

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
 Data File : VN078181.D
 Acq On : 13 Jun 2023 13:12
 Operator : JC\MD
 Sample : 03170-03
 Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1971

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_N\methods\82N060623W.M
 Title : SW846 8260

Signal : TIC: VN078181.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.442	411	423	444	rBV	2671032	8623858	48.75%	11.872%
2	8.171	1043	1057	1061	rBV	461006	1116649	6.31%	1.537%
3	8.224	1061	1066	1077	rVV2	1099676	2563678	14.49%	3.529%
4	8.330	1077	1084	1093	rVB3	107071	256924	1.45%	0.354%
5	8.447	1093	1104	1114	rBV	452002	1017384	5.75%	1.401%
6	8.582	1119	1127	1139	rVB	446151	1002725	5.67%	1.380%
7	8.971	1184	1193	1206	rVB	500769	976358	5.52%	1.344%
8	9.106	1206	1216	1228	rBV	1097566	2268089	12.82%	3.122%
9	10.571	1456	1465	1470	rBV	1599865	2994257	16.93%	4.122%
10	10.635	1470	1476	1490	rVV	9696275	17690638	100.00%	24.354%
11	11.870	1678	1686	1697	rBV	1549803	2769820	15.66%	3.813%
12	11.970	1697	1703	1708	rVV	195803	364188	2.06%	0.501%
13	12.076	1712	1721	1731	rVV2	866576	1852441	10.47%	2.550%
14	12.400	1765	1776	1785	rBV2	348878	854143	4.83%	1.176%
15	12.600	1796	1810	1812	rBV6	91402	302533	1.71%	0.416%
16	12.770	1832	1839	1842	rVV3	101163	246734	1.39%	0.340%
17	12.853	1847	1853	1862	rVB	1286504	2271332	12.84%	3.127%
18	13.041	1878	1885	1890	rBV	202912	412231	2.33%	0.567%
19	13.100	1890	1895	1899	rVV	570902	1027330	5.81%	1.414%
20	13.165	1899	1906	1914	rVB4	679612	1733415	9.80%	2.386%
21	13.341	1928	1936	1942	rBV	233507	488573	2.76%	0.673%
22	13.400	1942	1946	1953	rVV5	121601	224511	1.27%	0.309%
23	13.488	1954	1961	1973	rVB	943985	1639019	9.26%	2.256%
24	13.676	1987	1993	1998	rBV3	245455	452628	2.56%	0.623%
25	13.723	1998	2001	2008	rVV4	108091	223982	1.27%	0.308%
26	13.794	2008	2013	2022	rVV2	1515196	3038554	17.18%	4.183%
27	13.876	2022	2027	2033	rVB4	148068	318659	1.80%	0.439%
28	13.953	2033	2040	2042	rBV5	118805	206513	1.17%	0.284%
29	13.988	2042	2046	2049	rVV2	364350	638286	3.61%	0.879%
30	14.029	2050	2053	2062	rVV3	338150	734579	4.15%	1.011%
31	14.112	2062	2067	2073	rVV	573954	925591	5.23%	1.274%
32	14.188	2077	2080	2084	rVV	113490	178505	1.01%	0.246%
33	14.247	2086	2090	2093	rVV	202316	366128	2.07%	0.504%
34	14.276	2093	2095	2100	rVV	236161	333410	1.88%	0.459%
35	14.335	2100	2105	2113	rVB	369105	592487	3.35%	0.816%
36	14.447	2118	2124	2129	rVB3	267750	452820	2.56%	0.623%

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37	14.582	2140	2147	2151	rBV2	146501	277161	1.57%	0.382%
38	14.635	2151	2156	2157	rVV2	231429	343252	1.94%	0.473%
39	14.659	2158	2160	2163	rVV2	322938	446745	2.53%	0.615%
40	14.700	2163	2167	2171	rVV	403638	664138	3.75%	0.914%
41	14.770	2175	2179	2188	rVB	685846	1252129	7.08%	1.724%
42	14.882	2194	2198	2202	rVB2	138810	197603	1.12%	0.272%
43	14.964	2202	2212	2218	rVB7	361999	1050227	5.94%	1.446%
44	15.041	2218	2225	2227	rBV3	423996	830152	4.69%	1.143%
45	15.106	2233	2236	2246	rVB4	175309	329876	1.86%	0.454%
46	15.217	2249	2255	2261	rBV	386516	690653	3.90%	0.951%
47	15.323	2268	2273	2278	rBV3	199350	404635	2.29%	0.557%
48	15.441	2287	2293	2300	rVB4	199413	497959	2.81%	0.686%
49	15.706	2333	2338	2342	rBV	124415	192712	1.09%	0.265%
50	15.753	2342	2346	2351	rBV3	154944	280015	1.58%	0.385%
51	15.841	2357	2361	2371	rVB6	225297	533759	3.02%	0.735%
52	15.953	2371	2380	2387	rBV4	167089	418051	2.36%	0.576%
53	16.170	2413	2417	2425	rVB2	303917	608502	3.44%	0.838%
54	16.488	2462	2471	2484	rBV	806871	2076001	11.74%	2.858%
55	16.717	2503	2510	2517	rBV2	171446	388265	2.19%	0.534%

