

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
 Data File : VN078184.D
 Acq On : 13 Jun 2023 14:24
 Operator : JC\MD
 Sample : 03170-03 10X
 Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1971DL

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: VN078184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.853	141	153	162	rVB8	58201	221593	7.54%	0.982%
2	4.436	410	422	442	rBV	510742	1559870	53.07%	6.913%
3	8.177	1048	1058	1062	rBV	333606	810639	27.58%	3.593%
4	8.230	1062	1067	1077	rVV	636683	1401230	47.68%	6.210%
5	8.335	1079	1085	1091	rVB5	16944	36470	1.24%	0.162%
6	8.453	1096	1105	1116	rBV2	58397	136638	4.65%	0.606%
7	8.583	1118	1127	1137	rBV	338551	760865	25.89%	3.372%
8	8.977	1186	1194	1200	rBV3	60513	119974	4.08%	0.532%
9	9.106	1207	1216	1228	rBV	850132	1731364	58.91%	7.673%
10	10.571	1457	1465	1471	rBV	1296115	2400442	81.68%	10.639%
11	10.635	1471	1476	1490	rVV	1600218	2939000	100.00%	13.026%
12	11.276	1578	1585	1593	rBV9	14651	32728	1.11%	0.145%
13	11.647	1642	1648	1652	rBV4	20463	45106	1.53%	0.200%
14	11.747	1661	1665	1672	rVB3	19190	33827	1.15%	0.150%
15	11.871	1678	1686	1697	rVB	1131682	2003398	68.17%	8.879%
16	11.971	1698	1703	1708	rBV2	33294	53440	1.82%	0.237%
17	12.076	1713	1721	1727	rBV	156642	308561	10.50%	1.368%
18	12.406	1766	1777	1783	rVV3	62249	173735	5.91%	0.770%
19	12.488	1783	1791	1798	rVV5	44647	112226	3.82%	0.497%
20	12.594	1798	1809	1818	rVV5	22421	108073	3.68%	0.479%
21	12.706	1822	1828	1832	rVV4	20589	44444	1.51%	0.197%
22	12.776	1832	1840	1842	rVV8	36482	87026	2.96%	0.386%
23	12.806	1842	1845	1847	rVV4	37756	48458	1.65%	0.215%
24	12.853	1847	1853	1863	rVB	794279	1383849	47.09%	6.133%
25	13.041	1879	1885	1888	rBV	35865	63383	2.16%	0.281%
26	13.106	1891	1896	1899	rVV2	89059	159629	5.43%	0.707%
27	13.165	1899	1906	1913	rVB3	180358	389047	13.24%	1.724%
28	13.347	1928	1937	1942	rBV3	43665	124227	4.23%	0.551%
29	13.400	1942	1946	1952	rVB5	37866	53890	1.83%	0.239%
30	13.488	1954	1961	1966	rBV	151236	259373	8.83%	1.150%
31	13.676	1987	1993	1999	rBV8	51372	121428	4.13%	0.538%
32	13.723	1999	2001	2004	rVV4	26967	36196	1.23%	0.160%
33	13.794	2007	2013	2022	rVV	777697	1403815	47.77%	6.222%
34	13.876	2022	2027	2033	rVB4	37746	70822	2.41%	0.314%
35	13.988	2042	2046	2049	rVV2	46669	79206	2.69%	0.351%
36	14.023	2050	2052	2062	rVB4	68284	134016	4.56%	0.594%

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37	14.112	2062	2067	2073	rBV2	180069	307388	10.46%	1.362%
38	14.247	2087	2090	2092	rBV2	29748	36224	1.23%	0.161%
39	14.335	2100	2105	2110	rVB	55786	82849	2.82%	0.367%
40	14.441	2119	2123	2129	rVB6	44966	68848	2.34%	0.305%
41	14.582	2142	2147	2151	rBV5	36133	61885	2.11%	0.274%
42	14.629	2151	2155	2158	rBV4	55794	84600	2.88%	0.375%
43	14.700	2164	2167	2170	rVB	48593	60079	2.04%	0.266%
44	14.741	2170	2174	2175	rVV2	46694	55594	1.89%	0.246%
45	14.770	2175	2179	2189	rVB	173271	334237	11.37%	1.481%
46	14.964	2203	2212	2219	rVB6	135880	266585	9.07%	1.182%
47	15.041	2219	2225	2233	rBV8	77430	259881	8.84%	1.152%
48	15.217	2250	2255	2262	rVB6	72290	141503	4.81%	0.627%
49	15.323	2268	2273	2278	rBV5	43558	71564	2.43%	0.317%
50	15.435	2288	2292	2293	rBV4	34145	40317	1.37%	0.179%
51	15.600	2316	2320	2325	rBV6	29381	59547	2.03%	0.264%
52	15.753	2342	2346	2349	rBV5	32919	49321	1.68%	0.219%
53	15.841	2356	2361	2370	rVB5	80369	180722	6.15%	0.801%
54	16.176	2413	2418	2423	rVB4	44571	89615	3.05%	0.397%
55	16.482	2462	2470	2480	rBV	329495	776389	26.42%	3.441%
56	16.717	2504	2510	2516	rBV6	42659	88108	3.00%	0.390%

