

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011023\
 Data File : VN076189.D
 Acq On : 10 Jan 2023 18:00
 Operator : JC\MD
 Sample : 01061-04
 Misc : 5.08gr/10mL/100uL/5.0mL/MSVOA_N/MeOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SLUDGE-7

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\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN076189.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.818	120	130	133	rBV8	18263	53134	2.93%	0.348%
2	3.083	173	175	188	rVB6	28844	64446	3.55%	0.422%
3	5.265	537	546	556	rBV4	14434	45454	2.50%	0.298%
4	8.171	1028	1040	1044	rBV	237928	589297	32.47%	3.861%
5	8.224	1044	1049	1060	rVB	515278	1129285	62.23%	7.399%
6	8.447	1077	1087	1093	rBV3	12979	30708	1.69%	0.201%
7	8.583	1101	1110	1121	rBV	248601	565733	31.18%	3.707%
8	9.100	1189	1198	1212	rBV	658832	1359011	74.89%	8.904%
9	10.565	1439	1447	1455	rBV	974816	1814644	100.00%	11.890%
10	10.629	1455	1458	1465	rVB	41047	70981	3.91%	0.465%
11	10.747	1472	1478	1484	rBV4	17608	31968	1.76%	0.209%
12	11.865	1659	1668	1679	rVB	849015	1505340	82.96%	9.863%
13	11.965	1679	1685	1689	rBV2	13488	23043	1.27%	0.151%
14	12.071	1696	1703	1709	rBV	60827	120050	6.62%	0.787%
15	12.400	1751	1759	1764	rBV2	35073	62030	3.42%	0.406%
16	12.712	1803	1812	1817	rBV4	50236	123824	6.82%	0.811%
