

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101023\
 Data File : VN079495.D
 Acq On : 10 Oct 2023 16:01
 Operator : JC\MD
 Sample : 04770-01
 Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1037

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\82N100523W.M

Title : SW846 8260

Signal : TIC: VN079495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.224	1059	1066	1076	rVB2	1009271	2464721	1.99%	0.228%
2	8.441	1093	1103	1112	rBV	905158	2027063	1.63%	0.187%
3	8.759	1136	1157	1168	rBV	900455	2905790	2.34%	0.269%
4	8.965	1182	1192	1206	rVB	1475342	2859684	2.31%	0.264%
5	9.106	1207	1216	1224	rBV	672076	1426648	1.15%	0.132%
6	9.594	1285	1299	1304	rBV2	1382562	3542976	2.86%	0.328%
7	10.018	1359	1371	1380	rBV	1187648	2466976	1.99%	0.228%
8	10.147	1380	1393	1398	rBV	1715704	3528734	2.85%	0.326%
9	10.206	1398	1403	1408	rBV	1804897	3235370	2.61%	0.299%
10	10.347	1417	1427	1440	rBV	2159023	4873932	3.93%	0.451%
11	10.494	1442	1452	1458	rBV	894354	1736414	1.40%	0.161%
12	10.571	1458	1465	1469	rBV	2270764	4223545	3.41%	0.391%
13	10.635	1469	1476	1483	rVB	22299049	40316536	32.52%	3.729%
14	10.747	1489	1495	1503	rVB	4108221	7475440	6.03%	0.691%
15	11.012	1531	1540	1548	rBV3	1250117	2778945	2.24%	0.257%
16	11.176	1560	1568	1574	rBV	794383	1415121	1.14%	0.131%
17	11.276	1574	1585	1593	rBV	1096532	2787353	2.25%	0.258%
18	11.423	1606	1610	1614	rVV	1092934	1927814	1.55%	0.178%
19	11.470	1614	1618	1624	rVB	898853	1803363	1.45%	0.167%
20	11.576	1631	1636	1640	rBV	843900	1345961	1.09%	0.124%
21	11.647	1640	1648	1660	rVV3	3385783	8343364	6.73%	0.772%
22	11.747	1660	1665	1671	rVB	2739352	4255266	3.43%	0.394%
23	11.870	1681	1686	1691	rBV	883951	1461949	1.18%	0.135%
24	11.970	1695	1703	1712	rVV	14507190	25666414	20.70%	2.374%
25	12.076	1712	1721	1731	rVV2	64457524	123993415	100.00%	11.468%
26	12.159	1731	1735	1740	rVB2	1199181	2049600	1.65%	0.190%
27	12.406	1764	1777	1785	rBV	30001348	55664702	44.89%	5.148%
28	12.482	1785	1790	1795	rVB2	1213767	2176525	1.76%	0.201%
29	12.617	1795	1813	1818	rBV8	1465436	7079515	5.71%	0.655%
30	12.700	1822	1827	1832	rBV	2377355	4137923	3.34%	0.383%
31	12.882	1856	1858	1863	rVB	1343868	1651385	1.33%	0.153%
32	13.041	1878	1885	1890	rBV	9058140	14545881	11.73%	1.345%
33	13.106	1890	1896	1899	rVV2	34883510	60190063	48.54%	5.567%
34	13.135	1899	1901	1904	rVV	15935870	22591292	18.22%	2.089%
35	13.176	1904	1908	1914	rVB2	21639198	38023433	30.67%	3.517%
36	13.229	1914	1917	1923	rVB2	964165	1528741	1.23%	0.141%

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37	13.341	1926	1936	1943	rBV	14881655	26394792	21.29%	2.441%
38	13.488	1954	1961	1973	rVB3	73197120	120866893	97.48%	11.178%
39	13.617	1974	1983	1987	rBV3	1458634	3636428	2.93%	0.336%
40	13.676	1988	1993	1998	rVB2	3276387	5309199	4.28%	0.491%

41	13.729	1998	2002	2009	rVB3	1167962	2344327	1.89%	0.217%
42	13.823	2009	2018	2031	rVB	21287620	40628952	32.77%	3.758%
43	13.959	2032	2041	2042	rBV	4968403	7879969	6.36%	0.729%
44	13.994	2042	2047	2050	rVV2	16220227	31602831	25.49%	2.923%
45	14.023	2050	2052	2063	rVB3	17271860	33868794	27.31%	3.132%

46	14.111	2063	2067	2074	rBV3	4478802	7918853	6.39%	0.732%
47	14.188	2074	2080	2085	rBV	4761643	7064866	5.70%	0.653%
48	14.247	2085	2090	2093	rBV	9929727	16546020	13.34%	1.530%
49	14.276	2093	2095	2100	rVB	9221429	12517093	10.09%	1.158%
50	14.335	2100	2105	2111	rVB	17780009	26882319	21.68%	2.486%

51	14.400	2112	2116	2119	rBV	1347011	2131368	1.72%	0.197%
52	14.447	2119	2124	2130	rVB3	7519426	13156086	10.61%	1.217%
53	14.576	2141	2146	2151	rBV	4476598	7247257	5.84%	0.670%
54	14.658	2151	2160	2163	rBV	10751944	20432704	16.48%	1.890%
55	14.700	2163	2167	2171	rVB	13409885	18020485	14.53%	1.667%

56	14.741	2171	2174	2177	rVB	4890092	5931490	4.78%	0.549%
57	14.782	2177	2181	2188	rVB	3372735	6278830	5.06%	0.581%
58	14.847	2188	2192	2193	rBV	1183210	1515142	1.22%	0.140%
59	14.882	2193	2198	2202	rVB2	4420748	6395322	5.16%	0.591%
60	14.935	2202	2207	2211	rBV2	9383368	19634801	15.84%	1.816%

61	15.058	2218	2228	2233	rBV3	13882361	38194742	30.80%	3.532%
62	15.106	2233	2236	2249	rVB2	3739966	7177369	5.79%	0.664%
63	15.217	2250	2255	2261	rBV2	2689201	5050706	4.07%	0.467%
64	15.323	2268	2273	2286	rVB3	7252723	19793904	15.96%	1.831%
65	15.447	2286	2294	2300	rVB4	5908926	14128364	11.39%	1.307%

66	15.600	2314	2320	2322	rBV3	2070871	3716756	3.00%	0.344%
67	15.641	2322	2327	2333	rVB	8735559	16664973	13.44%	1.541%
68	15.705	2333	2338	2341	rBV2	1204746	2066621	1.67%	0.191%
69	15.753	2341	2346	2350	rVV3	3637235	5997358	4.84%	0.555%
70	15.835	2357	2360	2371	rVB3	4159402	9111570	7.35%	0.843%