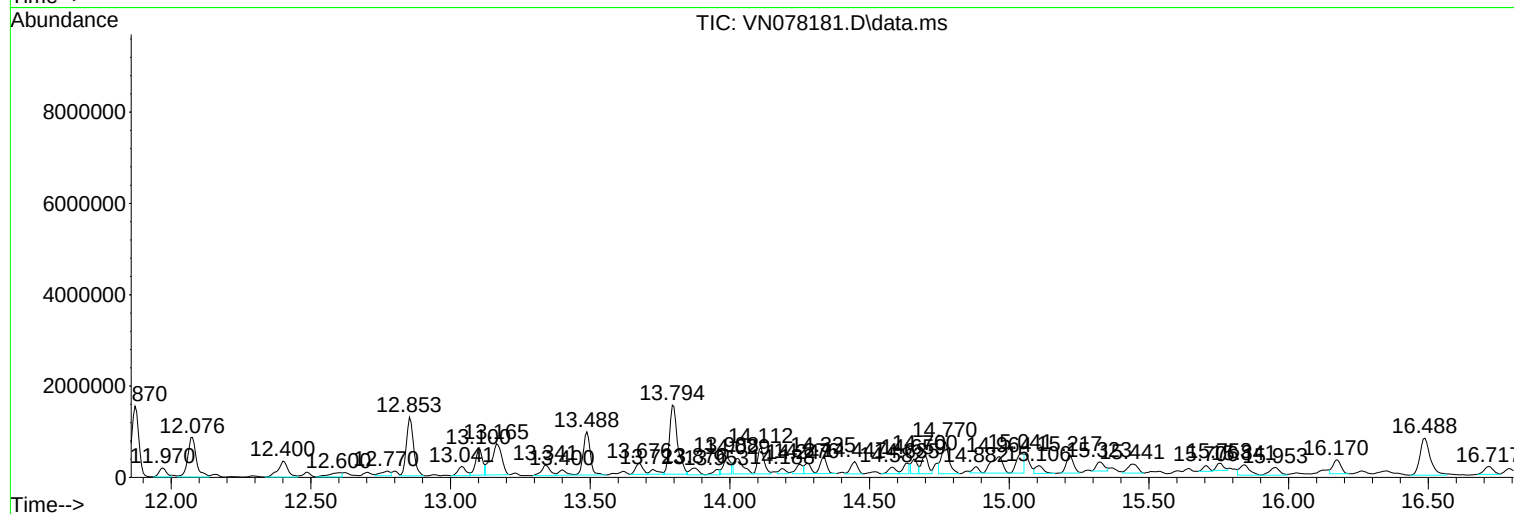
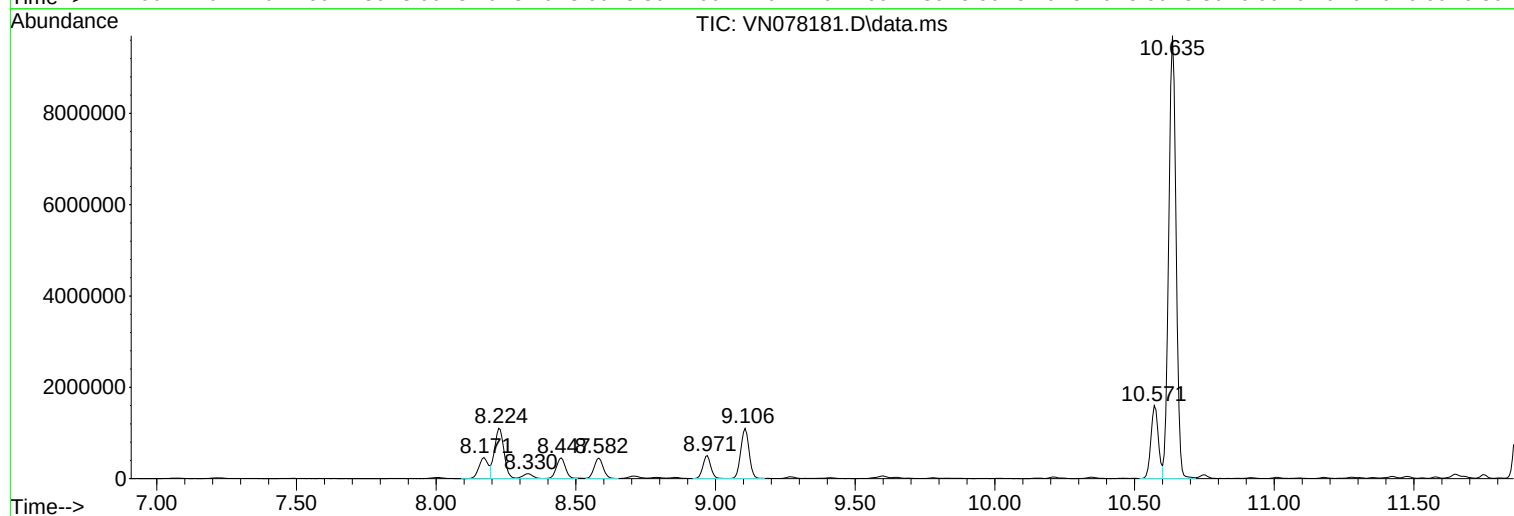
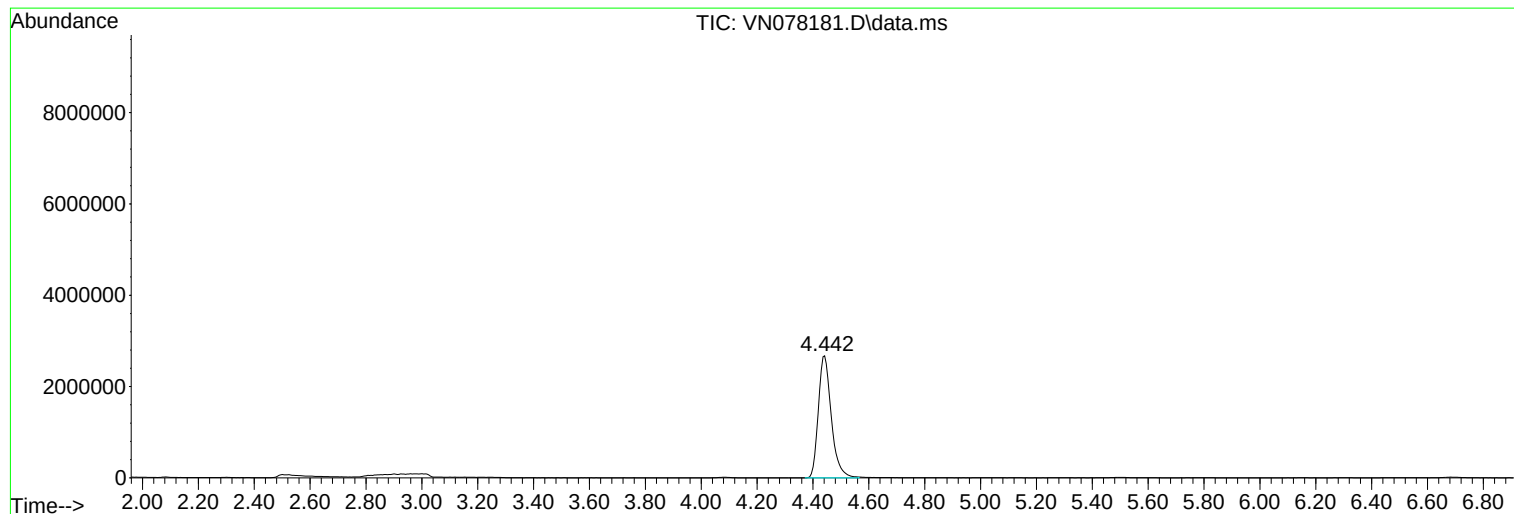
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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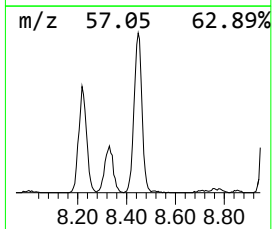
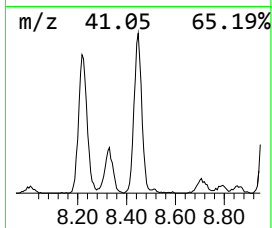
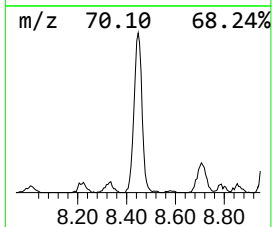
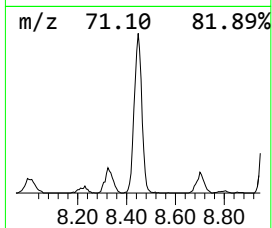
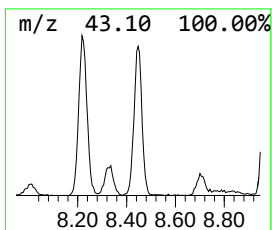
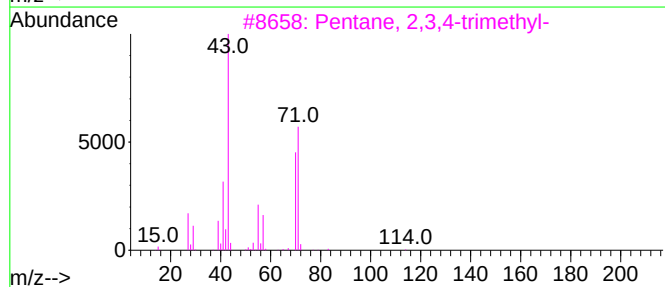
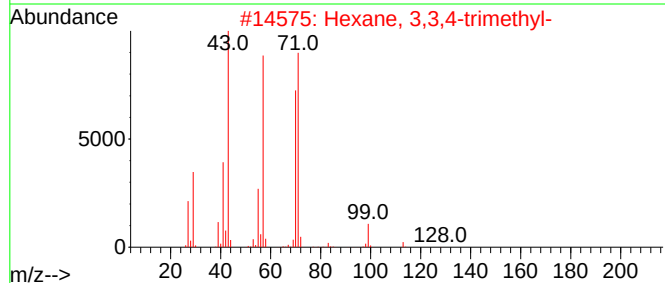
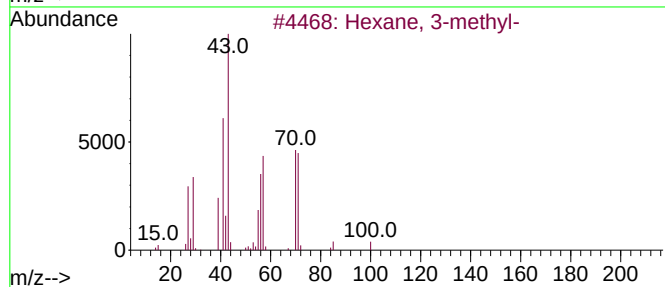
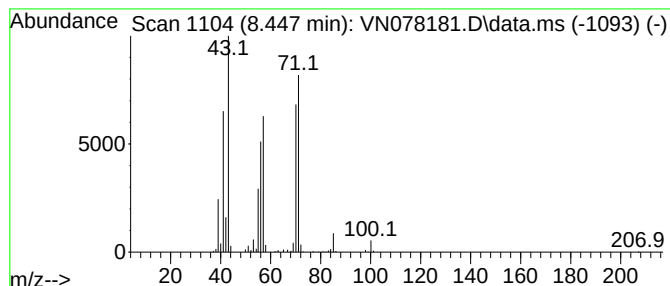
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Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.447	19.84 ug/l	1017380	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	59
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
4			Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	59
5			3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	53