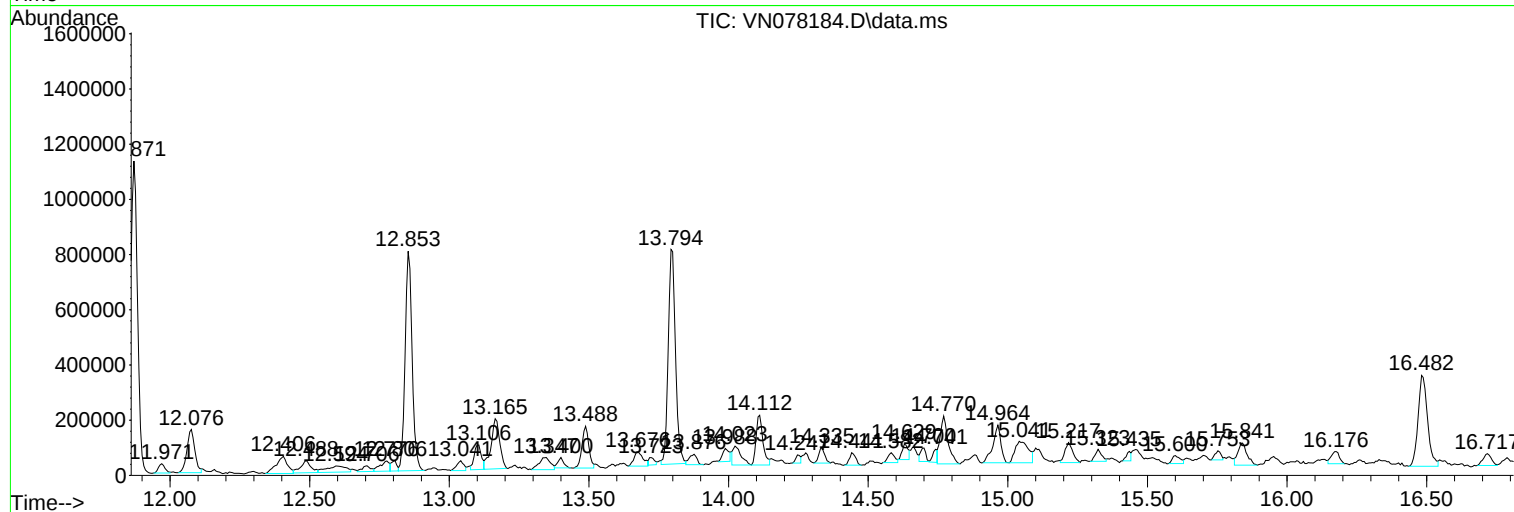
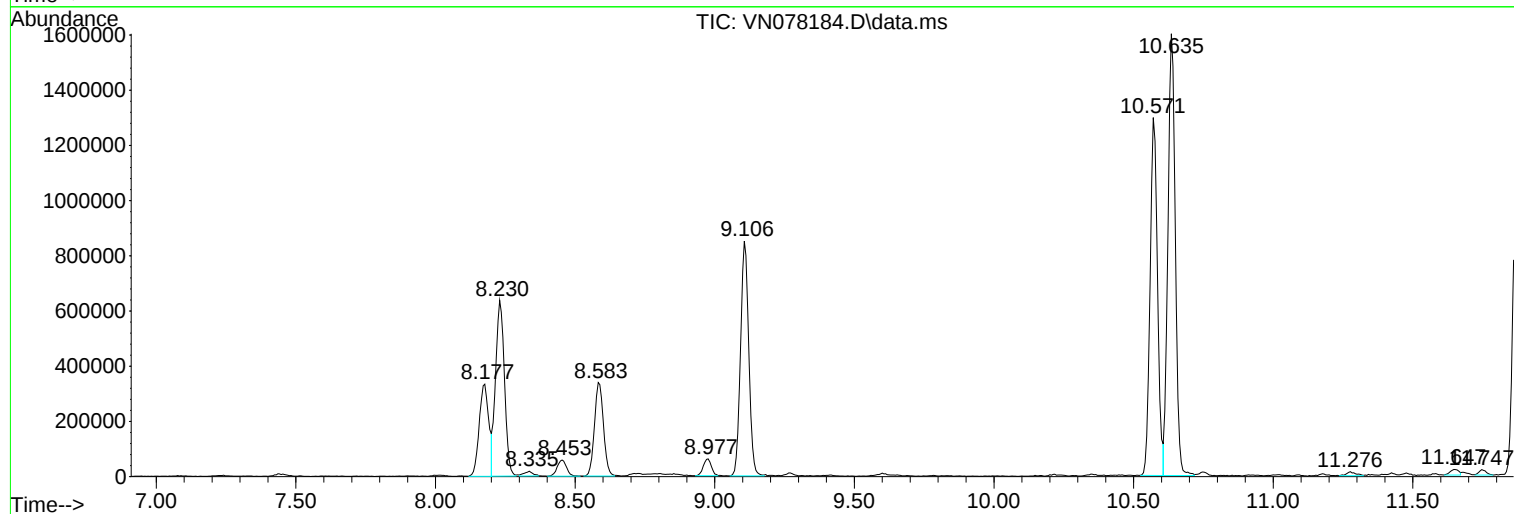
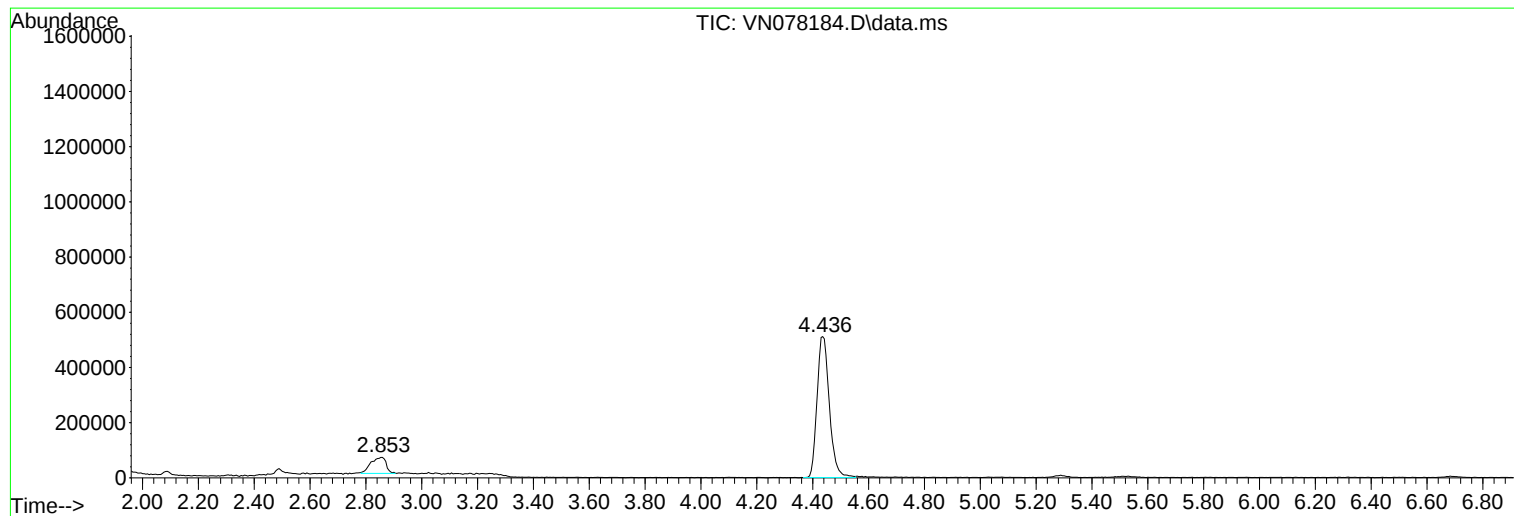
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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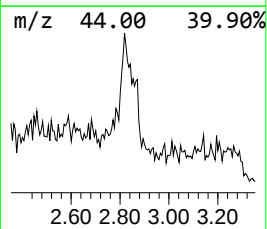
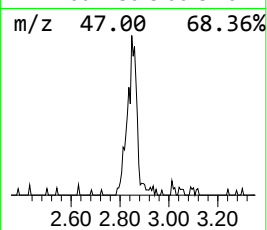
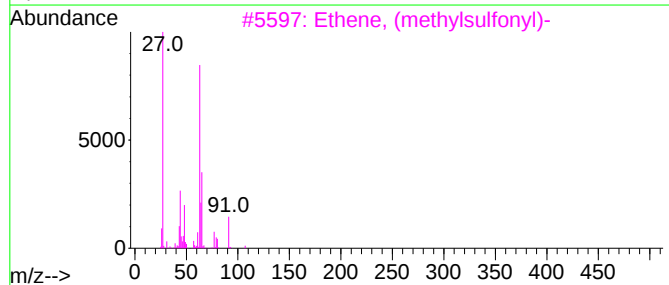
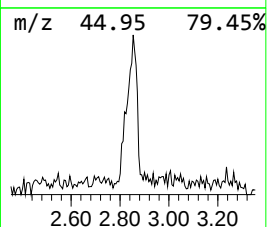
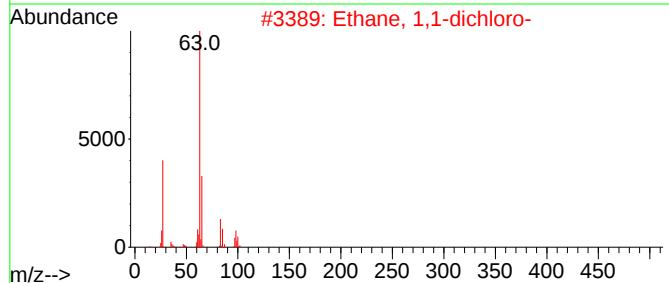
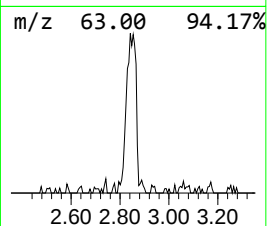
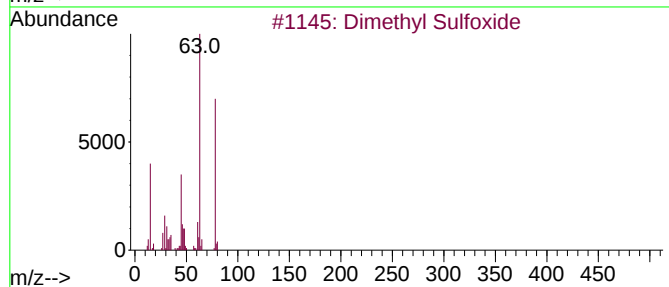
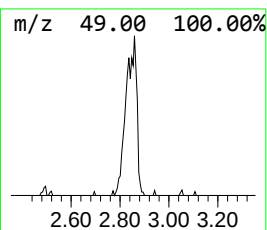
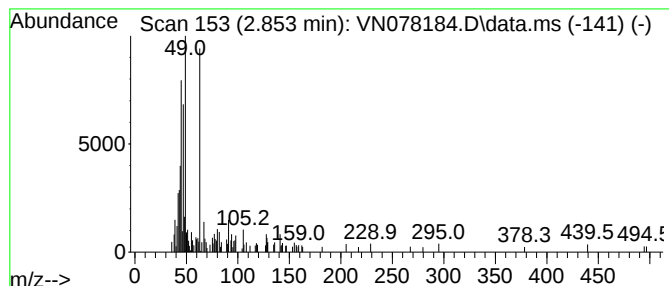
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.853 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.853	7.91 ug/l	221593	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl Sulfoxide	78	C2H6OS	000067-68-5	17
2			Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	12
3			Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	12
4			Propanoic acid, 2-chloro-, ethyl...	136	C5H9ClO2	000535-13-7	10
5			bis(chloromethyl) carbonate	158	C3H4Cl2O3	1000404-37-0	9