71	15.953	2371	2380	2387	rBV3	4499508	11014765	8.88%	1.019%
72	16.023	2388	2392	2397	rVB	697013	1267727	1.02%	0.117%
73	16.129	2403	2410	2412	rBV3	1720110	3648479	2.94%	0.337%
74	16.170	2413	2417	2426	rVB	3809120	7365122	5.94%	0.681%
75	16.258	2427	2432	2438	rVB2	1613169	2929784	2.36%	0.271%

76	16.347	2438	2447	2453	rBV4	2041035	5656985	4.56%	0.523%
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Title : SW846 8260

77	16.505	2464	2474	2480	rBV4	2328970	6727513	5.43%	0.622%
78	16.717	2499	2510	2515	rBV2	3113886	8039422	6.48%	0.744%

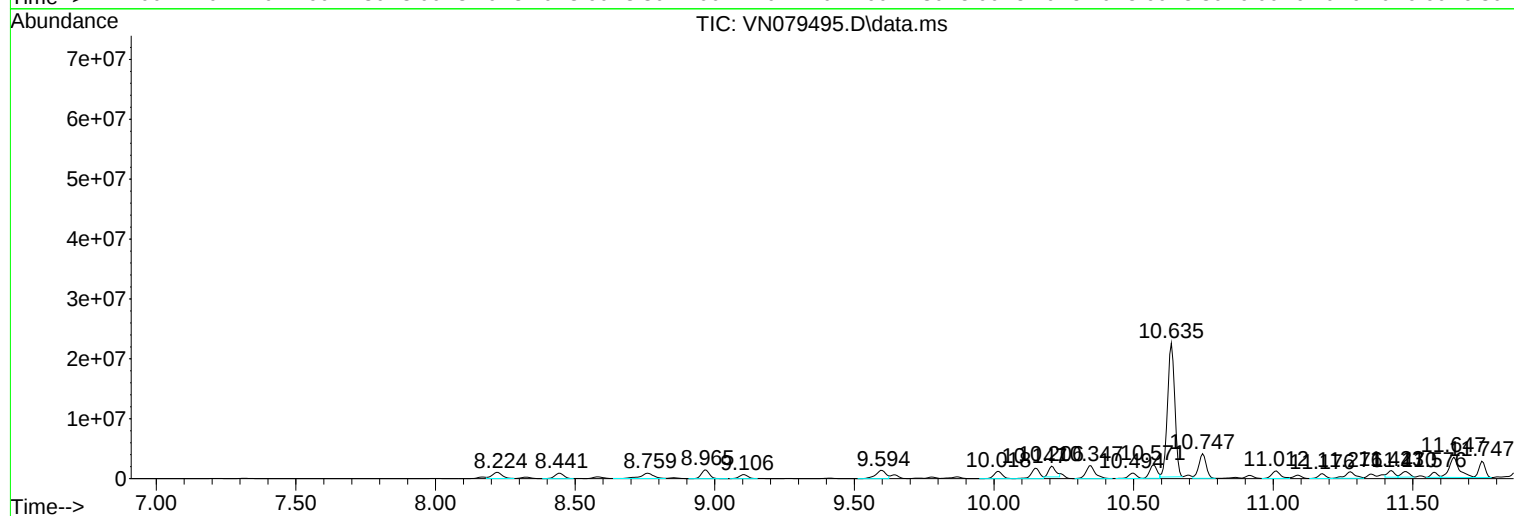
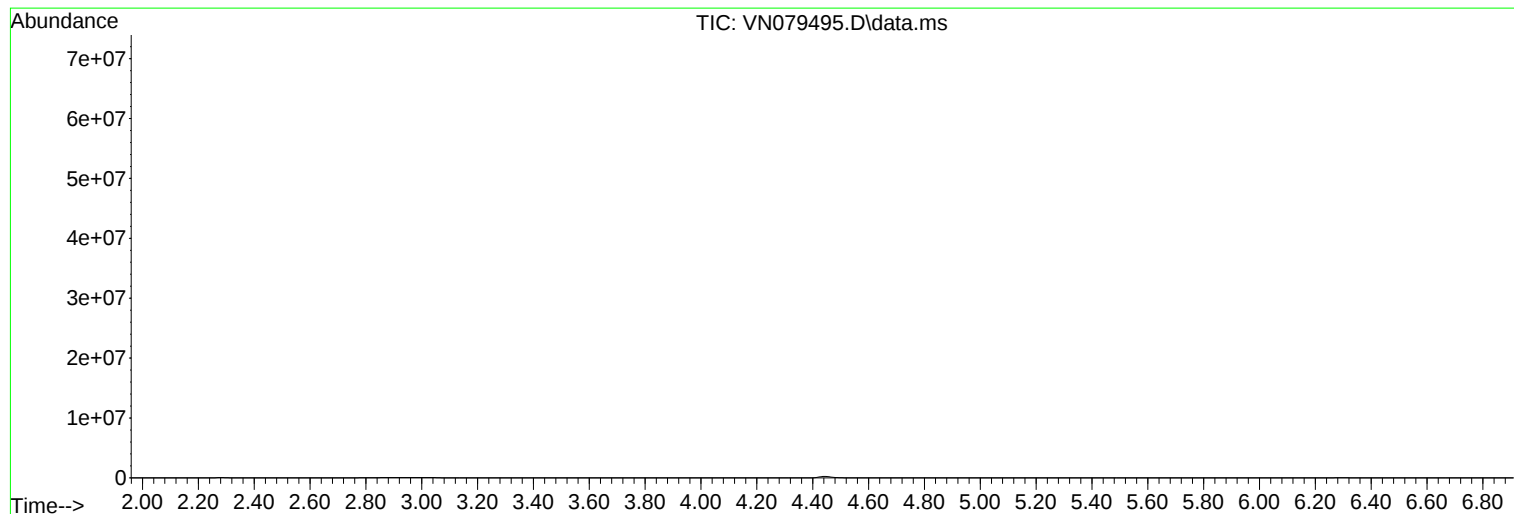
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
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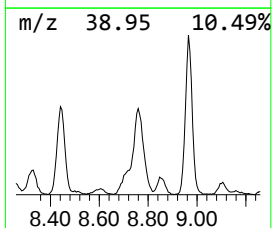
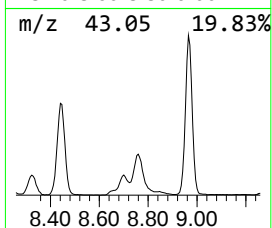
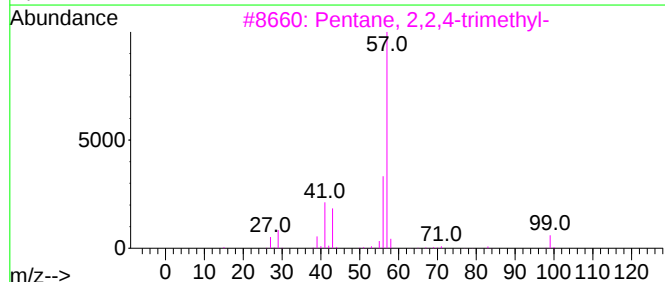
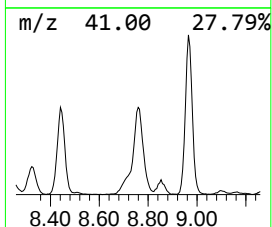
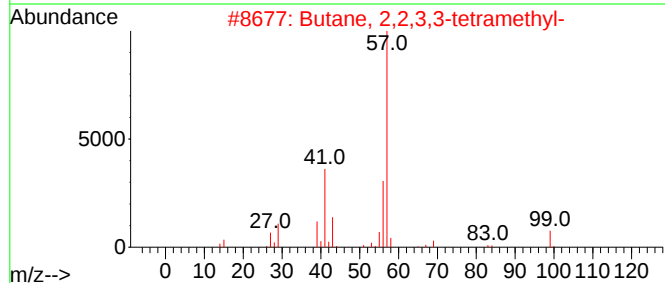
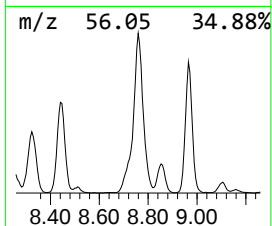
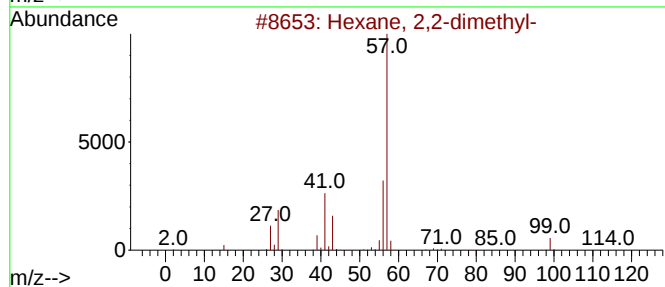
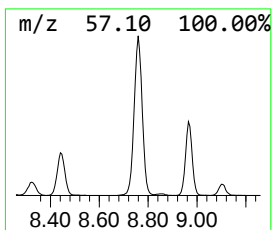
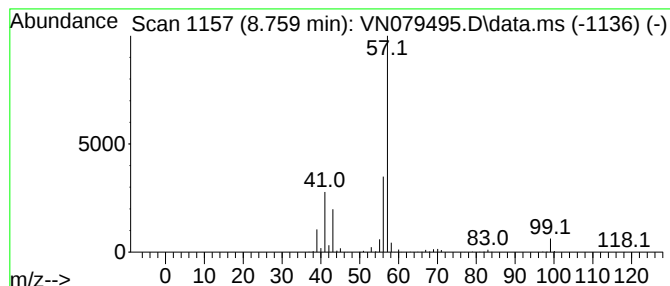
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.759	101.84 ug/l	2905790	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	59
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