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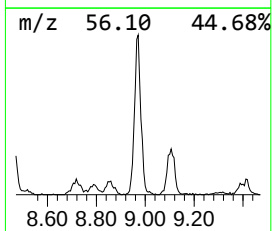
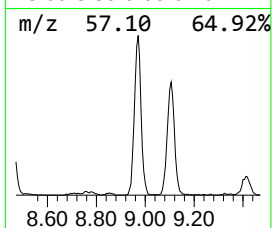
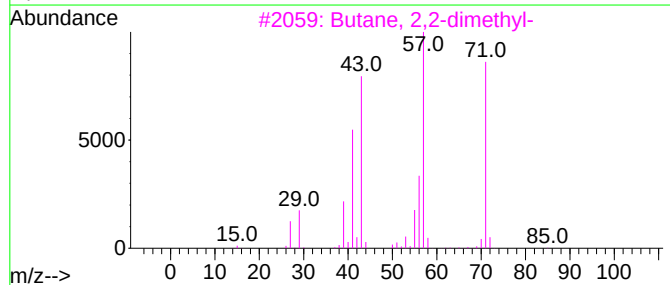
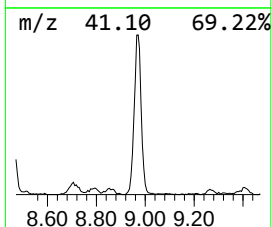
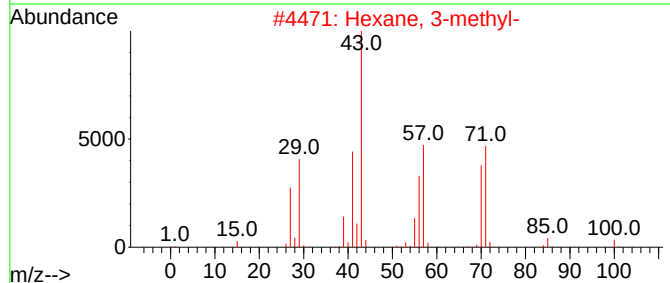
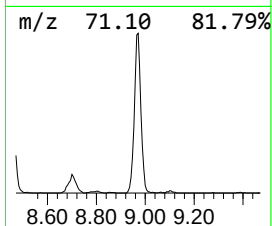
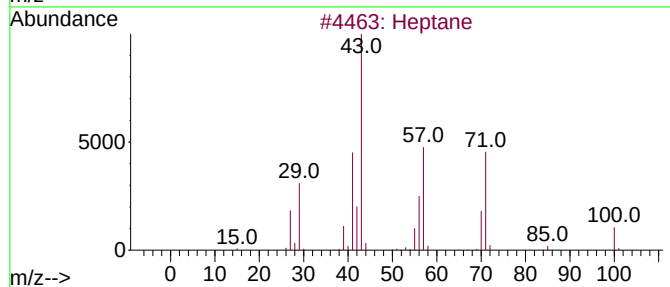
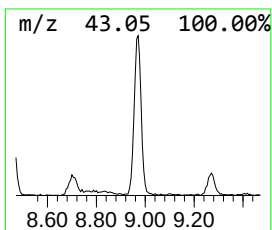
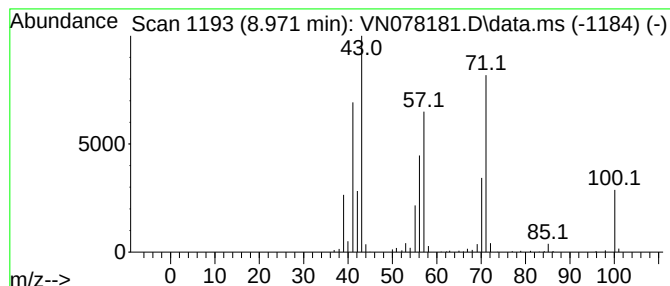
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.971	21.52 ug/l	976358	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	59
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
4			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38
5			3-Hexanone	100	C6H12O	000589-38-8	35



