

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
 Data File : VN083969.D
 Acq On : 18 Sep 2024 07:56
 Operator : JC\MD
 Sample : P3964-08
 Misc : 2.91g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 FDF-5

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\82N091024W.M
 Title : SW846 8260

Signal : TIC: VN083969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.218	1059	1065	1075	rVB2	343271	770611	2.12%	0.305%
2	8.577	1116	1126	1135	rBV	167100	375158	1.03%	0.148%
3	8.753	1139	1156	1168	rBV	653660	1596355	4.39%	0.632%
4	9.094	1206	1214	1222	rBV	427965	894632	2.46%	0.354%
5	9.582	1283	1297	1302	rBV	435677	907986	2.50%	0.359%
6	9.641	1302	1307	1314	rVB	311752	604233	1.66%	0.239%
7	10.012	1361	1370	1380	rBV	1077868	2157583	5.93%	0.854%
8	10.141	1380	1392	1398	rBV	1524207	3114081	8.56%	1.233%
9	10.200	1398	1402	1406	rBV	313901	503415	1.38%	0.199%
10	10.335	1416	1425	1438	rBV	475454	1153621	3.17%	0.457%
11	10.494	1438	1452	1458	rBV	1876194	3486778	9.58%	1.380%
12	10.565	1458	1464	1470	rBV	680737	1247946	3.43%	0.494%
13	10.741	1487	1494	1501	rVB	655148	1191273	3.27%	0.472%
14	11.012	1530	1540	1547	rVV2	469698	1032539	2.84%	0.409%
15	11.171	1558	1567	1574	rBV	259480	514974	1.42%	0.204%
16	11.271	1574	1584	1592	rBV	431118	911457	2.50%	0.361%
17	11.571	1630	1635	1639	rBV	229016	383200	1.05%	0.152%
18	11.641	1639	1647	1659	rVB2	1028908	2336908	6.42%	0.925%
19	11.741	1659	1664	1674	rBV	803394	1388679	3.82%	0.550%
20	11.859	1674	1684	1689	rBV3	900916	2528161	6.95%	1.001%
21	11.929	1689	1696	1697	rVV	522716	1001459	2.75%	0.396%
22	11.959	1697	1701	1708	rVV	2384783	4105746	11.28%	1.625%
23	12.065	1711	1719	1731	rVB	14189269	27734231	76.21%	10.977%
24	12.300	1748	1759	1764	rBV3	328095	717955	1.97%	0.284%
25	12.394	1766	1775	1782	rVV	6992979	12242269	33.64%	4.846%
26	12.476	1784	1789	1795	rVB	385200	715079	1.97%	0.283%
27	12.694	1820	1826	1831	rBV	1886667	3217054	8.84%	1.273%
28	12.823	1841	1848	1855	rVV2	1742067	3223660	8.86%	1.276%
29	12.876	1855	1857	1861	rVB	416356	479614	1.32%	0.190%
30	12.929	1861	1866	1871	rVB4	276566	508695	1.40%	0.201%
31	12.988	1871	1876	1879	rBV	592996	1078746	2.96%	0.427%
32	13.035	1879	1884	1889	rVV	3355170	5058146	13.90%	2.002%
33	13.100	1889	1895	1898	rVV	13430722	22970875	63.12%	9.092%
34	13.129	1898	1900	1903	rVV	5886409	7927956	21.79%	3.138%
35	13.170	1903	1907	1915	rVB	7447532	12986744	35.69%	5.140%
36	13.335	1926	1935	1942	rBV	5221408	8991245	24.71%	3.559%

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Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
 Title : SW846 8260

37	13.423	1942	1950	1954	rBV	1391062	2443946	6.72%	0.967%
38	13.482	1954	1960	1966	rBV	23358527	36390655	100.00%	14.404%
39	13.529	1966	1968	1974	rVB	619178	858169	2.36%	0.340%
40	13.641	1974	1987	1991	rBV3	1706347	4809508	13.22%	1.904%
41	13.823	2008	2018	2030	rVB2	5690011	14309074	39.32%	5.664%
42	13.953	2034	2040	2041	rBV2	1095953	1691692	4.65%	0.670%
43	13.988	2041	2046	2049	rBV2	3835762	7526637	20.68%	2.979%
44	14.106	2062	2066	2073	rVV3	442123	776041	2.13%	0.307%
45	14.182	2074	2079	2084	rVB	1214896	2030572	5.58%	0.804%
46	14.241	2084	2089	2092	rBV	1906939	3238672	8.90%	1.282%
47	14.270	2092	2094	2099	rVV	1741671	2204211	6.06%	0.872%
48	14.329	2099	2104	2112	rVB	3406699	5380127	14.78%	2.129%
49	14.441	2117	2123	2128	rVB3	817196	1411633	3.88%	0.559%
50	14.570	2140	2145	2151	rVB	720426	1152164	3.17%	0.456%
51	14.653	2151	2159	2162	rBV	2107794	3644758	10.02%	1.443%
52	14.688	2162	2165	2170	rVV	2544461	3862011	10.61%	1.529%
53	14.735	2170	2173	2177	rVB2	930507	1283299	3.53%	0.508%
54	14.806	2182	2185	2192	rVB	383635	582475	1.60%	0.231%
55	14.876	2192	2197	2200	rBV2	376005	507572	1.39%	0.201%
56	14.923	2200	2205	2209	rBV	1084149	1987795	5.46%	0.787%
57	15.029	2216	2223	2224	rBV3	1616860	2986588	8.21%	1.182%
58	15.094	2232	2234	2243	rVB2	404029	749108	2.06%	0.297%
59	15.211	2249	2254	2261	rVB4	201963	436661	1.20%	0.173%
60	15.317	2262	2272	2284	rVV3	673003	1937780	5.32%	0.767%
61	15.429	2286	2291	2300	rVB3	416285	1006498	2.77%	0.398%
62	15.635	2313	2326	2334	rBV	1749231	3885027	10.68%	1.538%
63	15.747	2339	2345	2349	rVV2	224483	448418	1.23%	0.177%
64	15.823	2350	2358	2370	rVB2	417665	1314932	3.61%	0.520%
65	15.941	2370	2378	2386	rBV	339633	839870	2.31%	0.332%
66	16.253	2426	2431	2437	rVV3	172247	375664	1.03%	0.149%
67	16.335	2439	2445	2452	rVB3	264899	623124	1.71%	0.247%
68	16.776	2513	2520	2522	rBV	1052152	1894852	5.21%	0.750%