17	12.853	1829	1836	1845	rVB	659887	1176679	64.84%	7.710%
18	13.094	1873	1877	1879	rBV3	15405	21789	1.20%	0.143%
19	13.159	1884	1888	1896	rVB6	27845	70979	3.91%	0.465%
20	13.265	1902	1906	1912	rVB4	29588	46592	2.57%	0.305%
21	13.488	1939	1944	1950	rBV2	25372	56184	3.10%	0.368%
22	13.594	1959	1962	1967	rVB7	17893	27316	1.51%	0.179%
23	13.706	1973	1981	1989	rBV	1120357	1808821	99.68%	11.851%
24	13.794	1990	1996	2003	rBV	813092	1359650	74.93%	8.908%
25	13.947	2019	2022	2026	rVB5	16095	23568	1.30%	0.154%
26	14.106	2045	2049	2053	rBV2	32045	49743	2.74%	0.326%
27	14.235	2066	2071	2077	rBV2	111590	182304	10.05%	1.194%
28	14.388	2093	2097	2101	rBV3	23380	40502	2.23%	0.265%
29	14.529	2116	2121	2133	rBV	110520	238515	13.14%	1.563%
30	14.635	2135	2139	2142	rBV5	31671	51208	2.82%	0.336%
31	14.741	2153	2157	2159	rBV4	43752	71942	3.96%	0.471%
32	14.776	2159	2163	2179	rVV4	159058	588931	32.45%	3.859%
33	14.894	2179	2183	2190	rVV2	65817	128363	7.07%	0.841%
34	14.959	2190	2194	2200	rVB	63663	113367	6.25%	0.743%
35	15.082	2210	2215	2217	rBV6	46836	84336	4.65%	0.553%
36	15.223	2234	2239	2241	rBV5	52410	92874	5.12%	0.609%

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37	15.259	2241	2245	2247	rBV3	73928	114865	6.33%	0.753%
38	15.329	2253	2257	2264	rVB5	137876	322335	17.76%	2.112%
39	15.406	2265	2270	2276	rBV3	114345	256623	14.14%	1.681%