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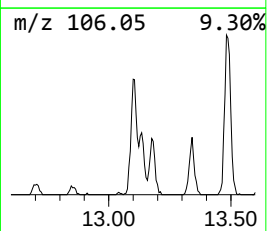
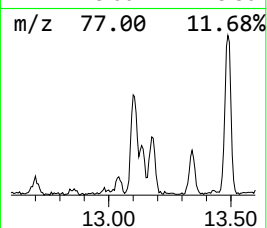
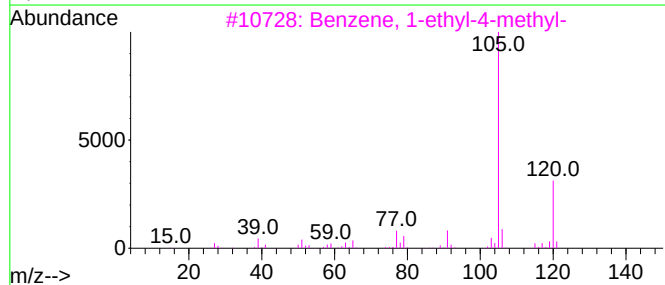
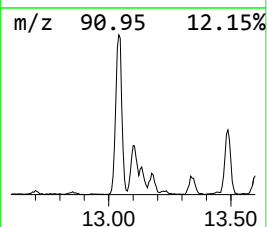
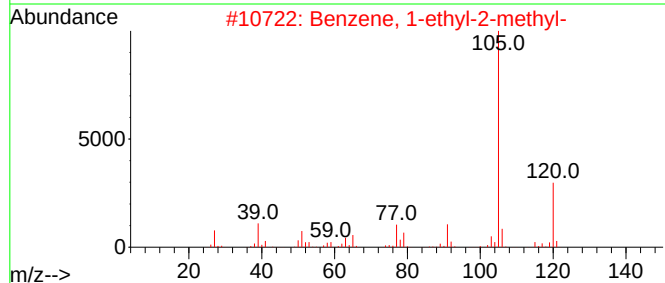
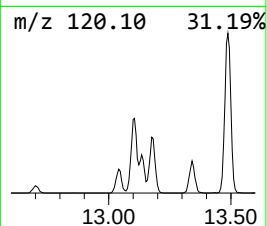
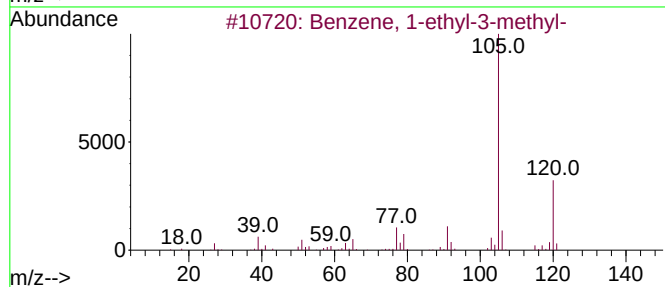
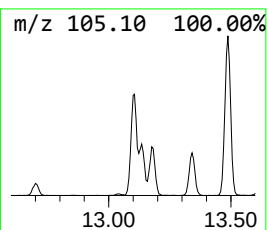
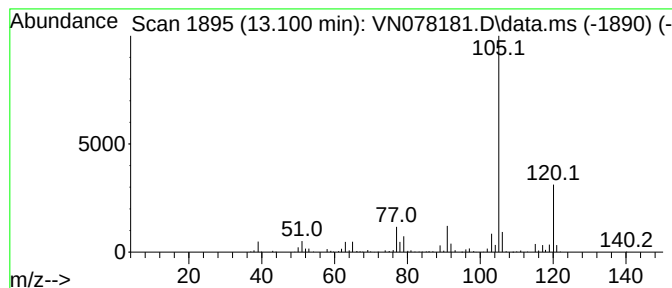
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	16.90 ug/l	1027330	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	90



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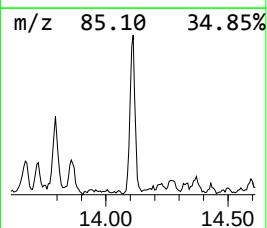
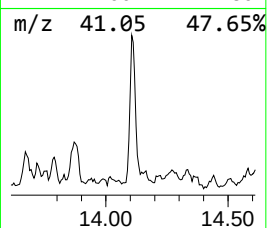
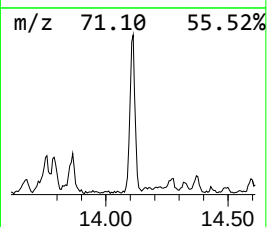
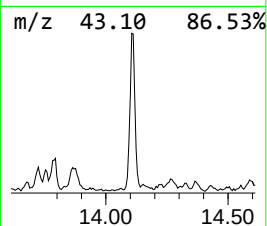
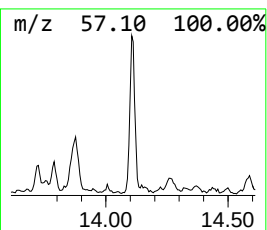
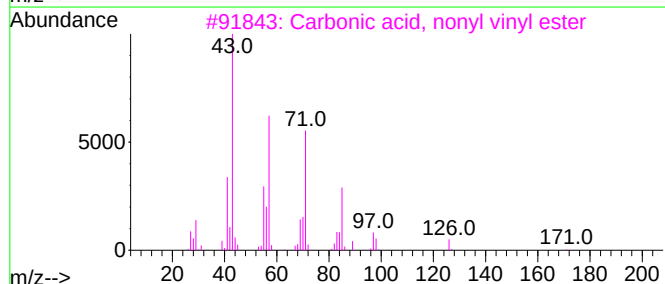
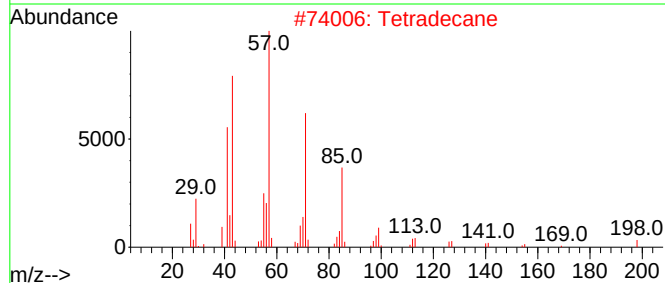
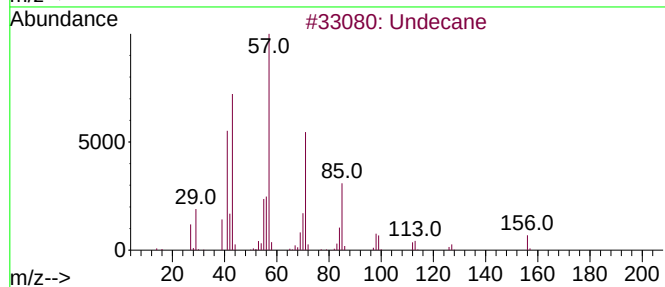
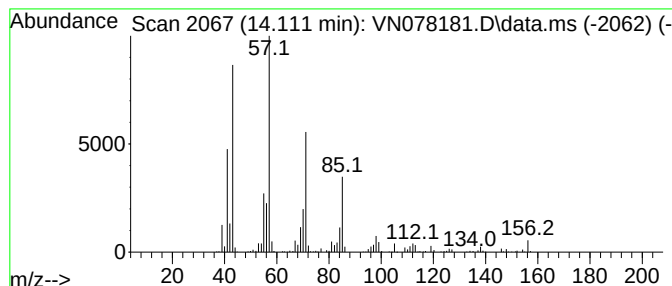
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Quant Title : SW846 8260