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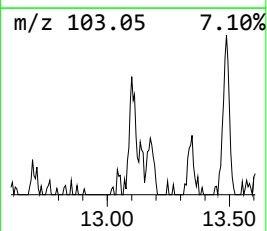
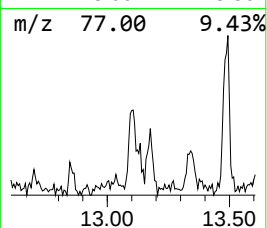
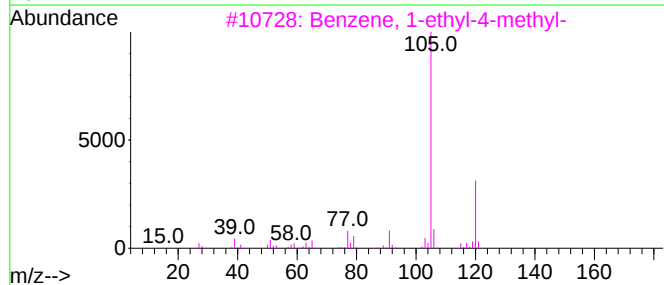
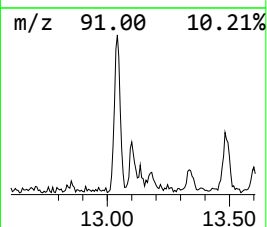
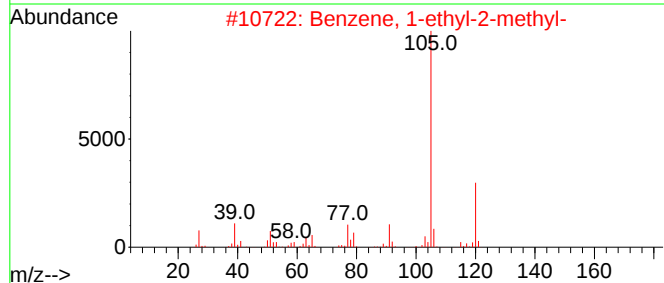
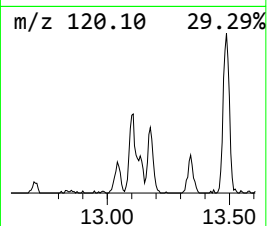
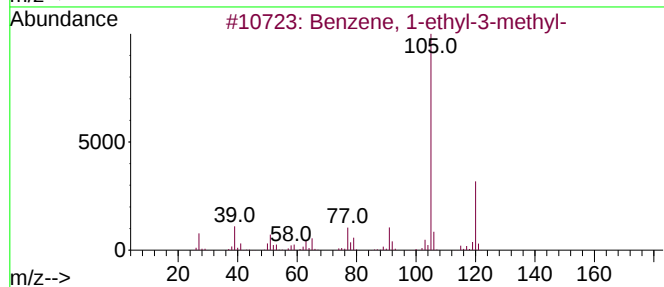
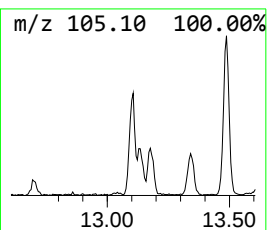
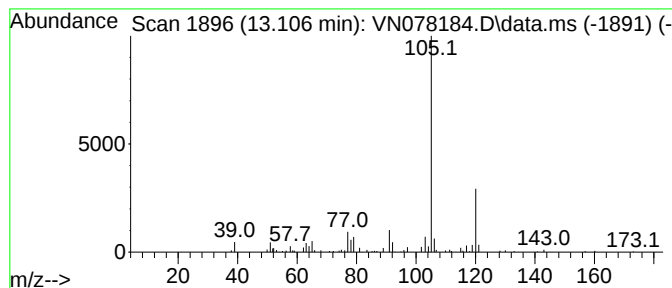
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060623W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.106	5.69 ug/l	159629	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	93
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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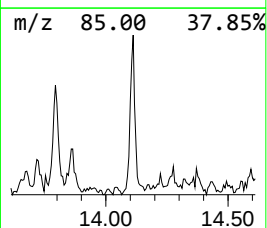
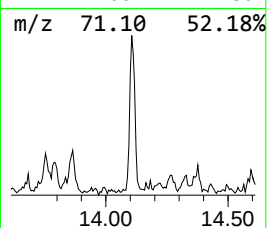
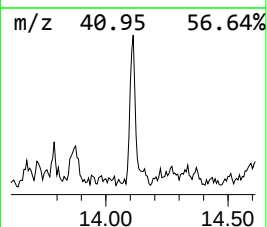
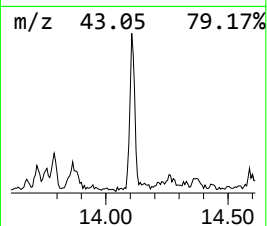
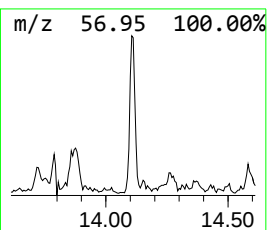
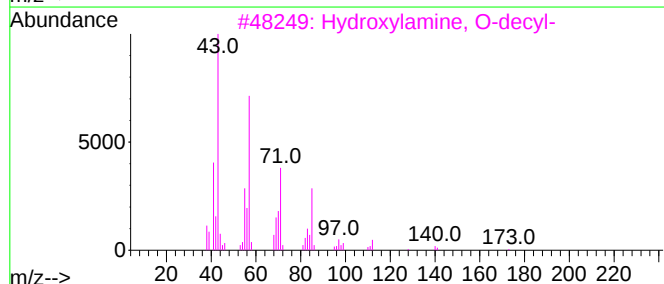
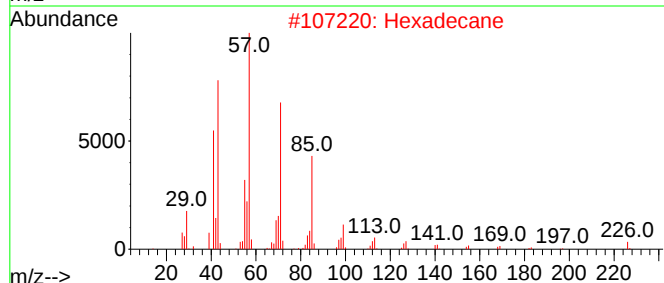
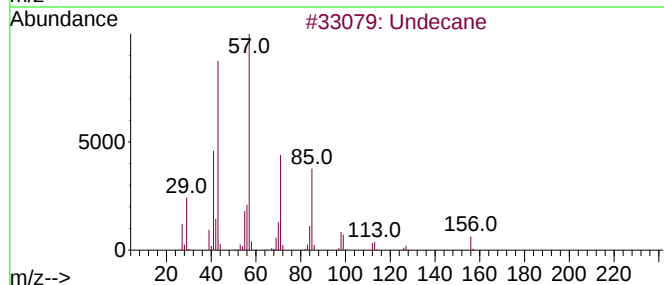
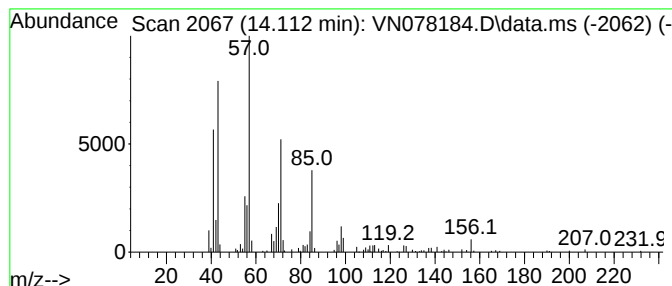
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.112	10.95 ug/l	307388	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	94
2			Hexadecane	226	C16H34	000544-76-3	80
3			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	80
4			Tetradecane	198	C14H30	000629-59-4	72
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64