40	15.564	2288	2297	2306	rBV5	104060	361723	19.93%	2.370%
41	15.641	2306	2310	2311	rBV2	61580	75363	4.15%	0.494%
42	15.835	2338	2343	2348	rVB2	77689	125386	6.91%	0.822%
43	16.011	2368	2373	2383	rBV4	53881	132739	7.31%	0.870%
44	16.623	2473	2477	2486	rVB8	23712	50852	2.80%	0.333%

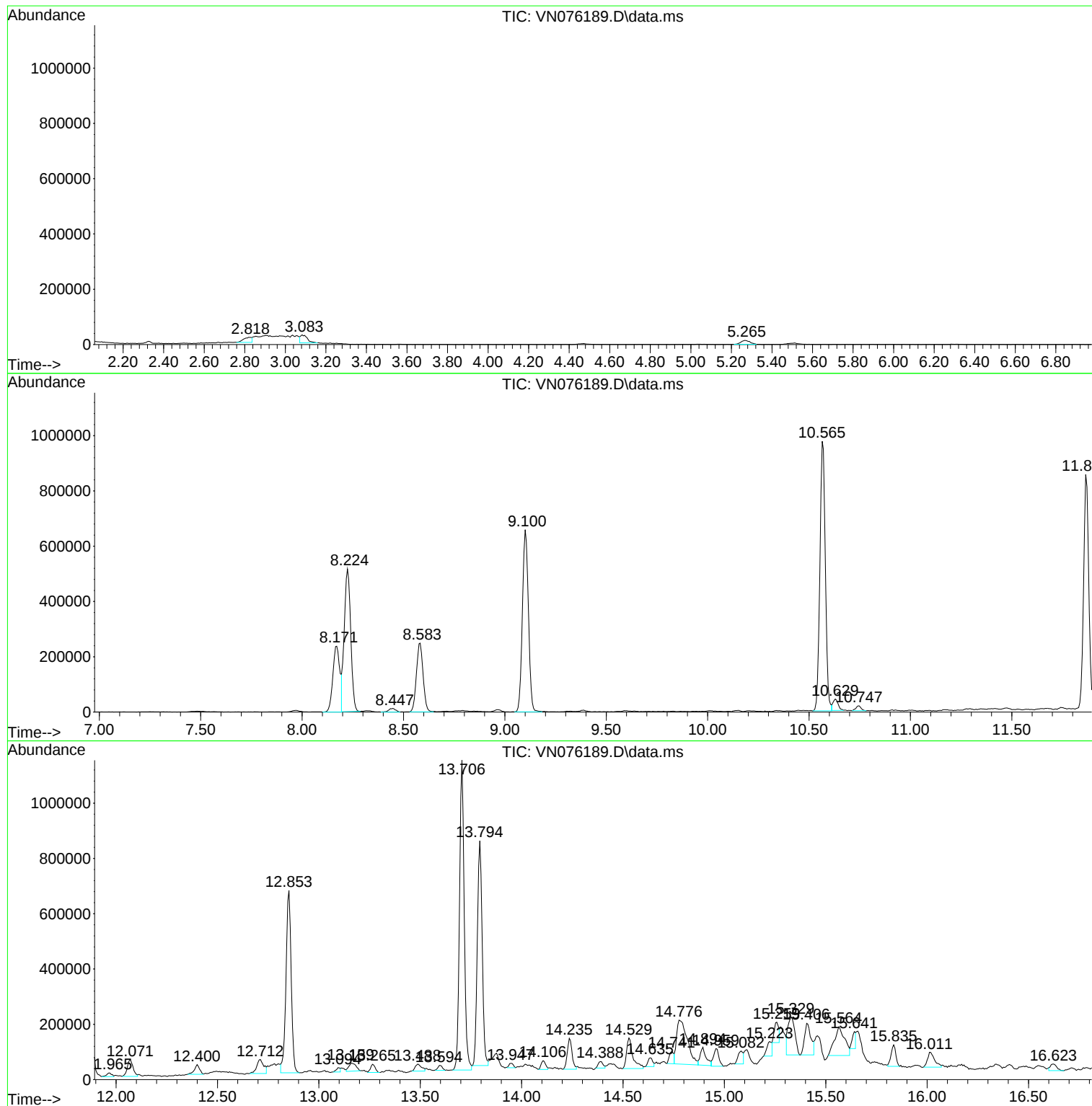
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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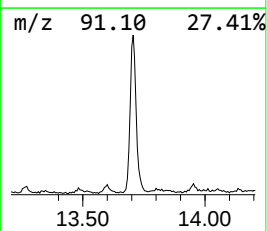
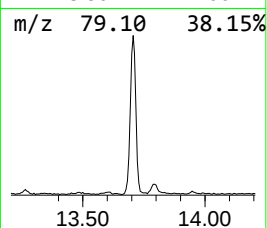
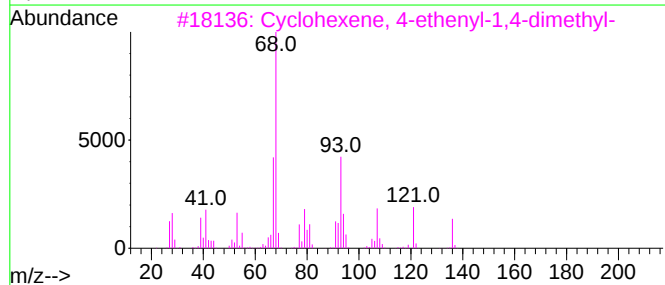
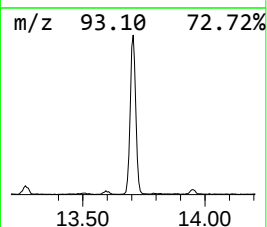
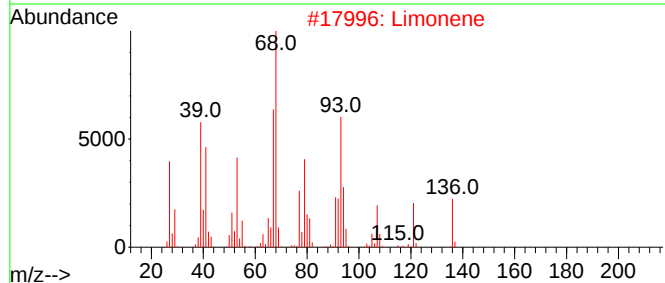
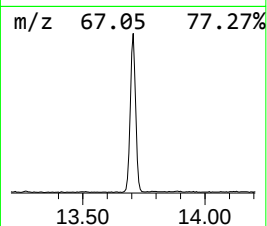
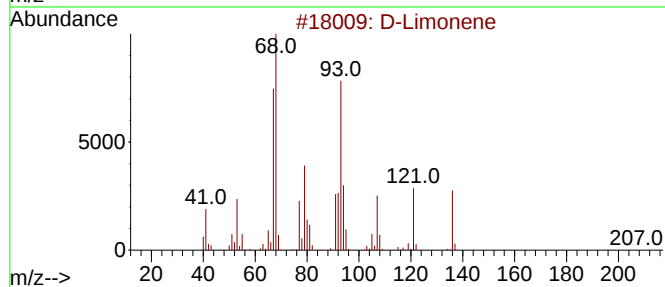
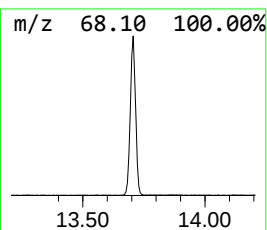
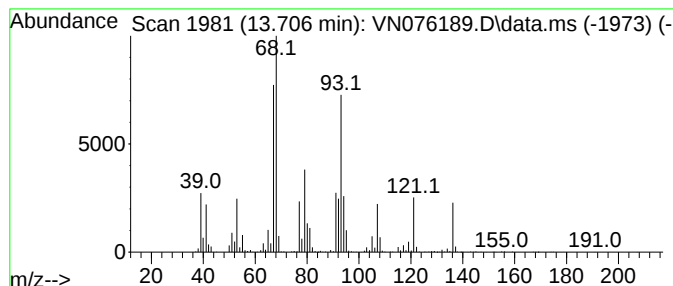
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 1 D-Limonene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.706	66.52 ug/l	1808820	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	99
2			Limonene	136	C10H16	000138-86-3	91
3			Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	86
4			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	86
5			Cyclohexanol, 1-methyl-4-(1-meth...	196	C12H20O2	010198-23-9	80