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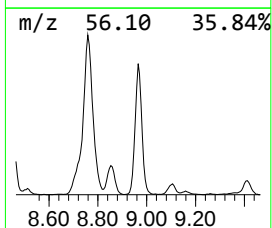
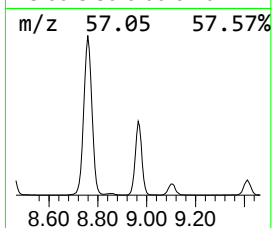
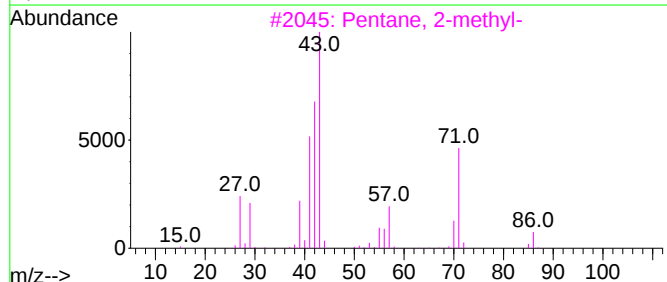
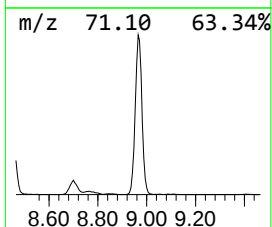
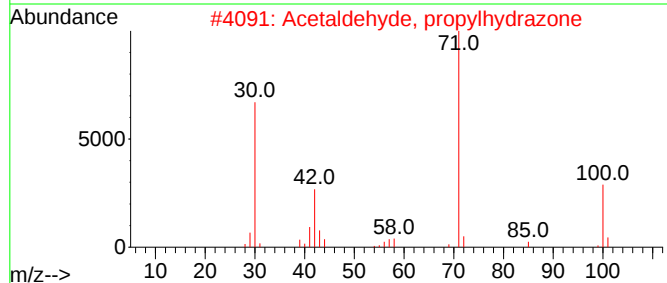
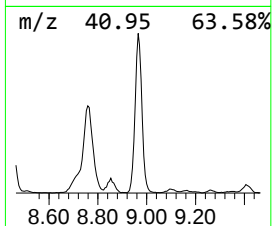
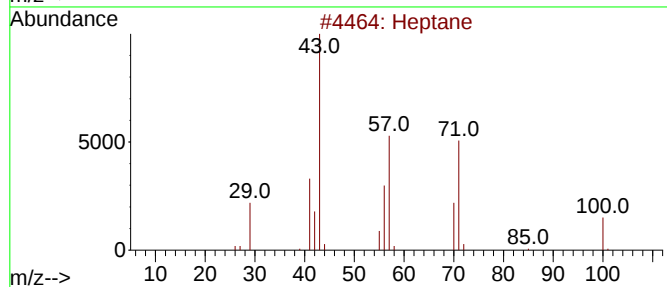
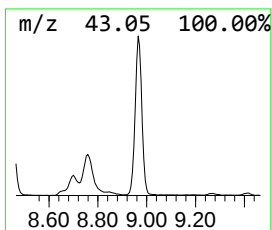
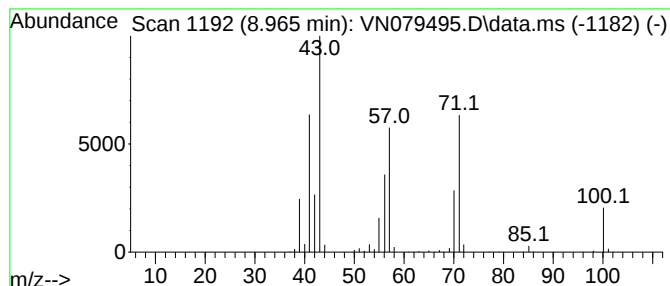
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.965	100.22 ug/l	2859680	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	43
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	43
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38