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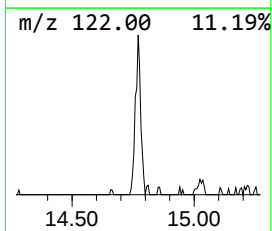
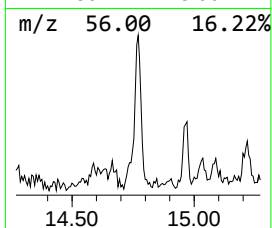
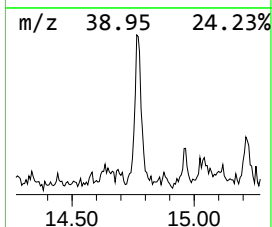
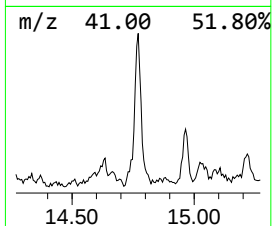
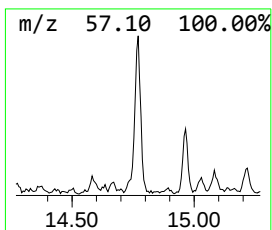
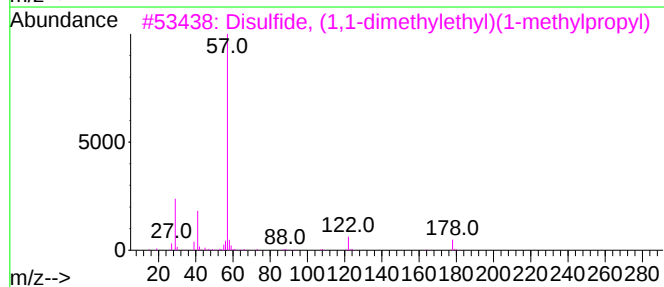
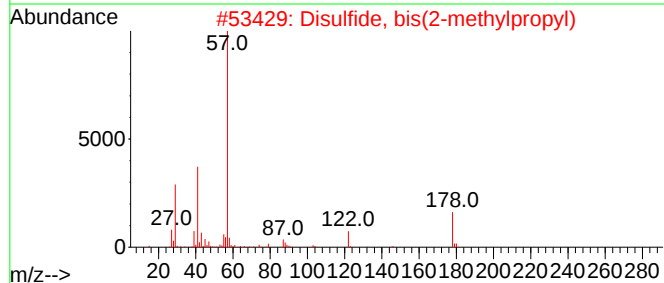
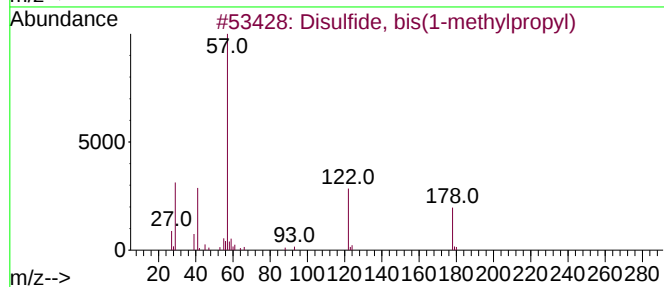
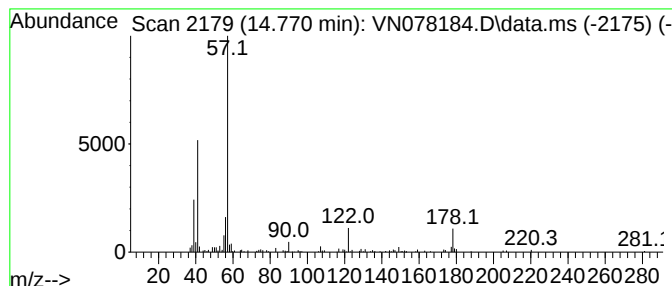
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Quant Title : SW846 8260