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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SLUDGE-7

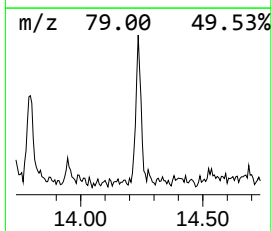
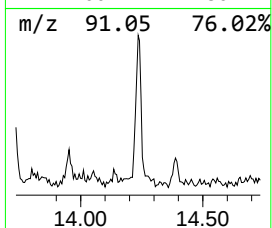
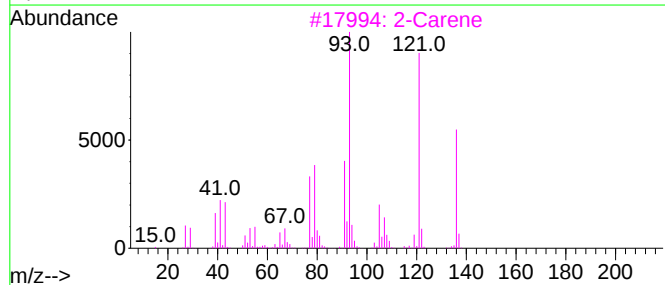
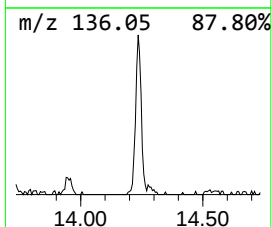
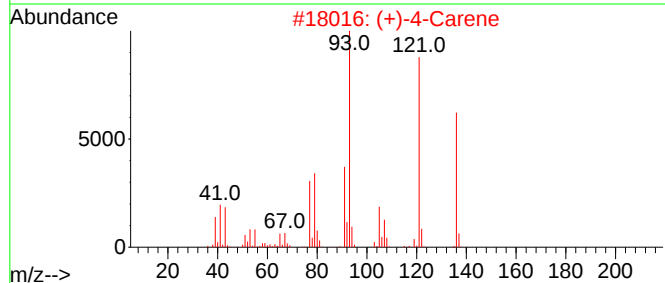
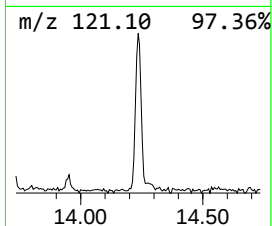
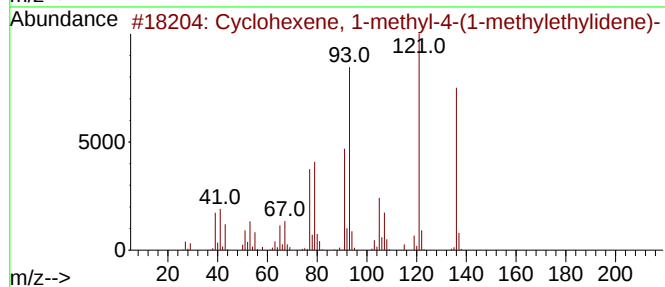
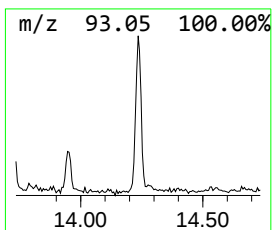
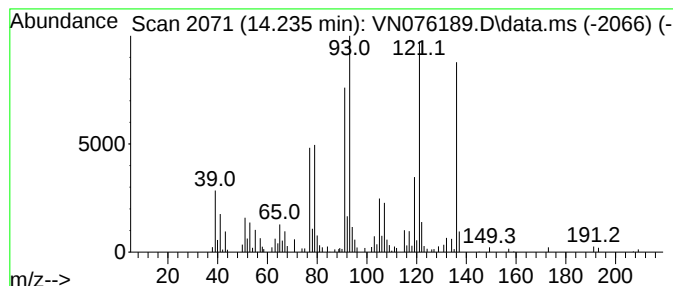
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.235	6.70 ug/l	182304	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	96
2			(+)-4-Carene	136	C10H16	029050-33-7	95
3			2-Carene	136	C10H16	000554-61-0	95
4			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	93
5			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	93



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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SLUDGE-7

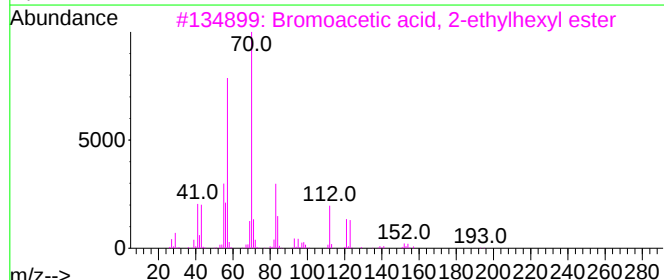
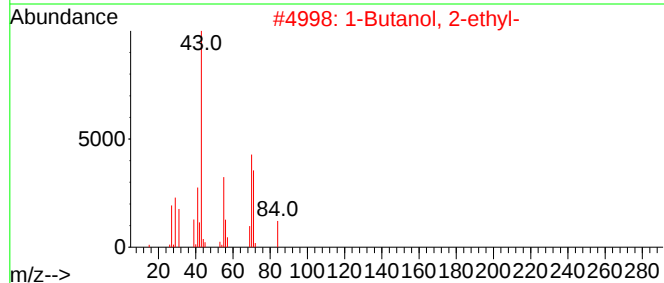
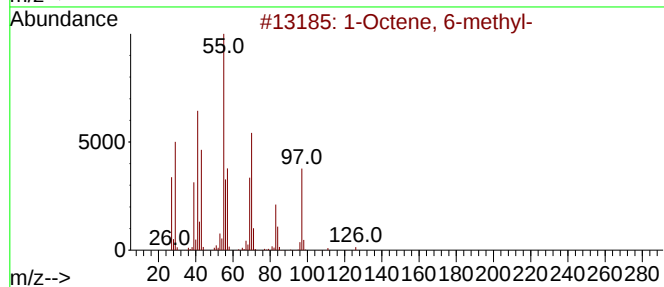
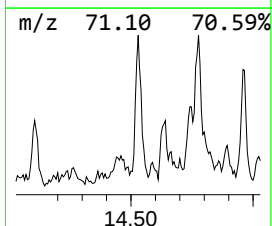
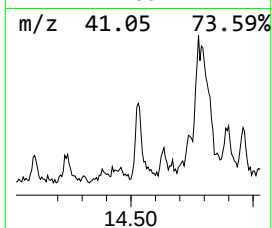
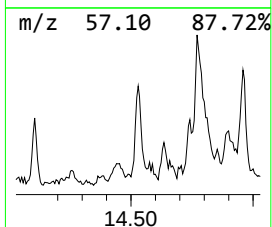
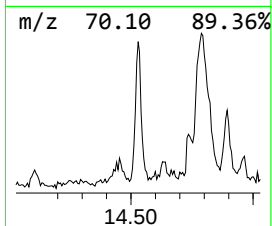
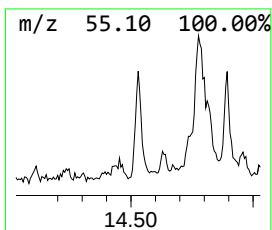
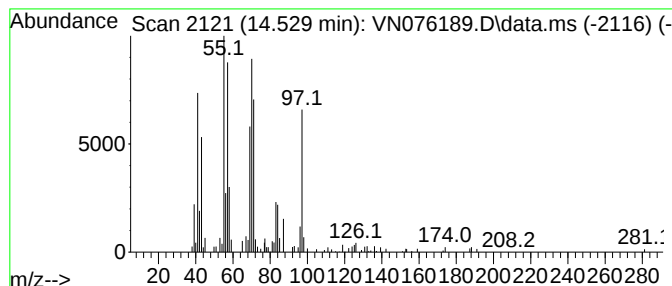