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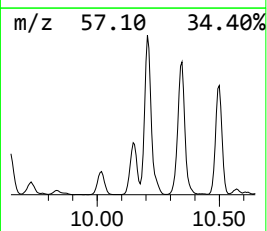
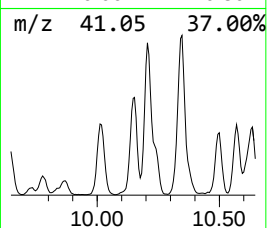
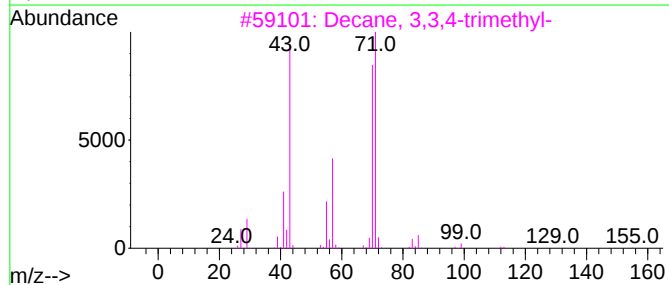
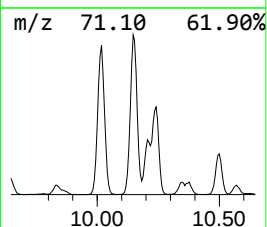
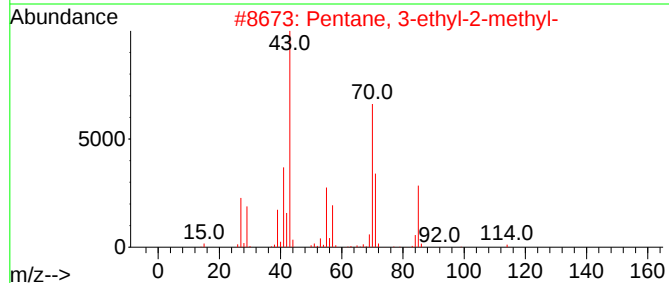
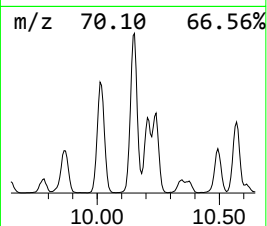
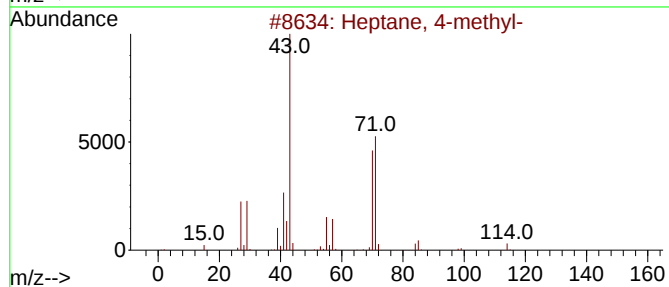
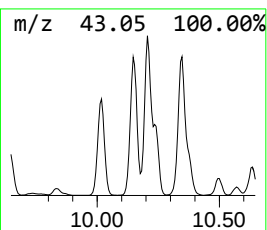
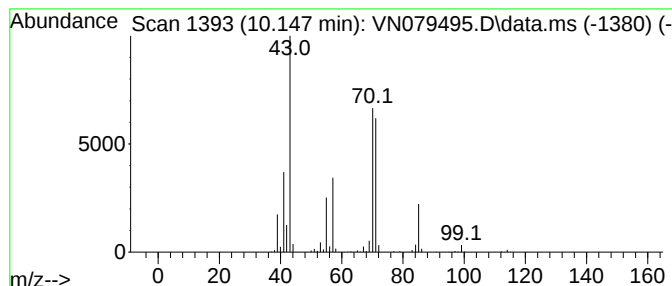
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.147	123.67 ug/l	3528730	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
2			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	64
3			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
4			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	64
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59



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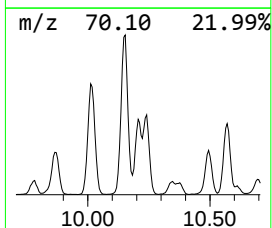
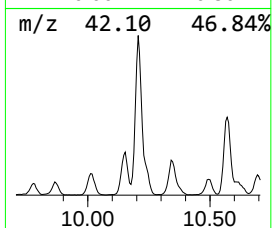
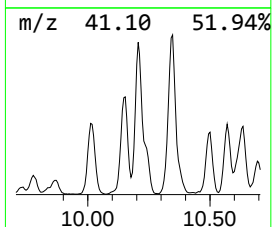
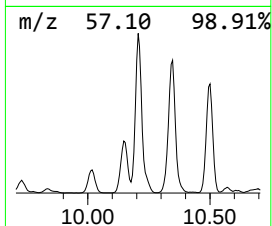
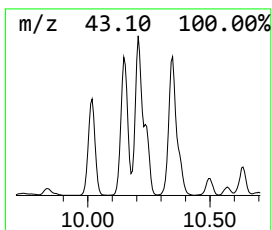
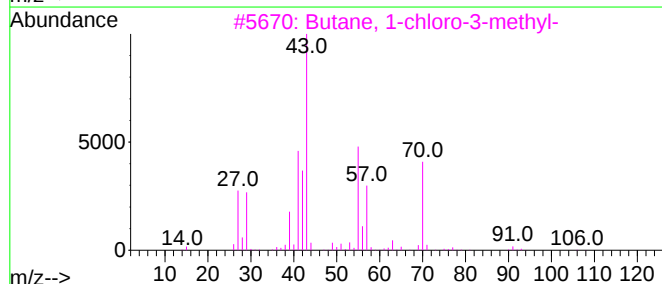
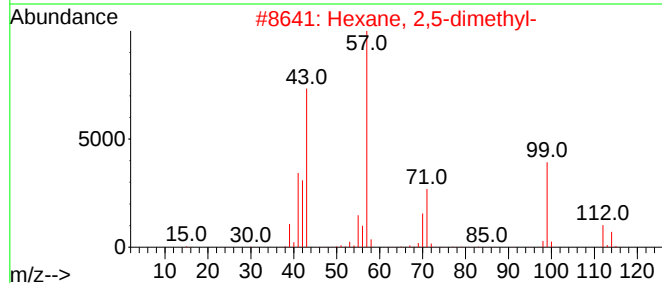
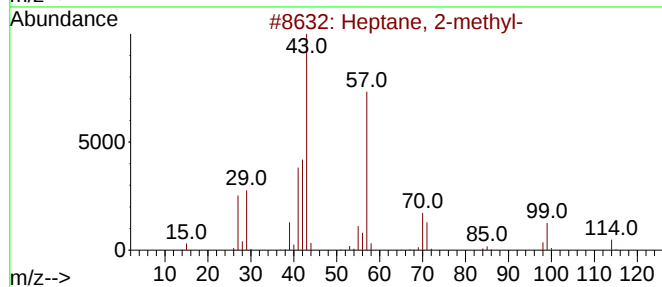
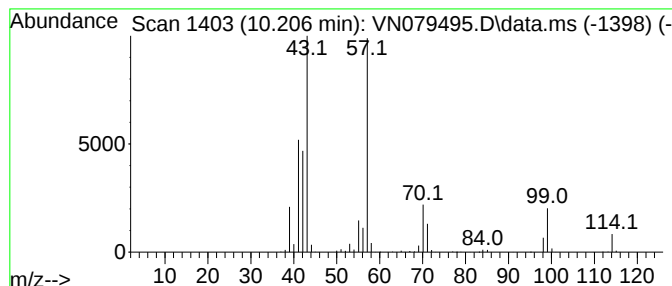
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Quant Title : SW846 8260