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

Peak Number 4 Disulfide, bis(1-methylpropyl) Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.770	11.90 ug/l	334237	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	53
2			Disulfide, bis(2-methylpropyl)	178	C8H18S2	001518-72-5	38
3			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	38
4			Disulfide, dibutyl	178	C8H18S2	000629-45-8	35
5			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	35



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Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971DL

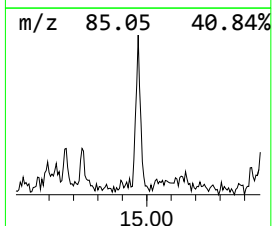
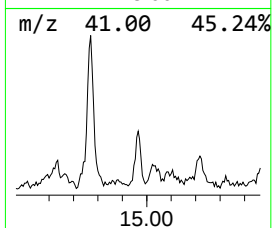
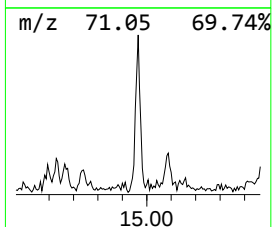
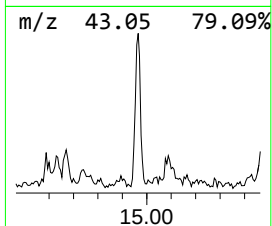
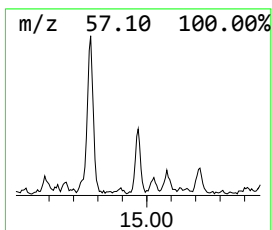
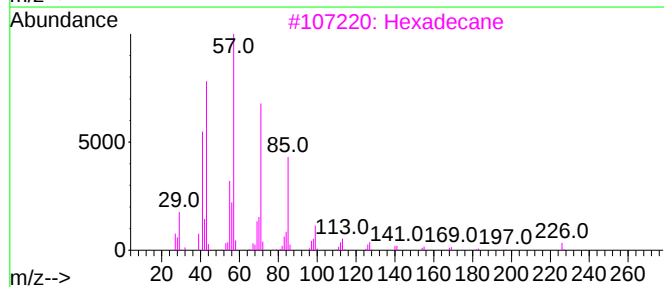
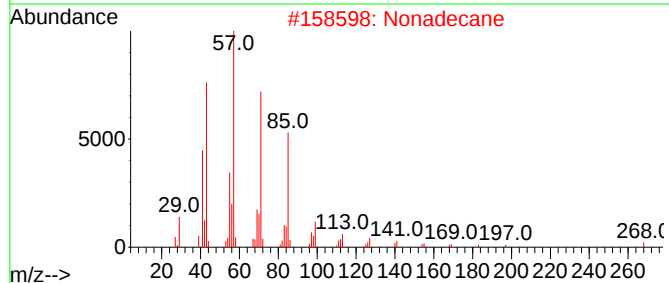
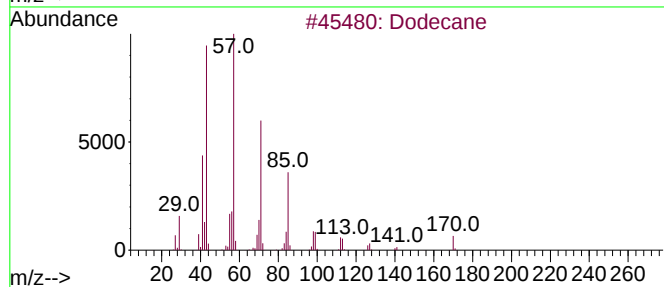
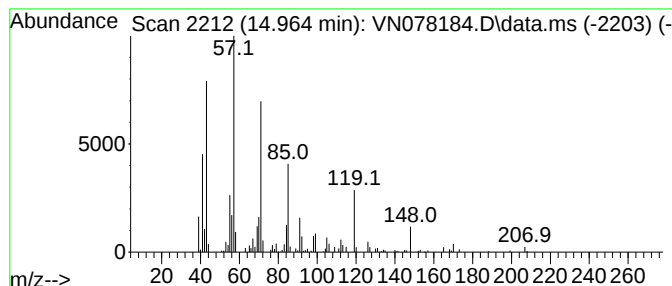
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Quant Title : SW846 8260