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown14.529 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.529	8.77 ug/l	238515	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octene, 6-methyl-	126	C9H18	013151-10-5	46
2			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	43
3			Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	43
4			1-Heptene, 5-methyl-	112	C8H16	013151-04-7	38
5			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	38



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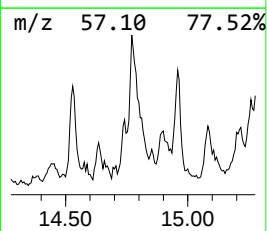
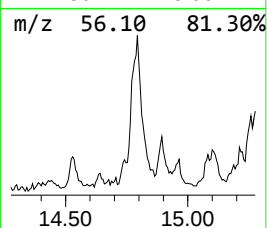
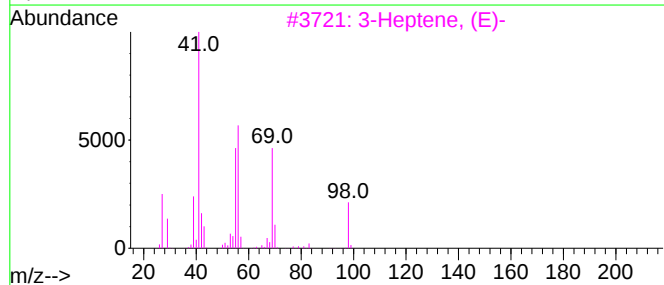
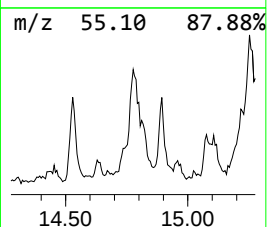
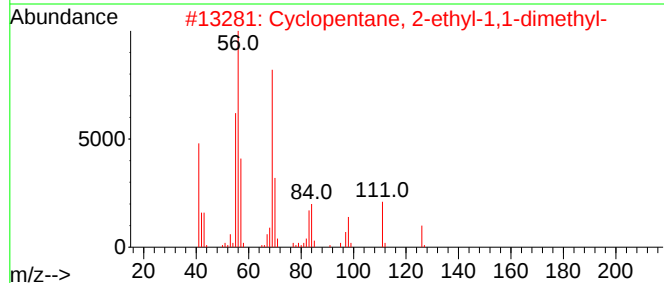
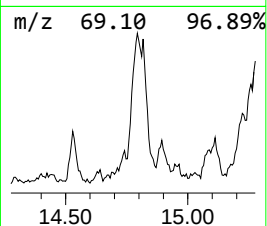
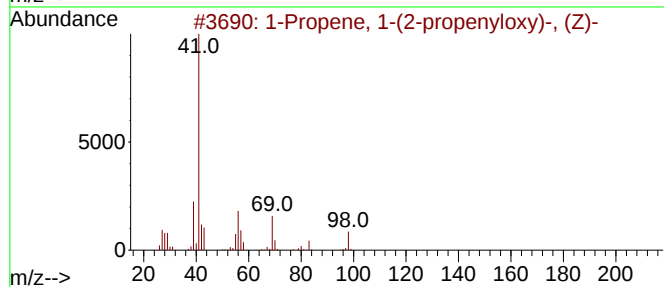
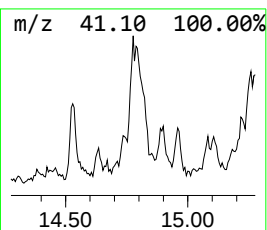
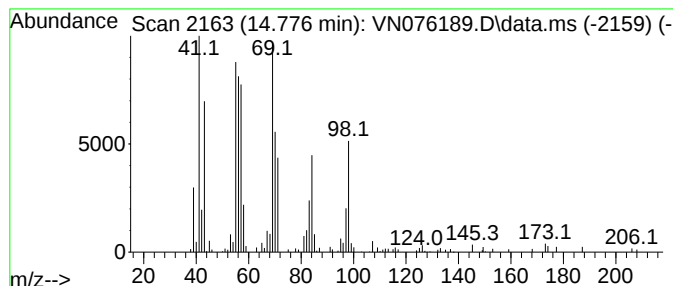
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propene, 1-(2-propenyloxy)... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.776	21.66 ug/l	588931	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propene, 1-(2-propenyloxy)-, (Z)-	98	C6H10O	061142-12-9	50
2			Cyclopentane, 2-ethyl-1,1-dimethyl-	126	C9H18	054549-80-3	49
3			3-Heptene, (E)-	98	C7H14	014686-14-7	46
4			(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	43
5			Cyclooctane, methyl-	126	C9H18	001502-38-1	41