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

Peak Number 4 Heptane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.206	113.39 ug/l	3235370	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	90
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	80
3			Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	38
4			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	38
5			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101023\
Data File : VN079495.D
Acq On : 10 Oct 2023 16:01
Operator : JC\MD
Sample : 04770-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1037

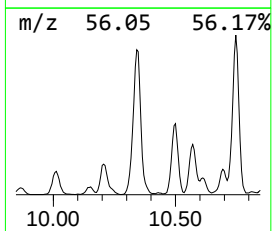
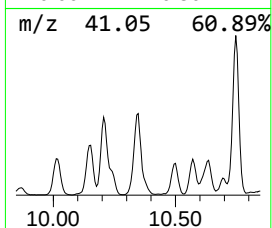
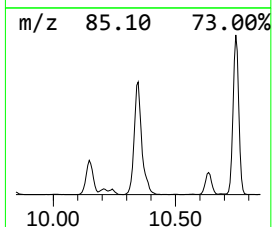
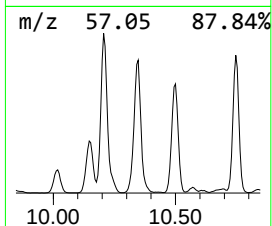
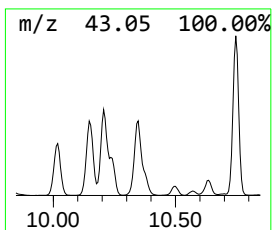
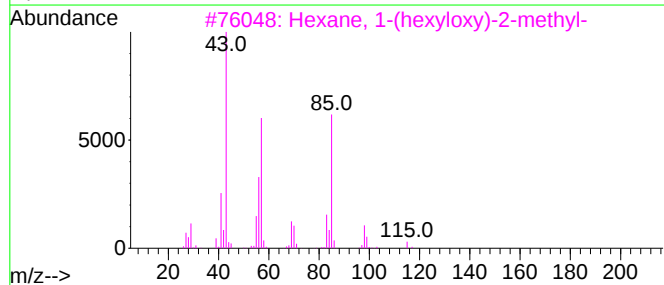
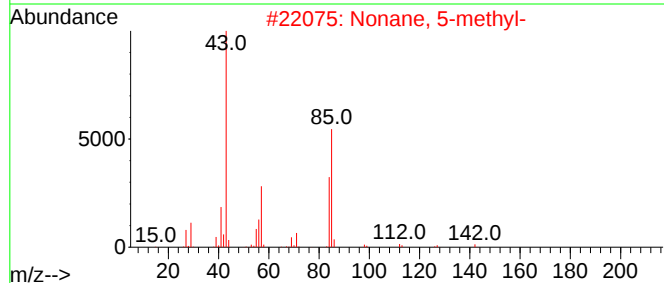
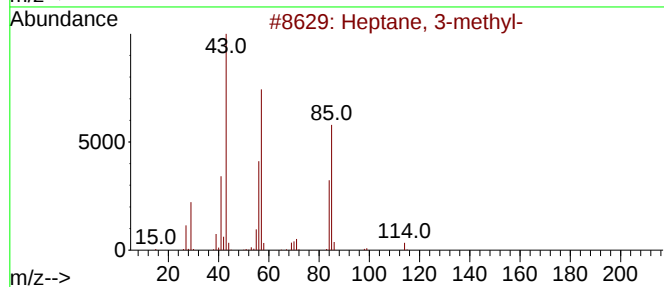
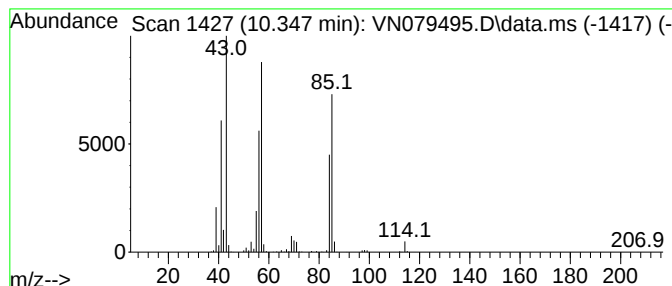
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Quant Title : SW846 8260