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

Peak Number 5 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.964	9.50 ug/l	266585	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	68
2			Nonadecane	268	C19H40	000629-92-5	58
3			Hexadecane	226	C16H34	000544-76-3	58
4			Tridecane	184	C13H28	000629-50-5	58
5			Tetradecane	198	C14H30	000629-59-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078184.D
Acq On : 13 Jun 2023 14:24
Operator : JC\MD
Sample : 03170-03 10X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971DL

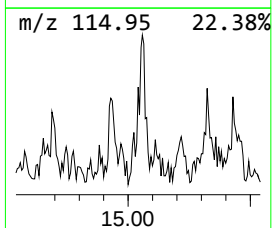
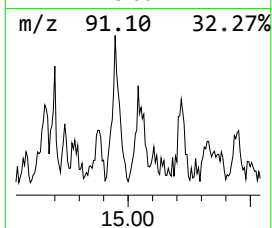
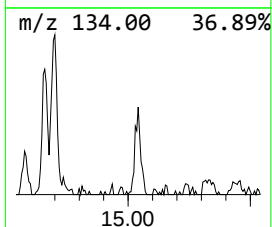
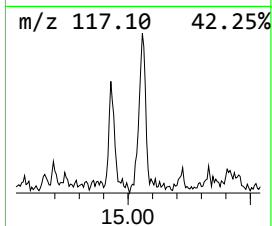
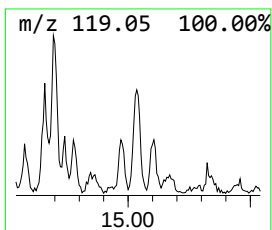
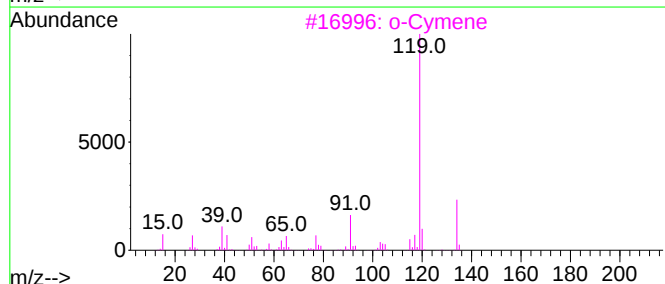
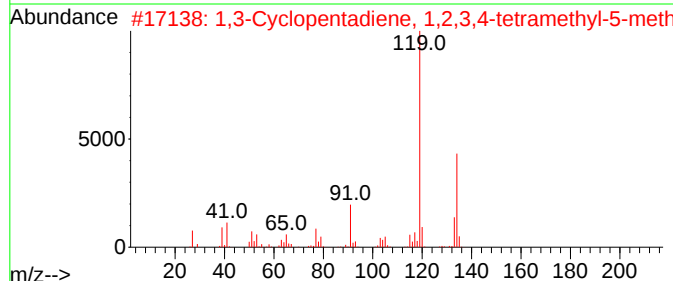
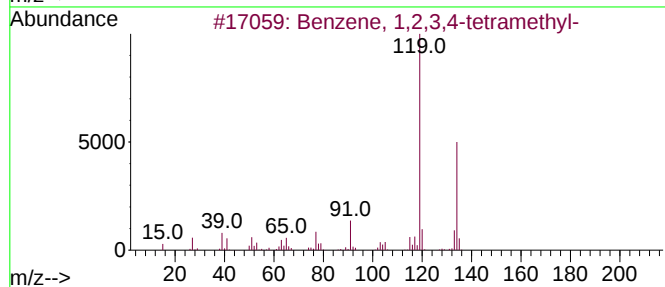
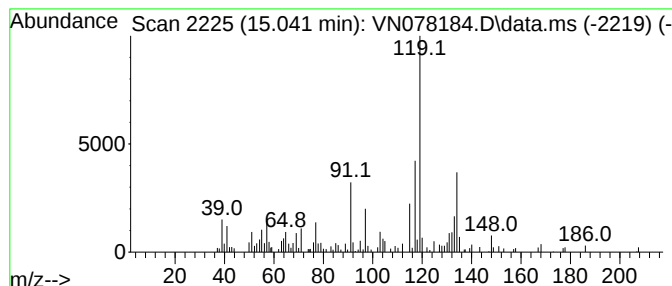
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	9.26 ug/l	259881	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	55
2			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	53
3			o-Cymene	134	C10H14	000527-84-4	49
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	49
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078184.D
Acq On : 13 Jun 2023 14:24
Operator : JC\MD
Sample : 03170-03 10X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971DL