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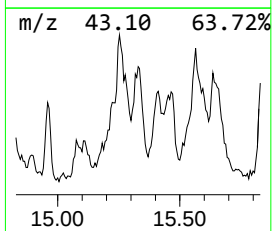
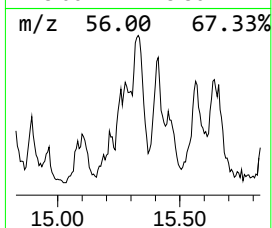
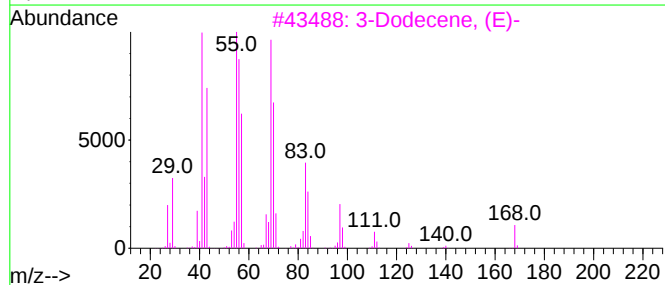
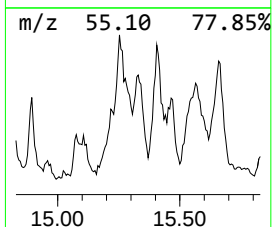
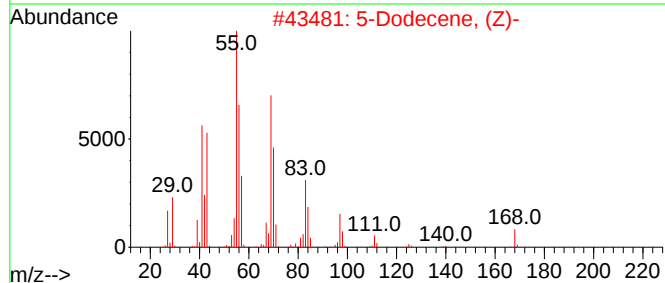
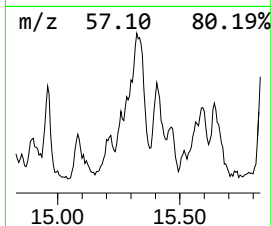
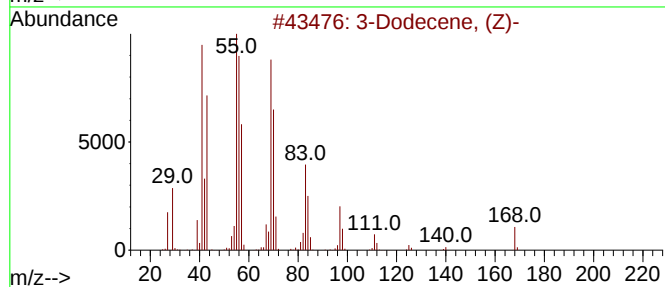
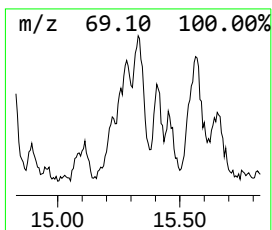
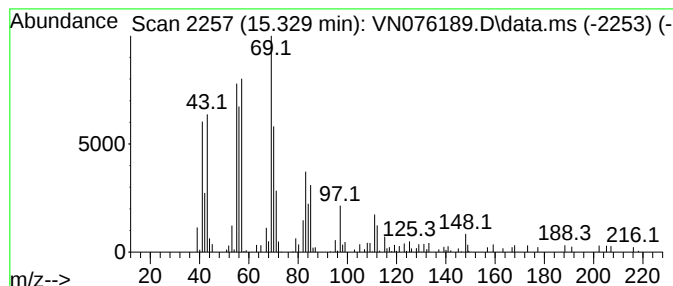
Instrument :
MSVOA_N
ClientSampleId :
SLUDGE-7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 5 3-Dodecene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.329	11.85 ug/l	322335	1,4-Dichlorobenzene-d4			13.794
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Dodecene, (Z)-		168	C12H24	007239-23-8	87
2	5-Dodecene, (Z)-		168	C12H24	007206-28-2	87
3	3-Dodecene, (E)-		168	C12H24	007206-14-6	83
4	6-Dodecene, (Z)-		168	C12H24	007206-29-3	72
5	Cyclooctane, 1,4-dimethyl-, cis-		140	C10H20	013151-99-0	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011023\
Data File : VN076189.D
Acq On : 10 Jan 2023 18:00
Operator : JC\MD
Sample : 01061-04
Misc : 5.08gr/10mL/100uL/5.0mL/MSVOA_N/MeOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SLUDGE-7

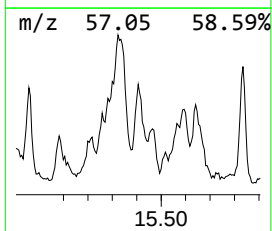
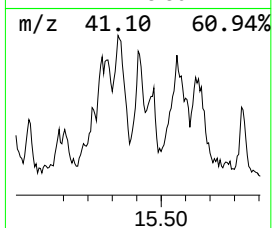
