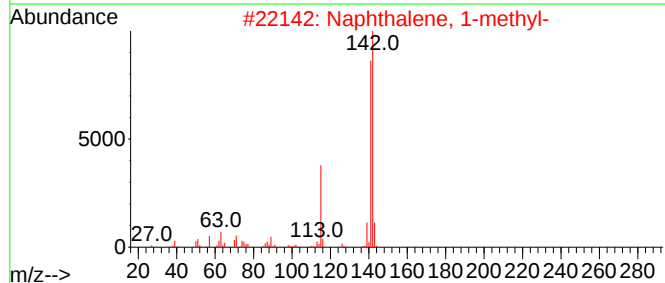
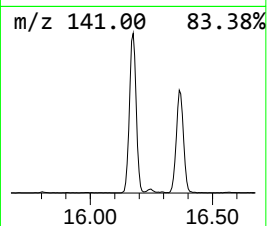
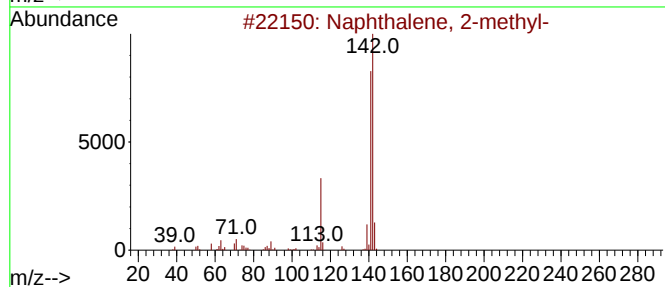
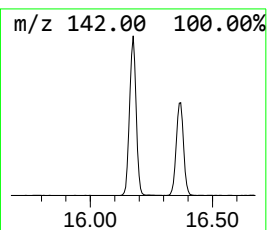
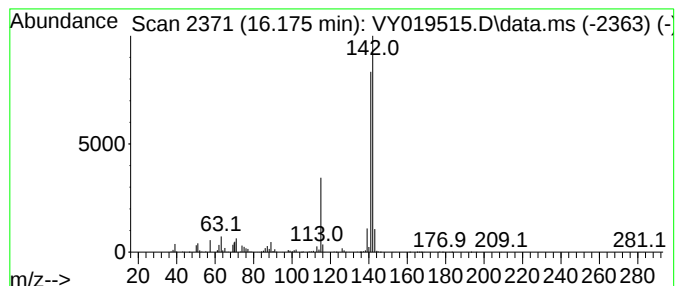
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.175	27.42 ug/l	1161500	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091124\
Data File : VY019515.D
Acq On : 11 Sep 2024 17:39
Operator : SY/MD
Sample : P3911-05
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