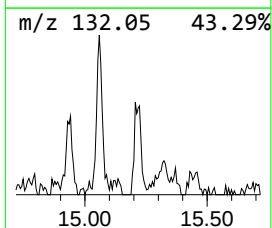
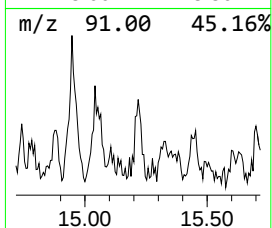
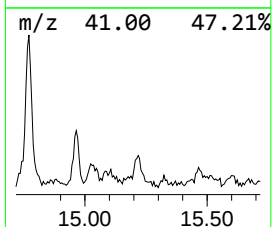
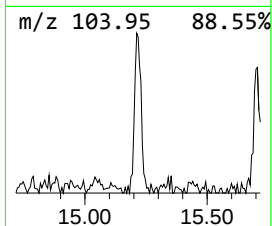
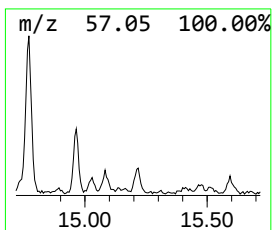
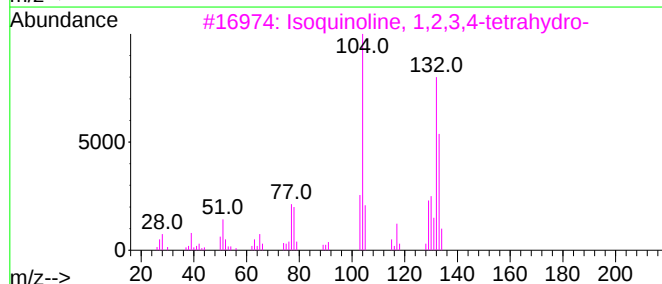
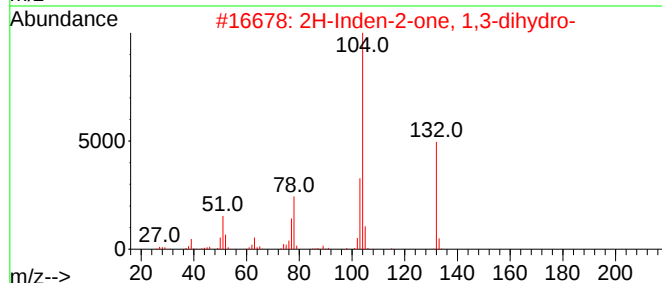
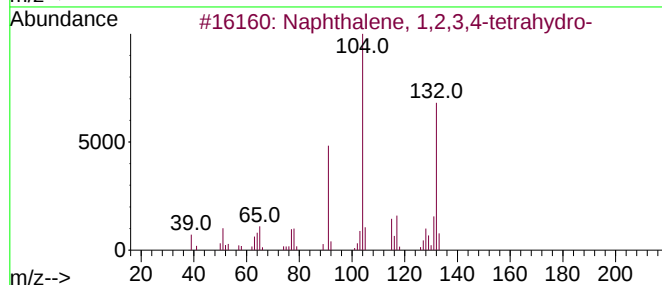
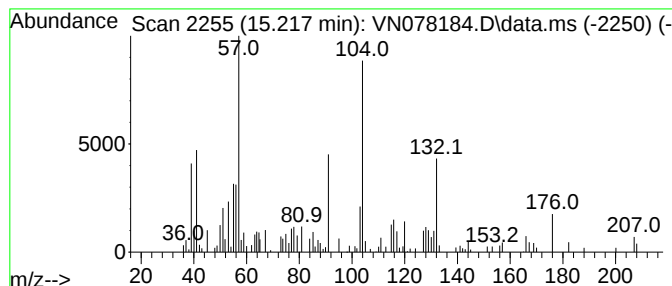
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.217	5.04 ug/l	141503	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	52
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	50
3			Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	42
4			2,5-Xylenesulfonamide	185	C8H11NO2S	006292-58-6	38
5			(3-Phenylpropionyl)glycine	207	C11H13NO3	056613-60-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078184.D
Acq On : 13 Jun 2023 14:24
Operator : JC\MD
Sample : 03170-03 10X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971DL

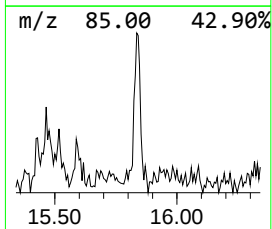
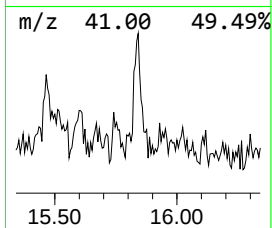
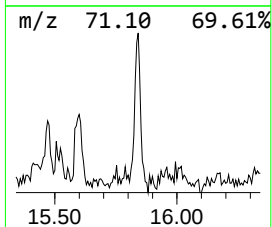
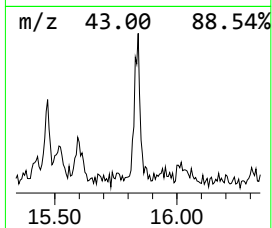
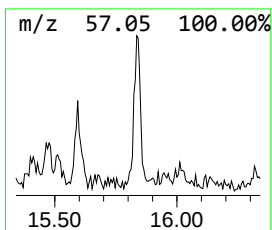
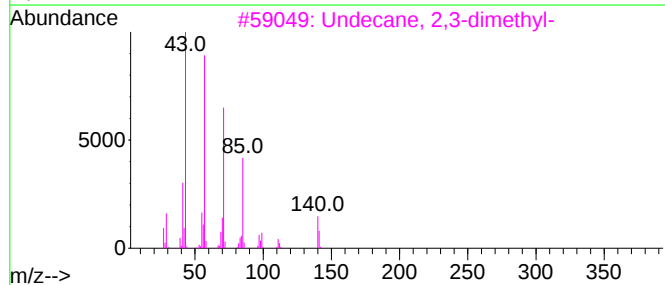
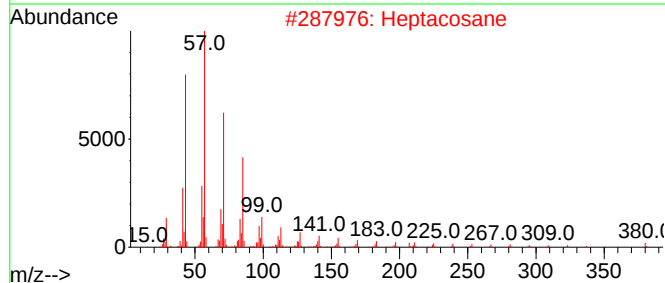
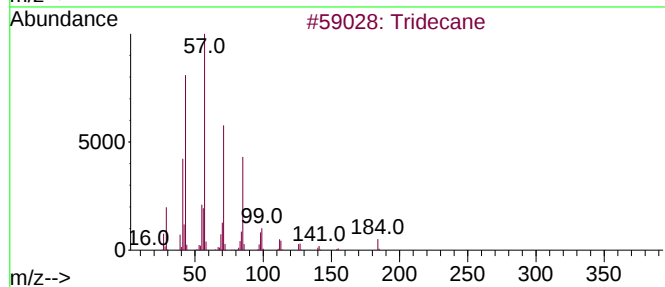
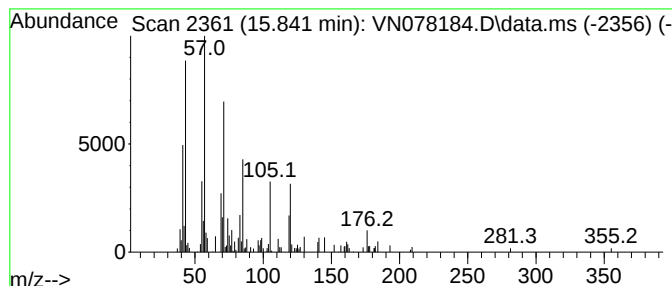
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Quant Title : SW846 8260