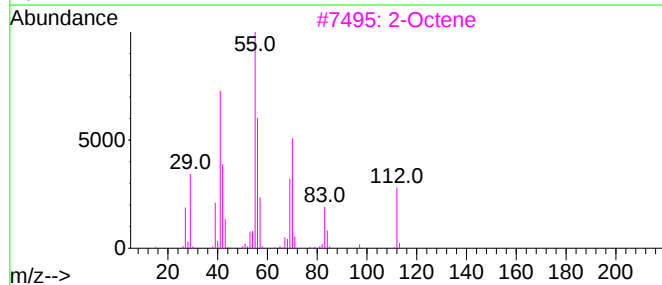
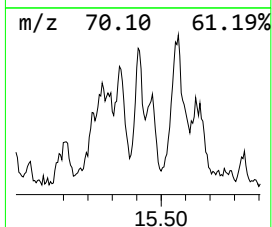
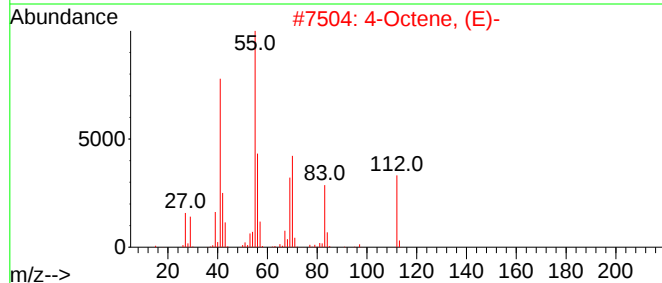
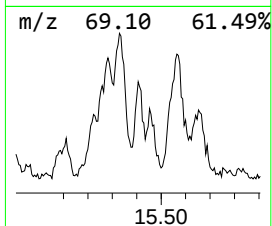
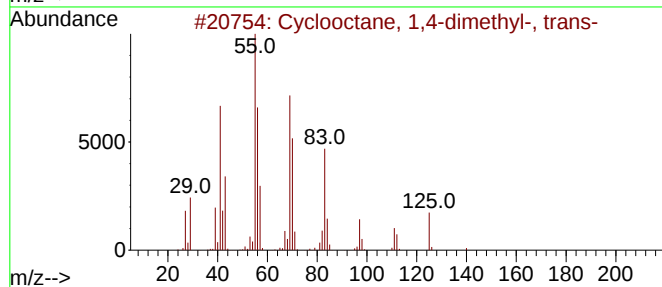
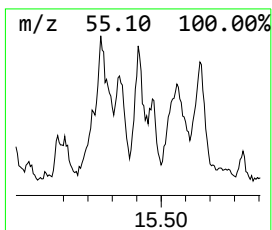
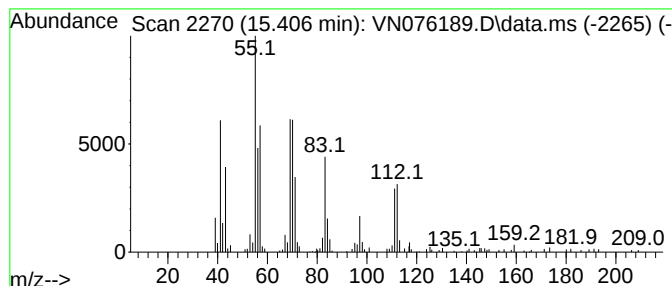
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Quant Title : SW846 8260

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

Peak Number 6 4-Octene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.406	9.44 ug/l	256623	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclooctane, 1,4-dimethyl-, trans-	140	C10H20	013151-98-9	76
2		4-Octene, (E)-	112	C8H16	014850-23-8	59
3		2-Octene	112	C8H16	000111-67-1	53
4		cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	52
5		trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011023\
Data File : VN076189.D
Acq On : 10 Jan 2023 18:00
Operator : JC\MD
Sample : 01061-04
Misc : 5.08gr/10mL/100uL/5.0mL/MSVOA_N/MeOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SLUDGE-7

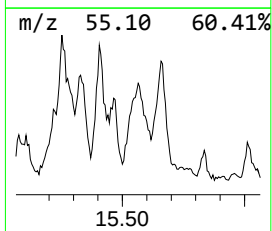
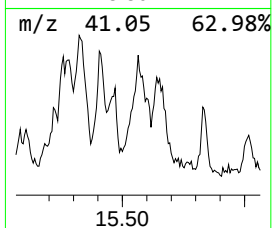
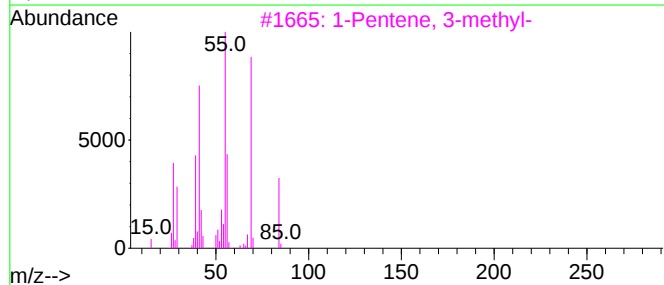
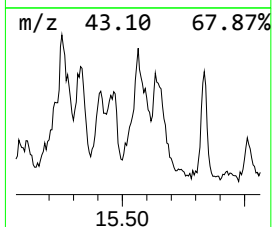
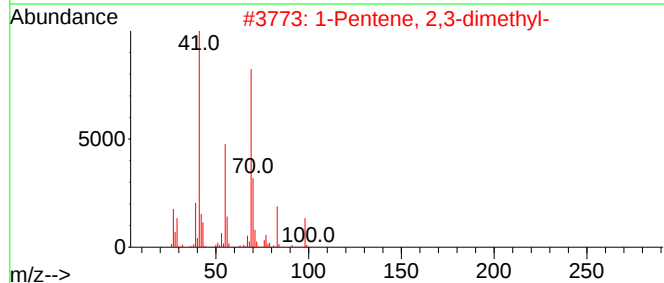
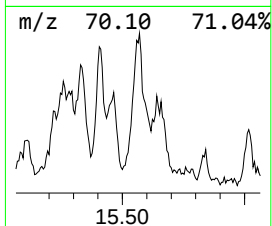
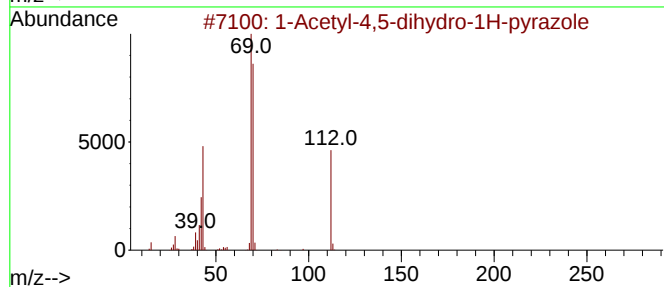