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

Peak Number 4 Undecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.111	15.23 ug/l	925591	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	90
2			Tetradecane	198	C14H30	000629-59-4	72
3			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	59
4			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	59
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	47



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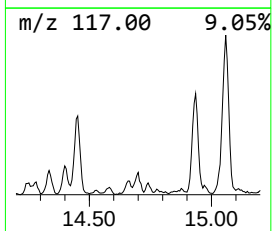
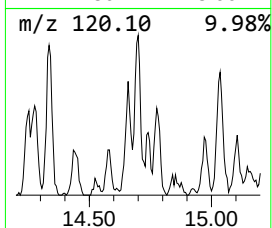
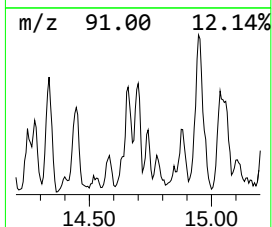
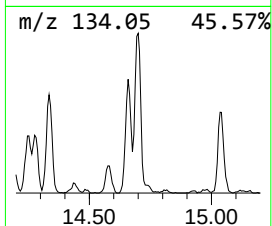
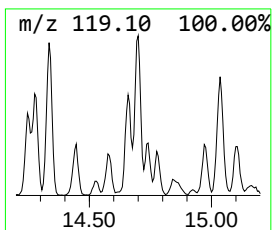
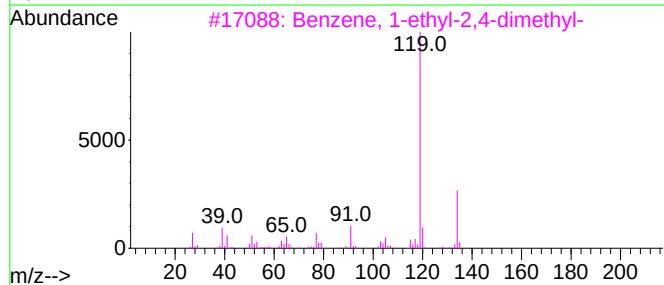
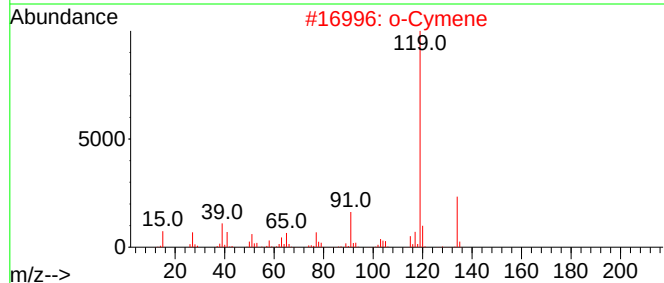
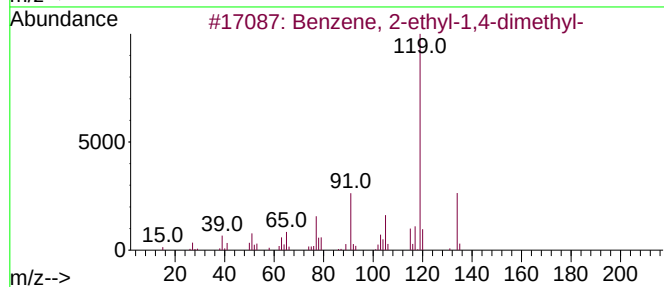
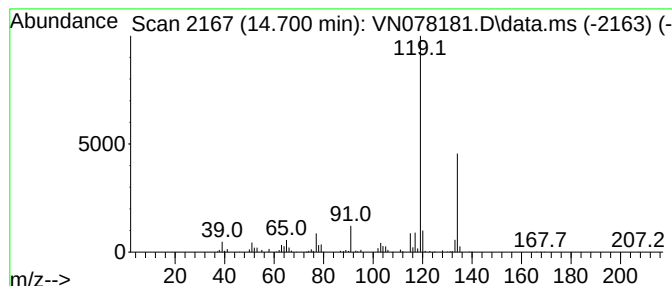
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.700	10.93 ug/l	664138	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
2			o-Cymene	134	C10H14	000527-84-4	91
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078181.D
Acq On : 13 Jun 2023 13:12
Operator : JC\MD
Sample : 03170-03
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971