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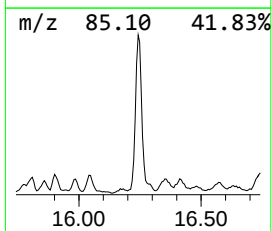
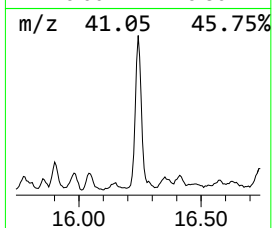
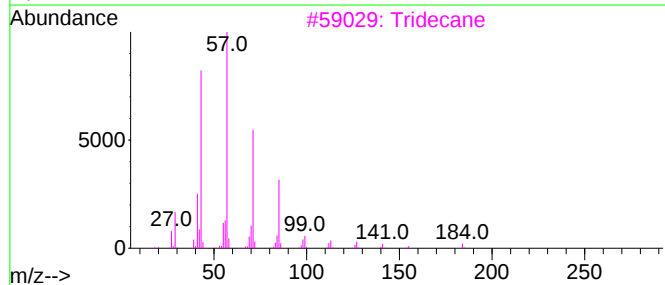
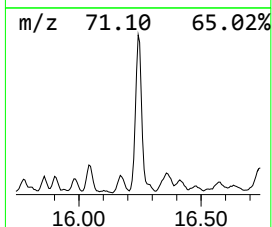
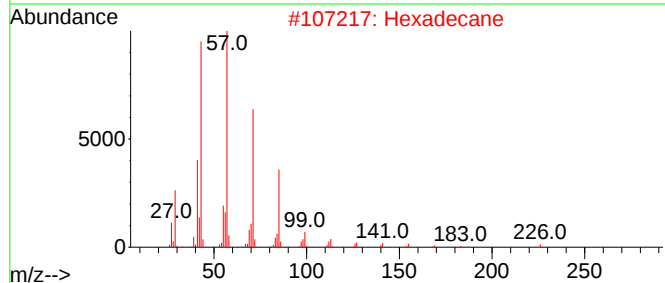
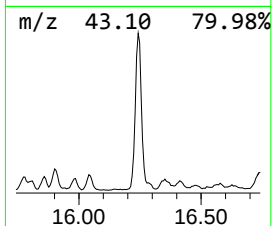
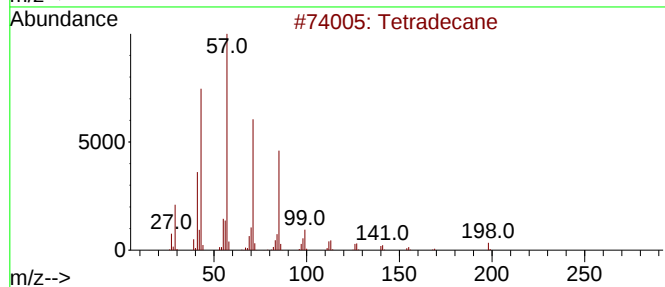
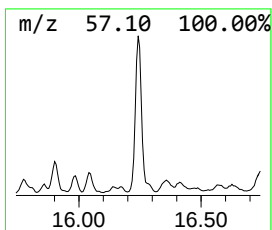
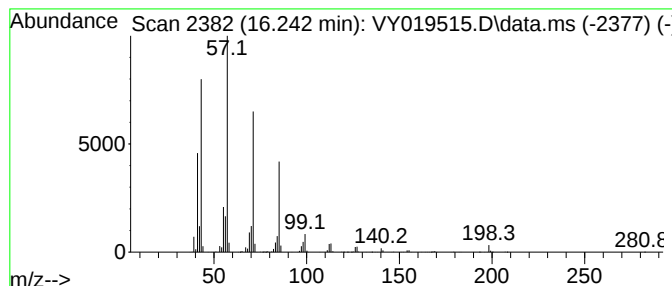
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Quant Title : SW846 8260