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

Peak Number 8 unknown15.841 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	6.44 ug/l	180722	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	49
2			Heptacosane	380	C27H56	000593-49-7	47
3			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	46
4			Decane, 3-bromo-	220	C10H21Br	030571-71-2	43
5			Hentriacontane	437	C31H64	000630-04-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078184.D
Acq On : 13 Jun 2023 14:24
Operator : JC\MD
Sample : 03170-03 10X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971DL

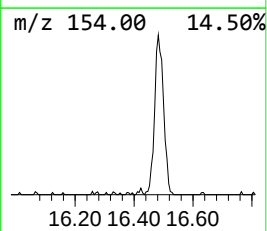
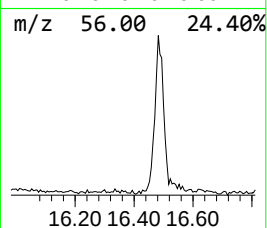
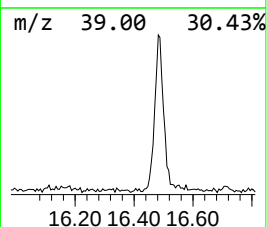
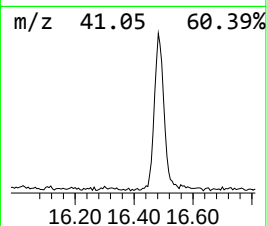
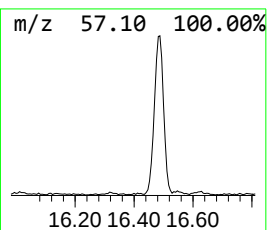
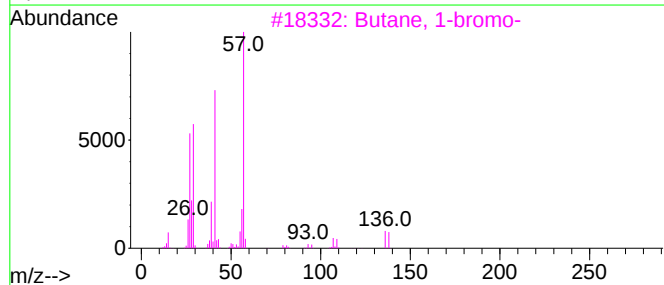
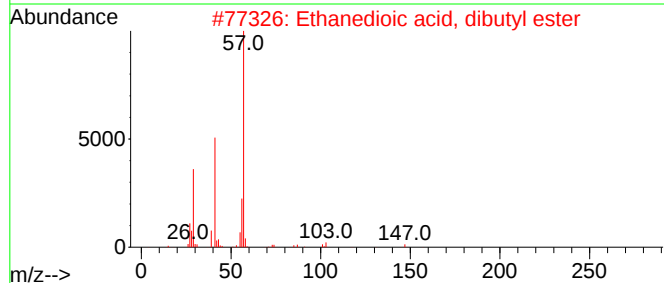
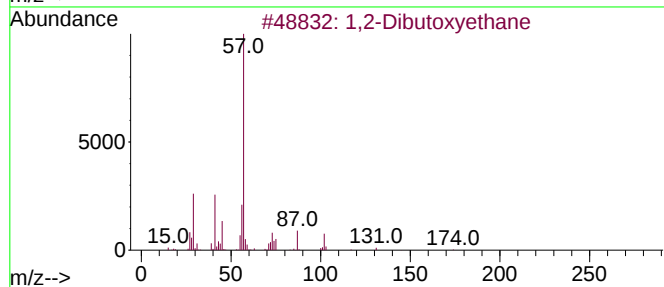
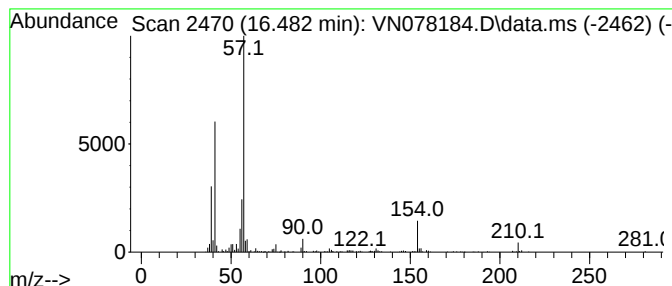
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.482 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.482	27.65 ug/l	776389	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dibutoxyethane	174	C10H22O2	000112-48-1	37
2			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	32
3			Butane, 1-bromo-	136	C4H9Br	000109-65-9	32
4			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	32
5			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061323\
Data File : VN078184.D
Acq On : 13 Jun 2023 14:24
Operator : JC\MD
Sample : 03170-03 10X
Misc : 5.04g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1971DL

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

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					#	RT	Resp	Conc
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Undecane	14.112	10.9	ug/l	307388	4	13.800	1403820	50.0
Disulfide, bis(...	14.770	11.9	ug/l	334237	4	13.800	1403820	50.0
Dodecane	14.964	9.5	ug/l	266585	4	13.800	1403820	50.0
Benzene, 1,2,3,...	15.041	9.3	ug/l	259881	4	13.800	1403820	50.0
Naphthalene, 1,...	15.217	5.0	ug/l	141503	4	13.800	1403820	50.0
unknown15.841	15.841	6.4	ug/l	180722	4	13.800	1403820	50.0
unknown16.482	16.482	27.6	ug/l	776389	4	13.800	1403820	50.0