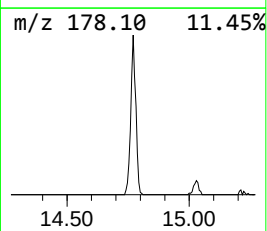
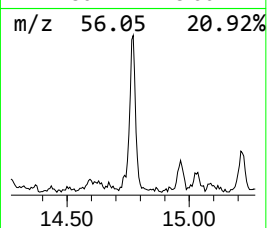
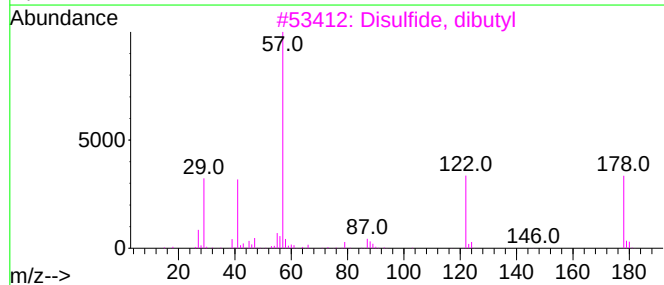
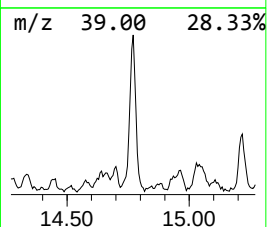
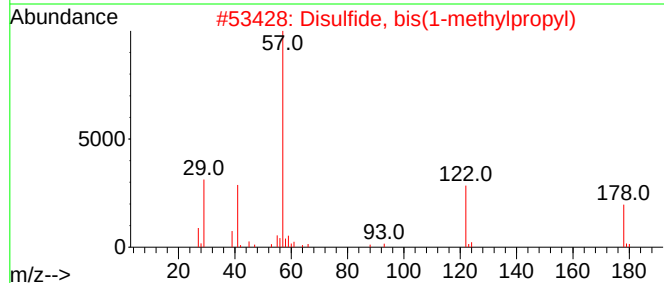
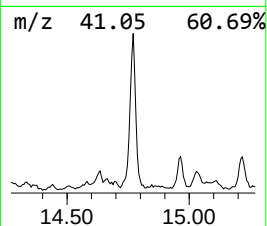
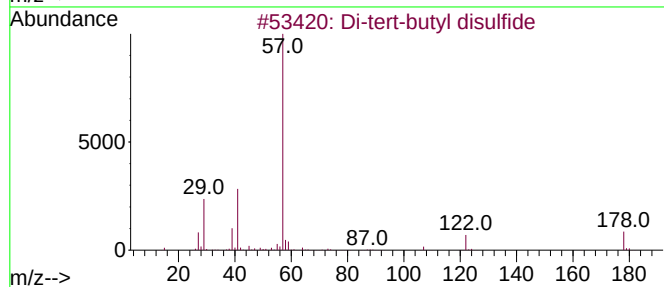
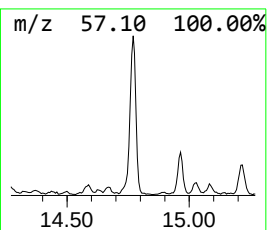
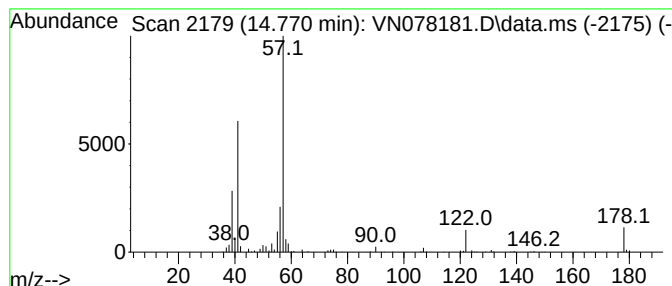
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Quant Title : SW846 8260

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

Peak Number 6 Di-tert-butyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.770	20.60 ug/l	1252130	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	58
2			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	50
3			Disulfide, dibutyl	178	C8H18S2	000629-45-8	46
4			Butane, 1-bromo-	136	C4H9Br	000109-65-9	32
5			1,2-Dibutoxyethane	174	C10H22O2	000112-48-1	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078181.D
Acq On : 13 Jun 2023 13:12
Operator : JC\MD
Sample : 03170-03
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971

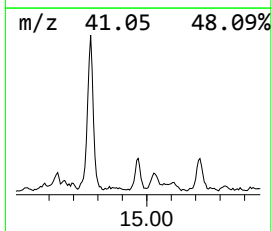
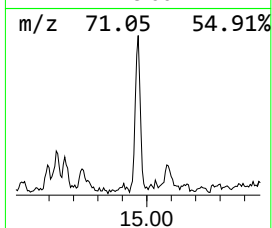
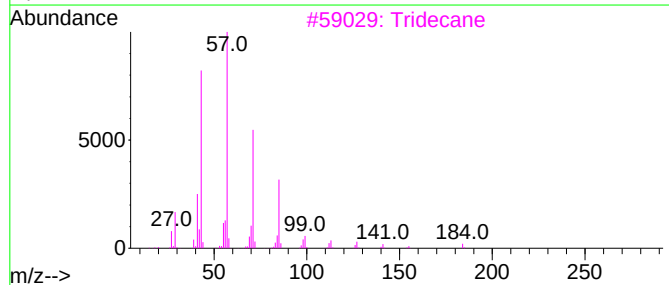
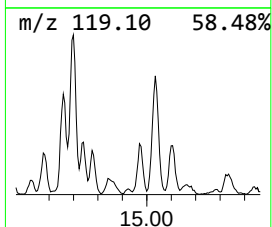
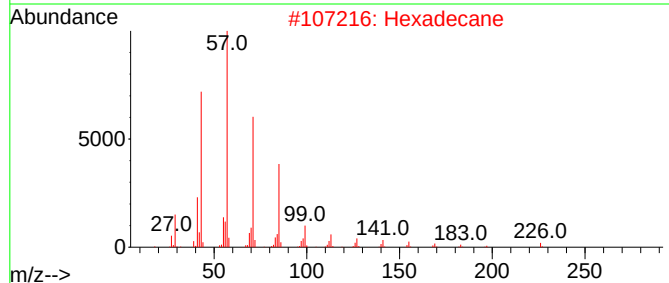
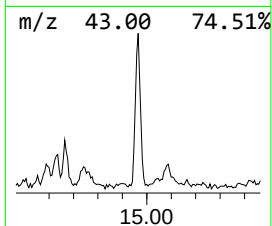
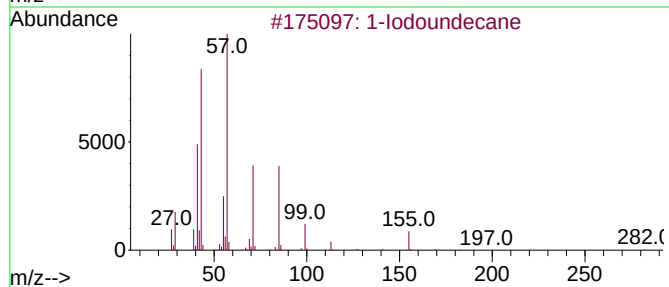
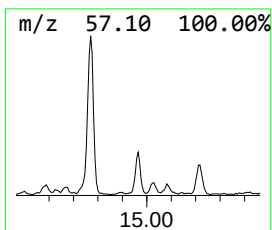
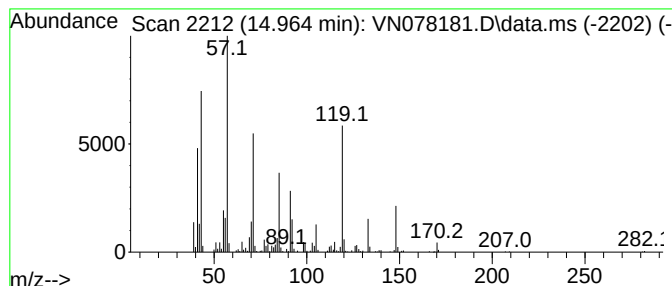
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.964 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.964	17.28 ug/l	1050230	1,4-Dichlorobenzene-d4	13.800