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

Peak Number 8 Tetradecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.242	38.18 ug/l	1617770	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	97
2			Hexadecane	226	C16H34	000544-76-3	90
3			Tridecane	184	C13H28	000629-50-5	90
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091124\
Data File : VY019515.D
Acq On : 11 Sep 2024 17:39
Operator : SY/MD
Sample : P3911-05
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SP-3

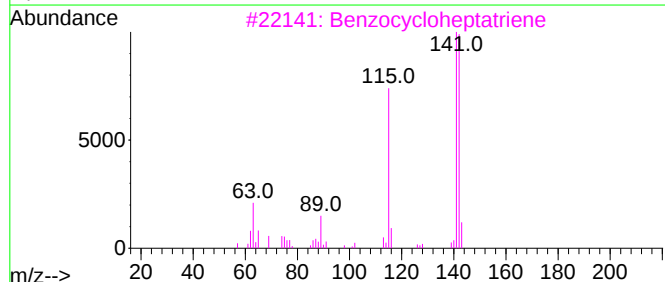
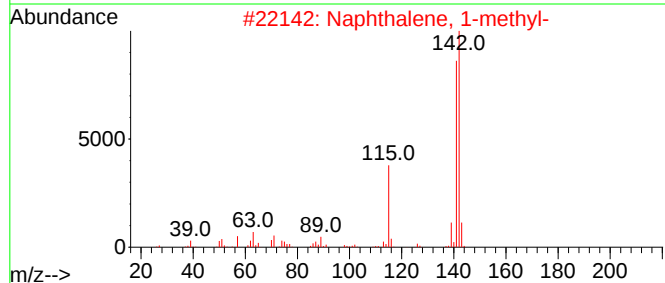
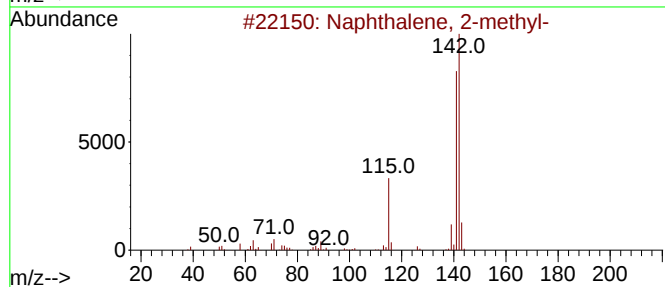
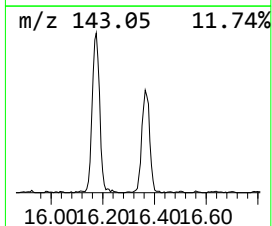
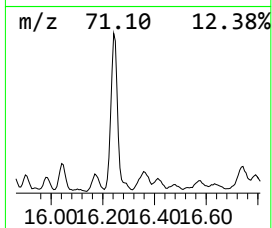
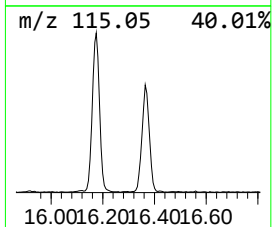
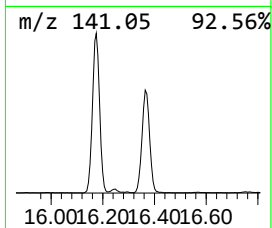
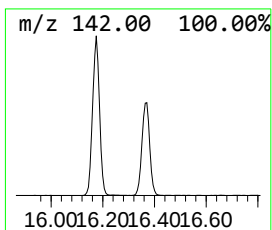
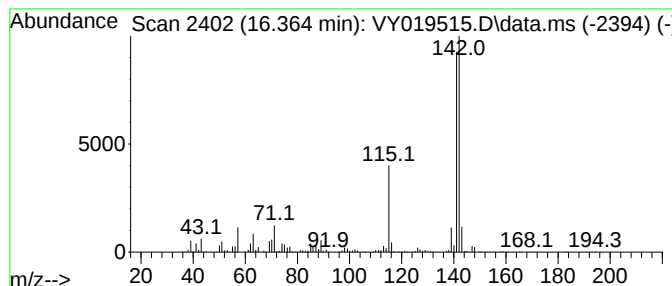
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.364	24.17 ug/l	1023830	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	93
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091124\
Data File : VY019515.D
Acq On : 11 Sep 2024 17:39
Operator : SY/MD
Sample : P3911-05
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SP-3