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

Peak Number 5 Heptane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.347	170.82 ug/l	4873930	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	90
2			Nonane, 5-methyl-	142	C10H22	015869-85-9	64
3			Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	59
4			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	59
5			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101023\
Data File : VN079495.D
Acq On : 10 Oct 2023 16:01
Operator : JC\MD
Sample : 04770-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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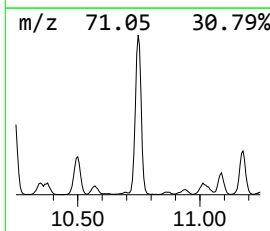
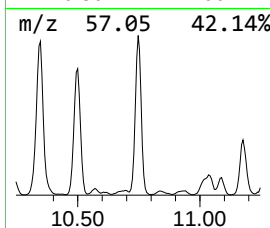
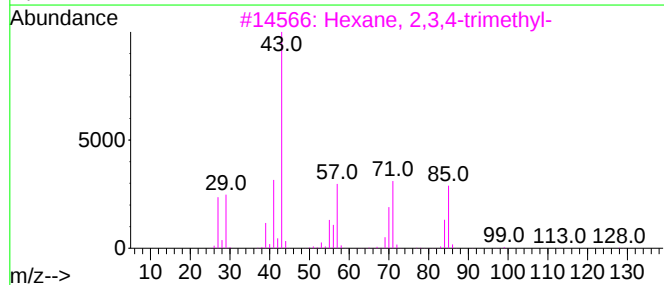
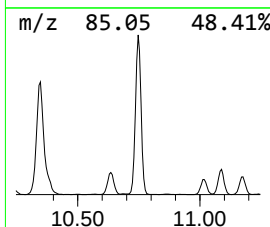
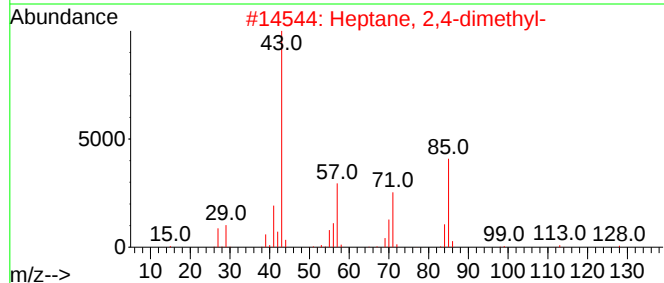
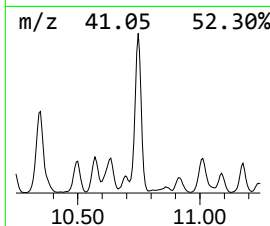
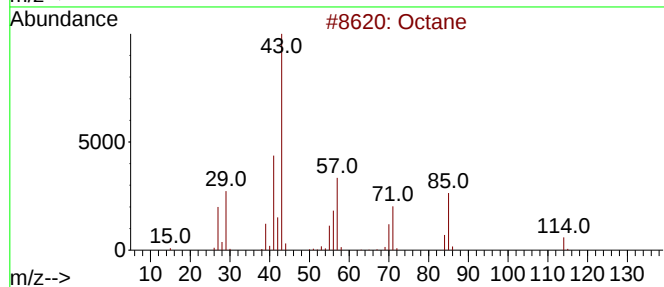
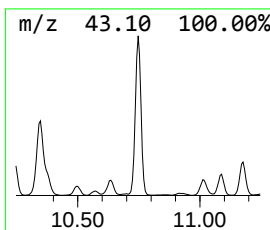
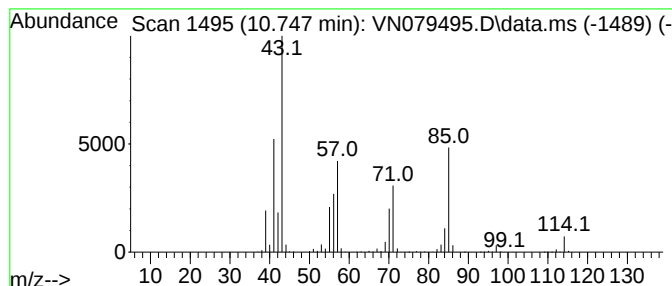
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Quant Title : SW846 8260

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

Peak Number 6 Octane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.747	255.67 ug/l	7475440	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	91
2			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	80
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
4			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	53
5			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101023\
Data File : VN079495.D
Acq On : 10 Oct 2023 16:01
Operator : JC\MD
Sample : 04770-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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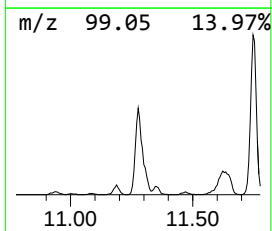
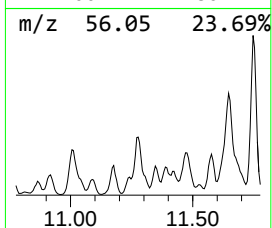
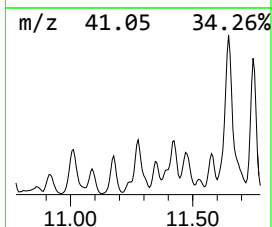
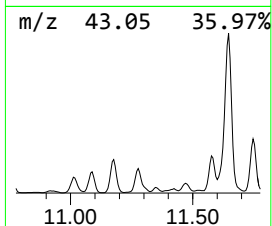
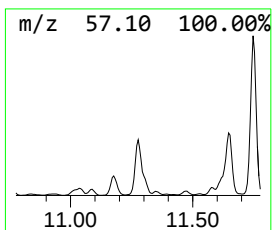
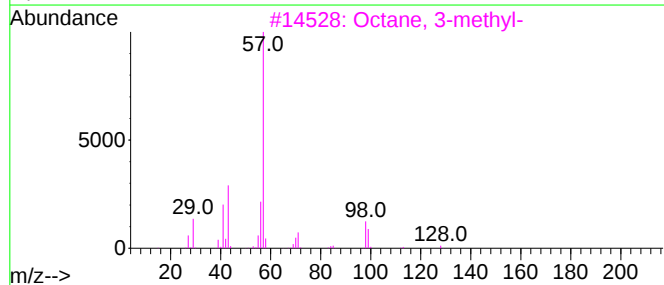
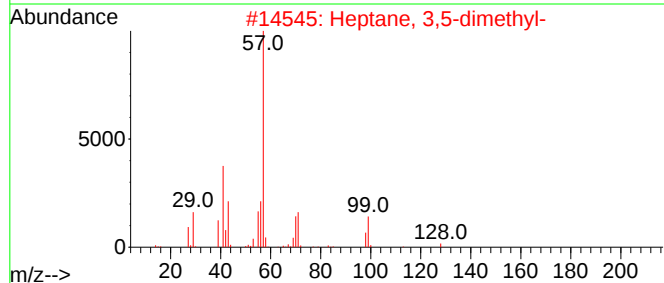
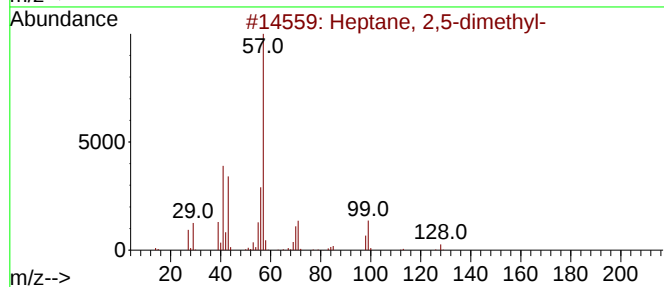
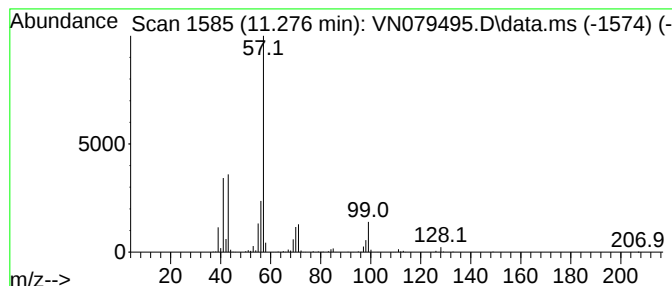
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Quant Title : SW846 8260