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Iodoundecane	282	C11H23I	004282-44-4	38
2		Hexadecane	226	C16H34	000544-76-3	35
3		Tridecane	184	C13H28	000629-50-5	35
4		Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	35
5		Tetradecane	198	C14H30	000629-59-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078181.D
Acq On : 13 Jun 2023 13:12
Operator : JC\MD
Sample : 03170-03
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971

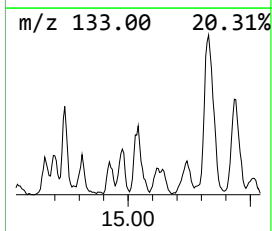
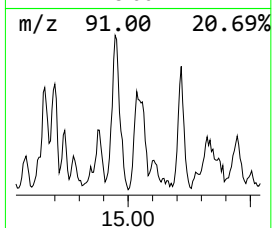
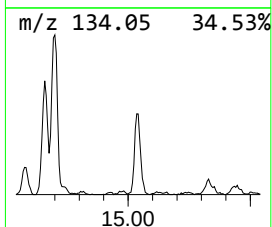
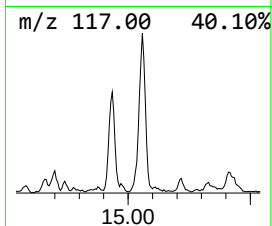
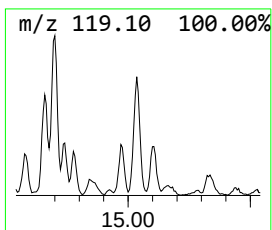
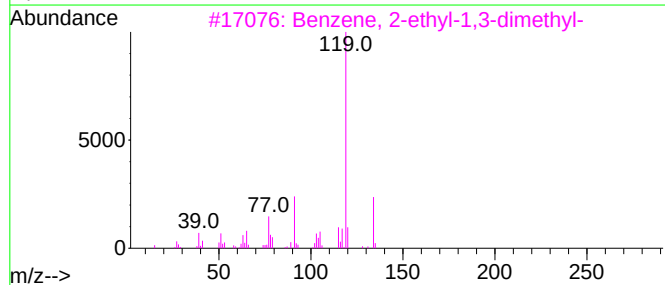
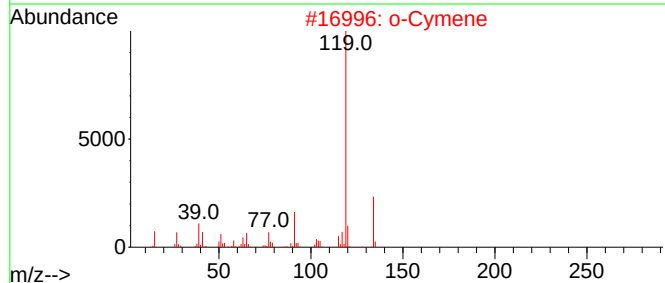
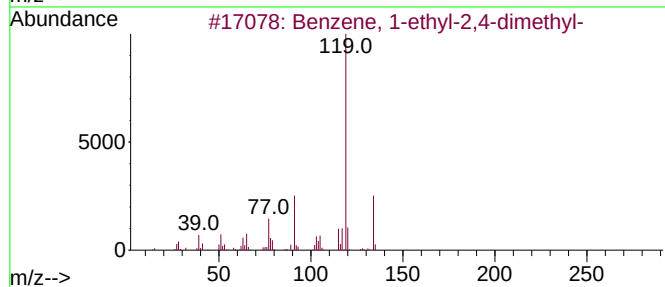
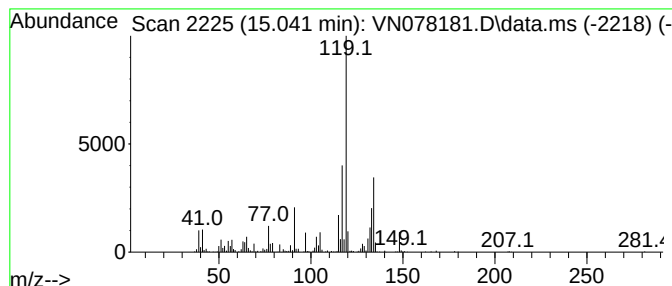
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	13.66 ug/l	830152	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	55
2			o-Cymene	134	C10H14	000527-84-4	55
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	55
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	55
5			p-Cymene	134	C10H14	000099-87-6	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078181.D
Acq On : 13 Jun 2023 13:12
Operator : JC\MD
Sample : 03170-03
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971

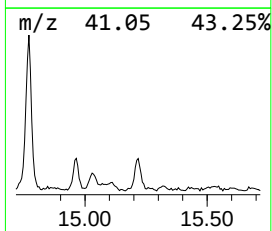
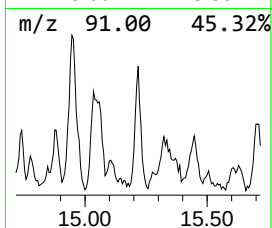
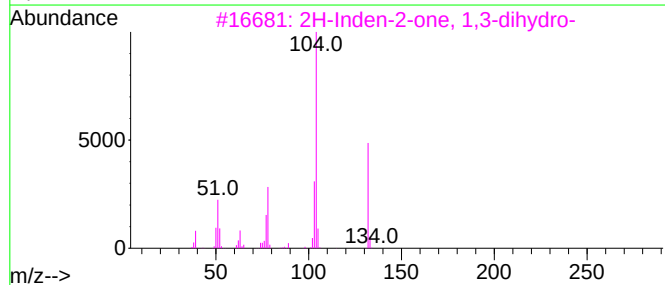
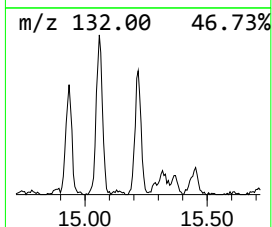
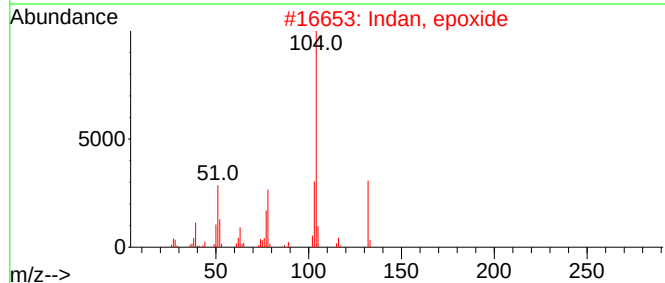
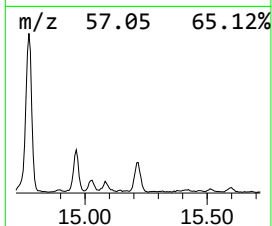
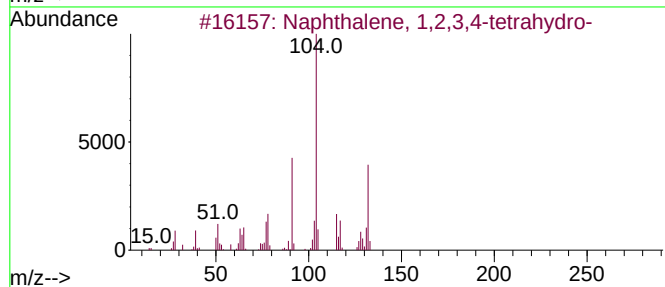
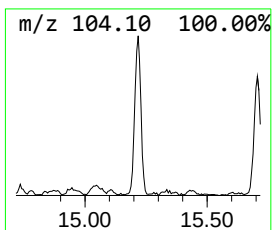
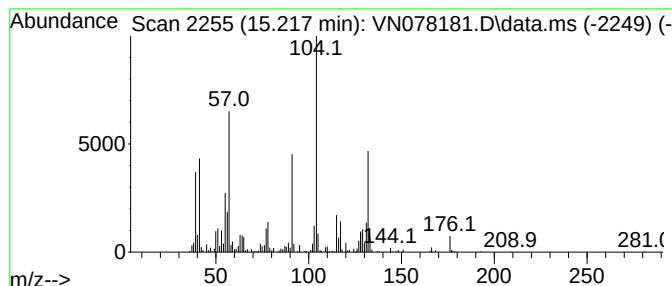
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.217	11.36 ug/l	690653	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	97
2			Indan, epoxide	132	C9H8O	000768-22-9	52
3			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	52
4			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	43
5			Benzeneethanol, .alpha.,.alpha.-...	162	C11H14O	025982-72-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078181.D
Acq On : 13 Jun 2023 13:12
Operator : JC\MD
Sample : 03170-03
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971