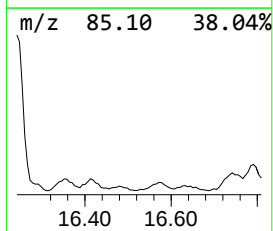
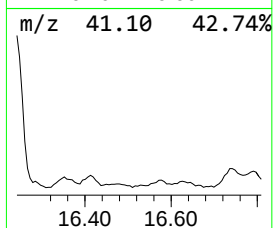
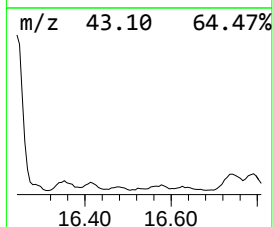
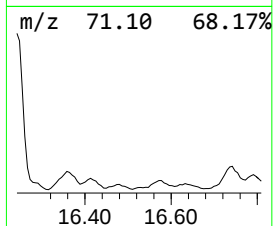
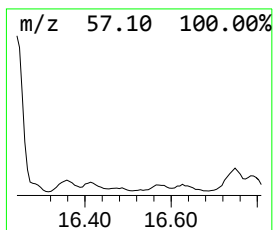
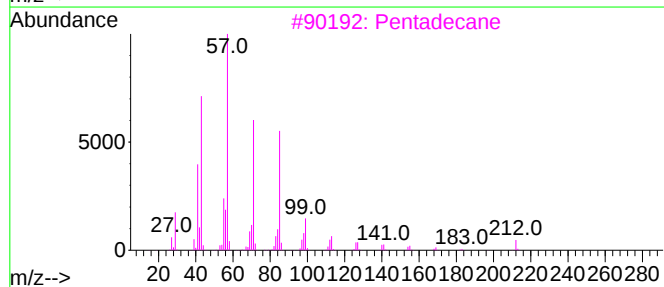
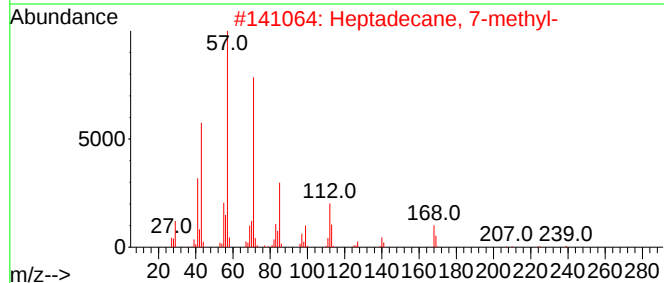
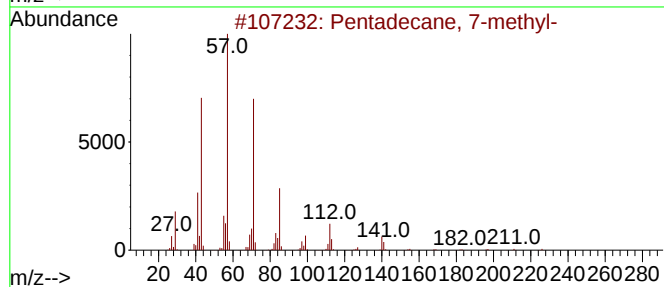
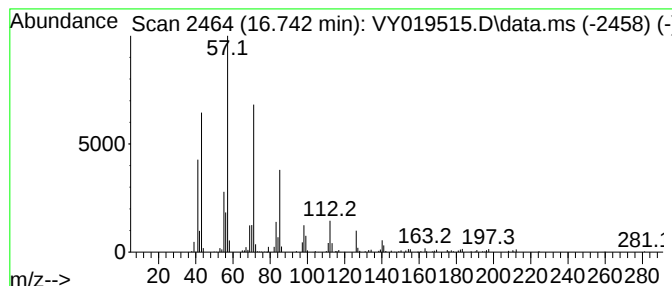
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Quant Title : SW846 8260

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

Peak Number 10 Pentadecane, 7-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.742	6.38 ug/l	270467	1,4-Dichlorobenzene-d4	13.346

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 7-methyl-	226	C16H34	006165-40-8	80
2		Heptadecane, 7-methyl-	254	C18H38	020959-33-5	64
3		Pentadecane	212	C15H32	000629-62-9	60
4		Dodecane	170	C12H26	000112-40-3	59
5		1-Decene, 4-methyl-	154	C11H22	013151-29-6	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY091124\
Data File : VY019515.D
Acq On : 11 Sep 2024 17:39
Operator : SY/MD
Sample : P3911-05
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SP-3

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-ethy...	12.657	6.4	ug/l	270183	4	13.346	2118330	50.0
Indene	13.724	10.0	ug/l	425416	4	13.346	2118330	50.0
Disulfide, (1-m...	14.163	6.8	ug/l	290023	4	13.346	2118330	50.0
Tridecane	15.340	17.2	ug/l	729740	4	13.346	2118330	50.0
Pentadecane, 6-...	15.901	6.1	ug/l	259324	4	13.346	2118330	50.0
Naphthalene, 2-...	16.175	27.4	ug/l	1161500	4	13.346	2118330	50.0
Tetradecane	16.242	38.2	ug/l	1617770	4	13.346	2118330	50.0
Naphthalene, 1-...	16.364	24.2	ug/l	1023830	4	13.346	2118330	50.0
Pentadecane, 7-...	16.742	6.4	ug/l	270467	4	13.346	2118330	50.0