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

Peak Number 7 Heptane, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.276	95.33 ug/l	2787350	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	93
2			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	81
3			Octane, 3-methyl-	128	C9H20	002216-33-3	72
4			Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	53
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101023\
Data File : VN079495.D
Acq On : 10 Oct 2023 16:01
Operator : JC\MD
Sample : 04770-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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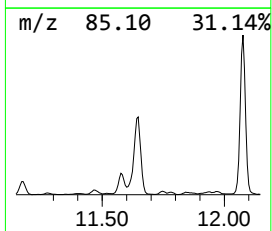
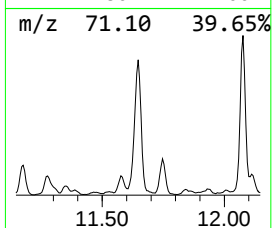
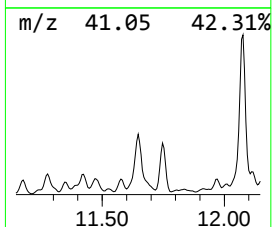
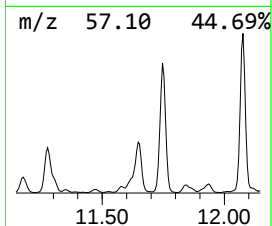
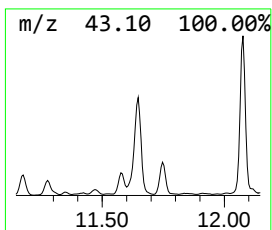
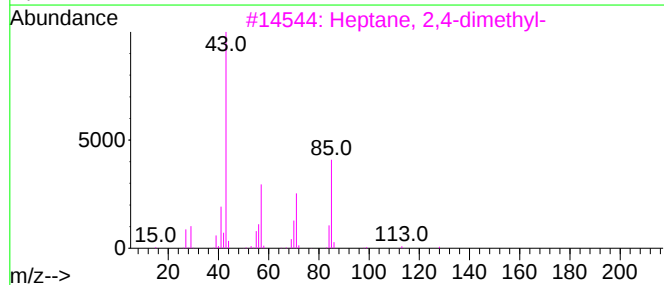
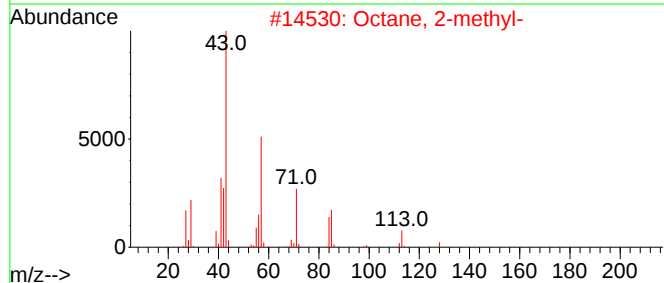
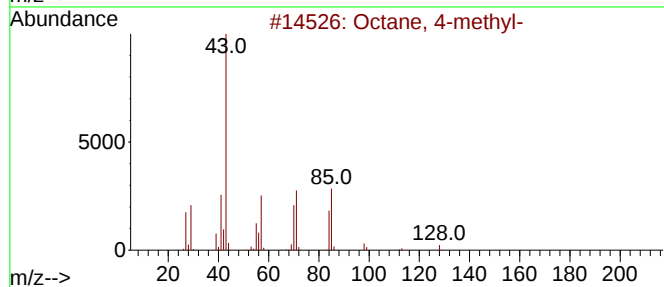
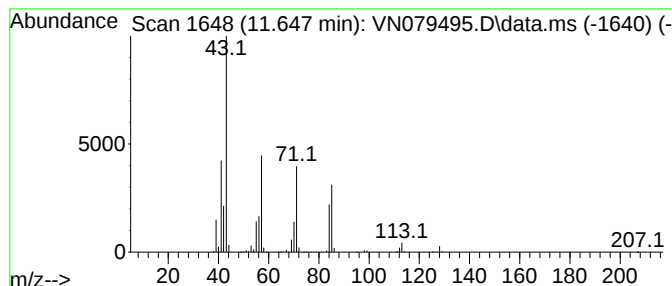
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Quant Title : SW846 8260

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

Peak Number 8 Octane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.647	285.35 ug/l	8343360	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 4-methyl-	128	C9H20	002216-34-4	72
2			Octane, 2-methyl-	128	C9H20	003221-61-2	64
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101023\
Data File : VN079495.D
Acq On : 10 Oct 2023 16:01
Operator : JC\MD
Sample : 04770-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1037

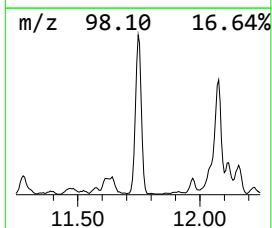
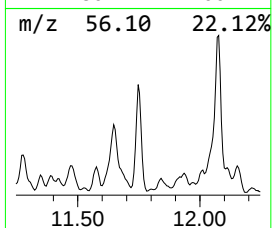
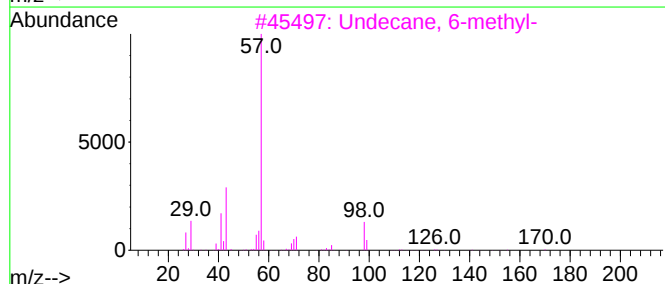
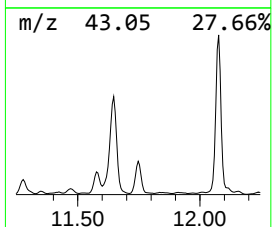
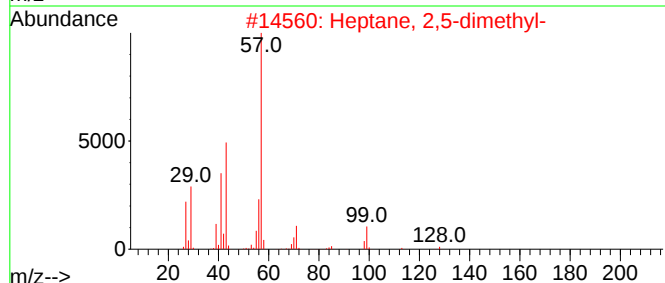
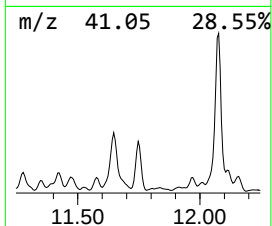
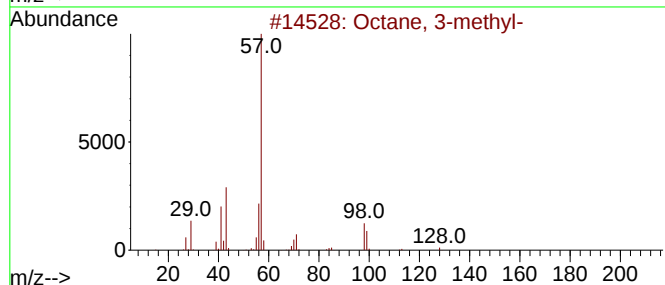
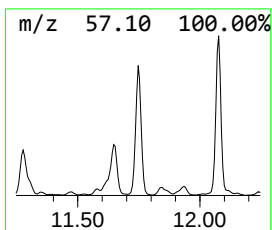
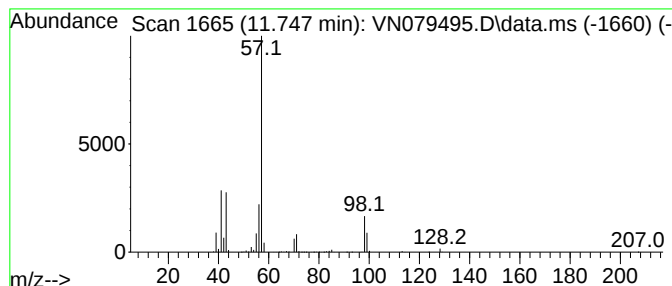
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Quant Title : SW846 8260