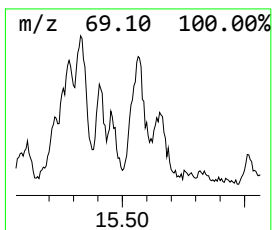
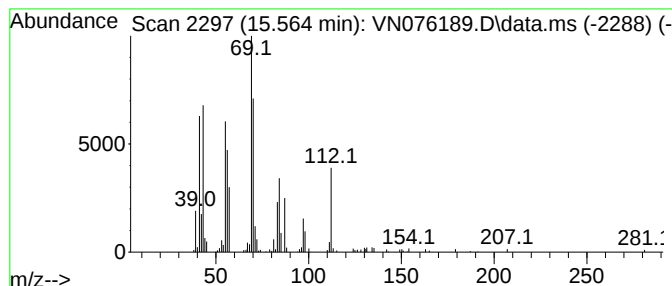
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.564 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.564	13.30 ug/l	361723	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Acetyl-4,5-dihydro-1H-pyrazole	112	C5H8N2O	1000373-42-6	46
2			1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	43
3			1-Pentene, 3-methyl-	84	C6H12	000760-20-3	43
4			3-Ethyl-4-methylpentan-1-ol	130	C8H18O	038514-13-5	35
5			1-Nonene	126	C9H18	000124-11-8	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011023\
Data File : VN076189.D
Acq On : 10 Jan 2023 18:00
Operator : JC\MD
Sample : 01061-04
Misc : 5.08gr/10mL/100uL/5.0mL/MSVOA_N/MeOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
SLUDGE-7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.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
D-Limonene	13.706	66.5	ug/l	1808820	4	13.794	1359650	50.0
Cyclohexene, 1-...	14.235	6.7	ug/l	182304	4	13.794	1359650	50.0
unknown14.529	14.529	8.8	ug/l	238515	4	13.794	1359650	50.0
1-Propene, 1-(2...	14.776	21.7	ug/l	588931	4	13.794	1359650	50.0
3-Dodecene, (Z)-	15.329	11.9	ug/l	322335	4	13.794	1359650	50.0
4-Octene, (E)-	15.406	9.4	ug/l	256623	4	13.794	1359650	50.0
unknown15.564	15.564	13.3	ug/l	361723	4	13.794	1359650	50.0