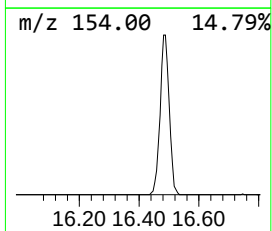
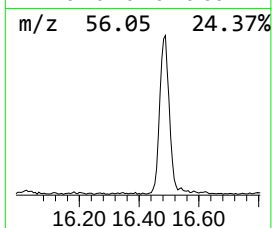
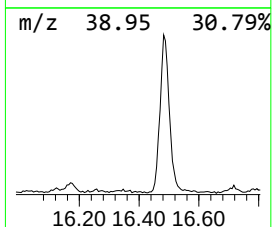
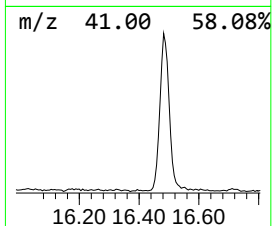
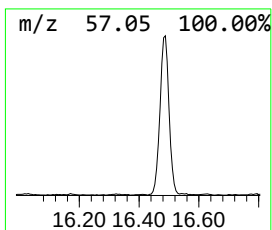
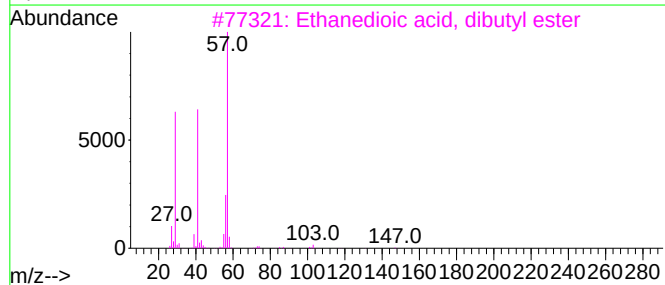
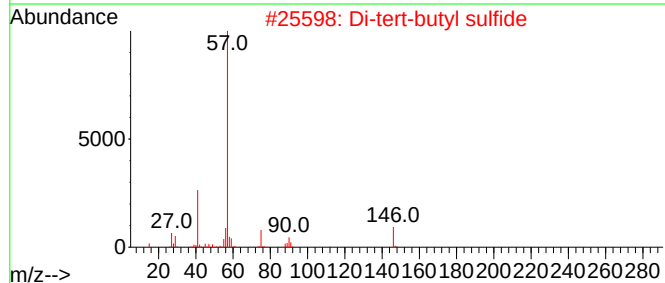
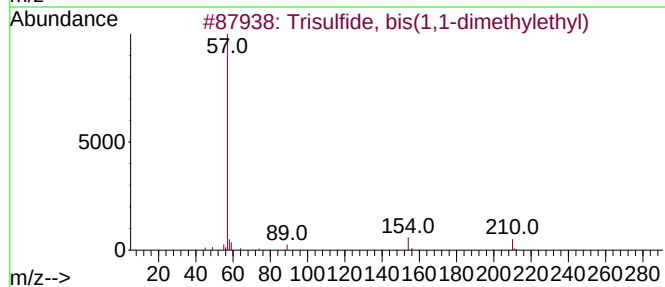
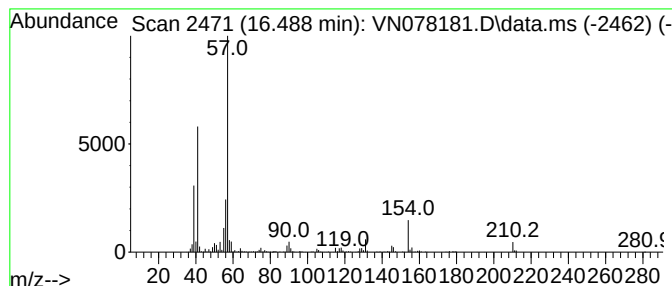
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

Peak Number 10 unknown16.488 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.488	34.16 ug/l	2076000	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	43
2			Di-tert-butyl sulfide	146	C8H18S	000107-47-1	35
3			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	32
4			Butane, 1-bromo-	136	C4H9Br	000109-65-9	32
5			1-[(chloromethyl)sulfonyl]butane	170	C5H11ClO2S	1000404-59-5	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078181.D
Acq On : 13 Jun 2023 13:12
Operator : JC\MD
Sample : 03170-03
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.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	8.971	21.5	ug/l	976358	2	9.106	2268090	50.0
Benzene, 1-ethy...	13.100	16.9	ug/l	1027330	4	13.800	3038550	50.0
Undecane	14.111	15.2	ug/l	925591	4	13.800	3038550	50.0
Benzene, 2-ethy...	14.700	10.9	ug/l	664138	4	13.800	3038550	50.0
Di-tert-butyl d...	14.770	20.6	ug/l	1252130	4	13.800	3038550	50.0
unknown14.964	14.964	17.3	ug/l	1050230	4	13.800	3038550	50.0
Benzene, 1-ethy...	15.041	13.7	ug/l	830152	4	13.800	3038550	50.0
Naphthalene, 1,...	15.217	11.4	ug/l	690653	4	13.800	3038550	50.0
unknown16.488	16.488	34.2	ug/l	2076000	4	13.800	3038550	50.0