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

Peak Number 9 Octane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.747	145.53 ug/l	4255270	Chlorobenzene-d5	11.870

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octane, 3-methyl-	128	C9H20	002216-33-3	91
2		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	72
3		Undecane, 6-methyl-	170	C12H26	017302-33-9	59
4		Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	56
5		Heptane, 4-propyl-	142	C10H22	003178-29-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101023\
Data File : VN079495.D
Acq On : 10 Oct 2023 16:01
Operator : JC\MD
Sample : 04770-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1037

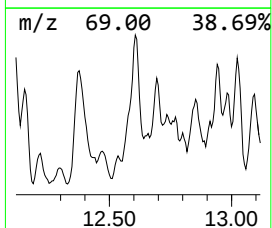
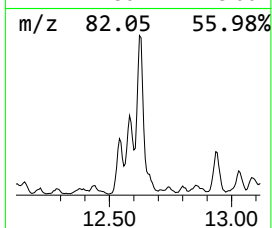
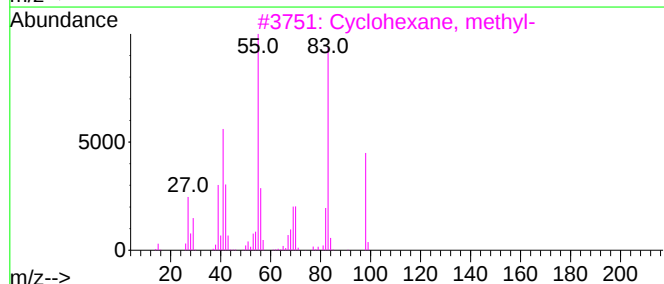
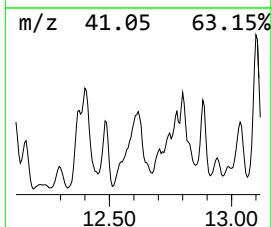
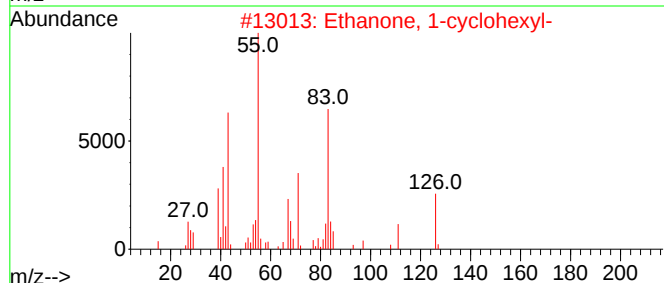
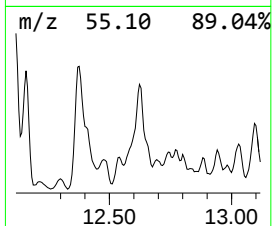
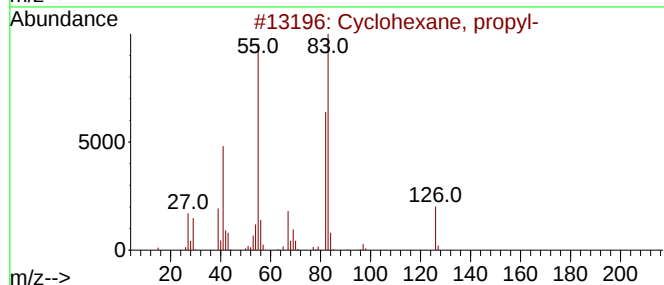
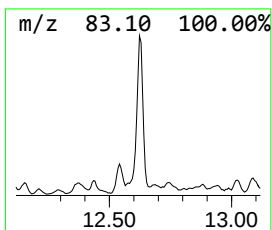
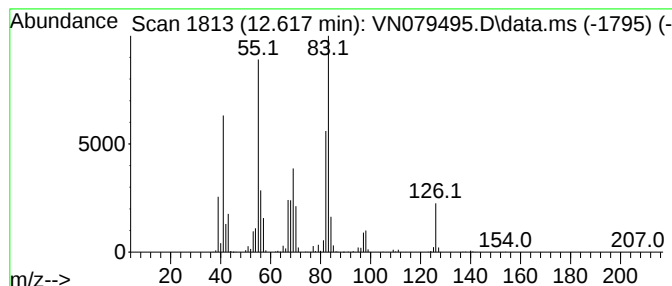
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Quant Title : SW846 8260

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

Peak Number 10 Cyclohexane, propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.617	242.13 ug/l	7079520	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	58
2			Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	49
3			Cyclohexane, methyl-	98	C7H14	000108-87-2	43
4			2-Butyl-.delta.1-pyrroline	125	C8H15N	064319-86-4	43
5			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101023\
Data File : VN079495.D
Acq On : 10 Oct 2023 16:01
Operator : JC\MD
Sample : 04770-01
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1037

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.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
Hexane, 2,2-dim...	8.759	101.8	ug/l	2905790	2	9.106	1426650	50.0
Heptane	8.965	100.2	ug/l	2859680	2	9.106	1426650	50.0
Heptane, 4-methyl-	10.147	123.7	ug/l	3528730	2	9.106	1426650	50.0
Heptane, 2-methyl-	10.206	113.4	ug/l	3235370	2	9.106	1426650	50.0
Heptane, 3-methyl-	10.347	170.8	ug/l	4873930	2	9.106	1426650	50.0
Octane	10.747	255.7	ug/l	7475440	3	11.870	1461950	50.0
Heptane, 2,5-di...	11.276	95.3	ug/l	2787350	3	11.870	1461950	50.0
Octane, 4-methyl-	11.647	285.4	ug/l	8343360	3	11.870	1461950	50.0
Octane, 3-methyl-	11.747	145.5	ug/l	4255270	3	11.870	1461950	50.0
Cyclohexane, pr...	12.617	242.1	ug/l	7079520	3	11.870	1461950	50.0