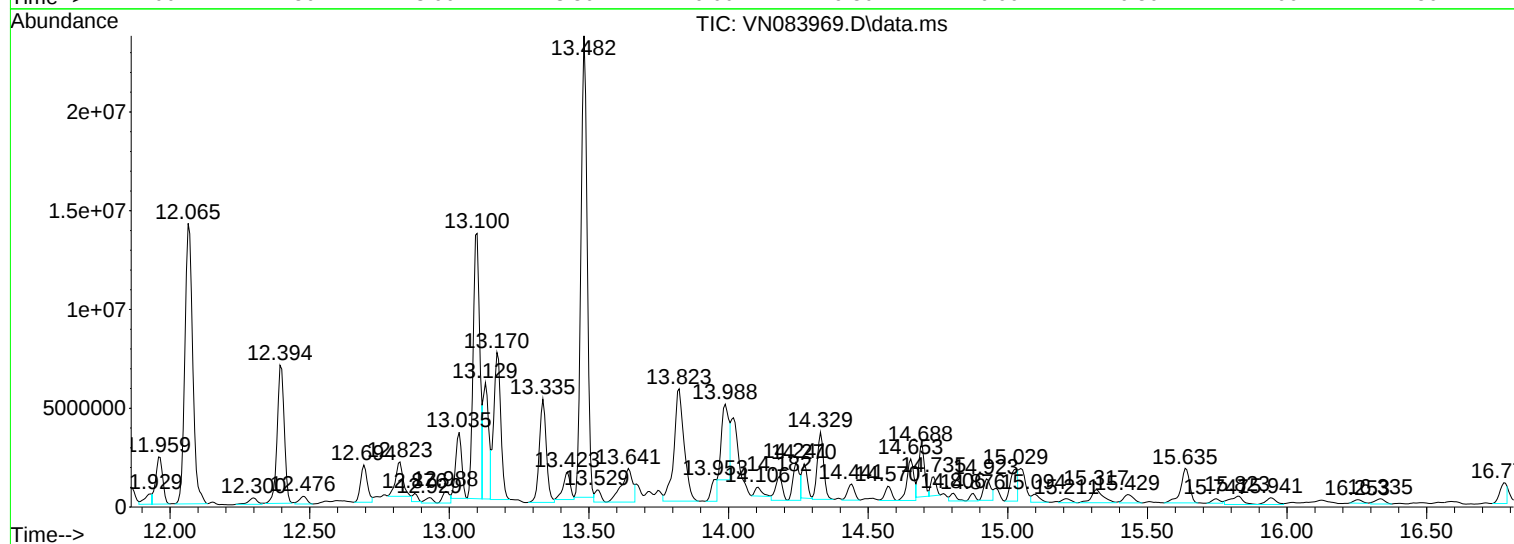
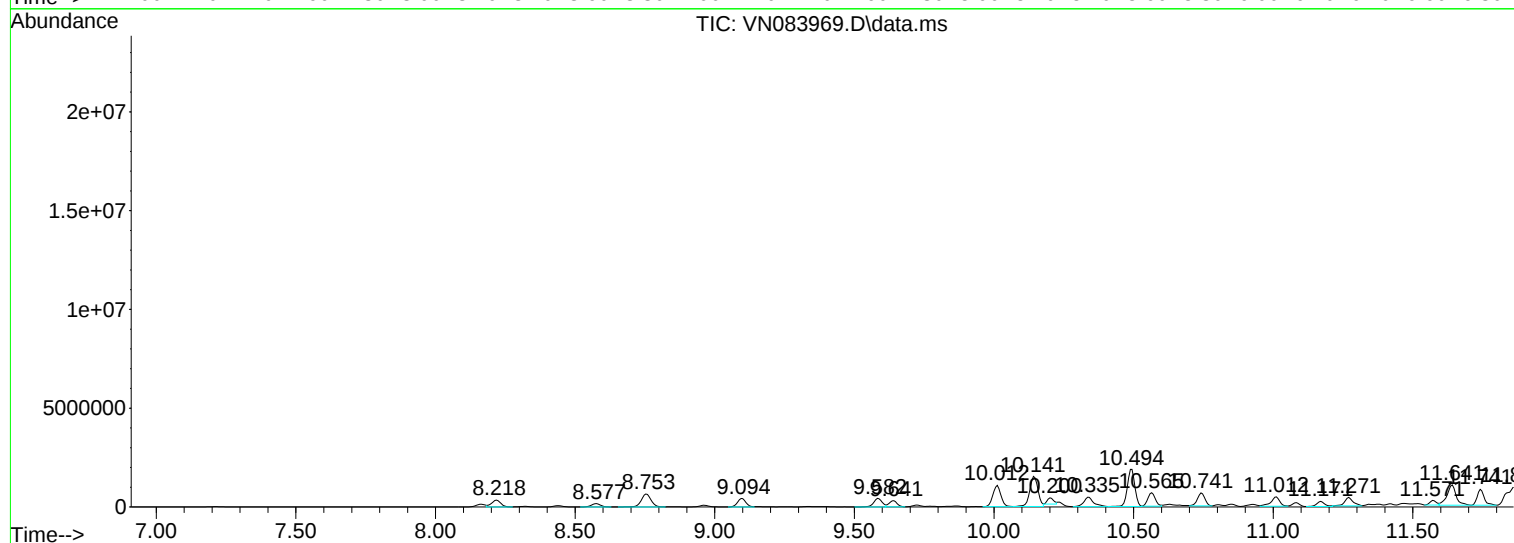
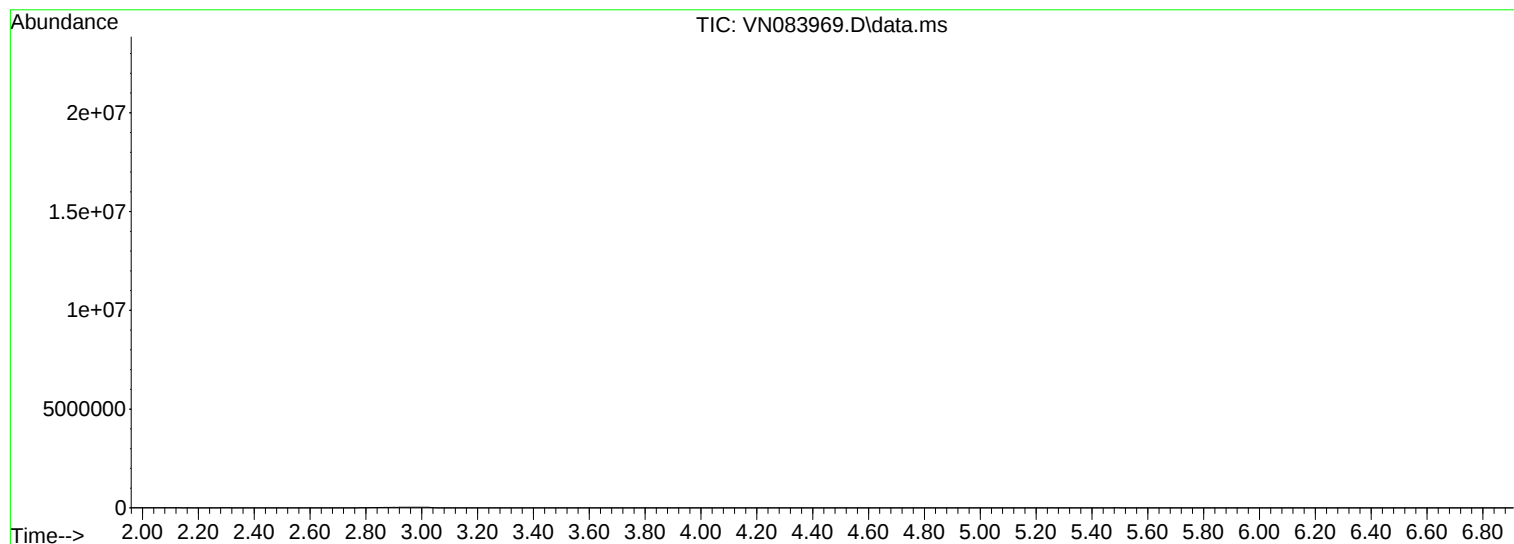
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Instrument :
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ClientSampleId :
FDF-5

Quant Title :

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



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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-5

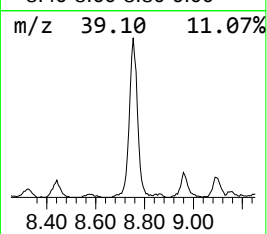
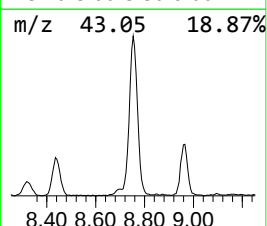
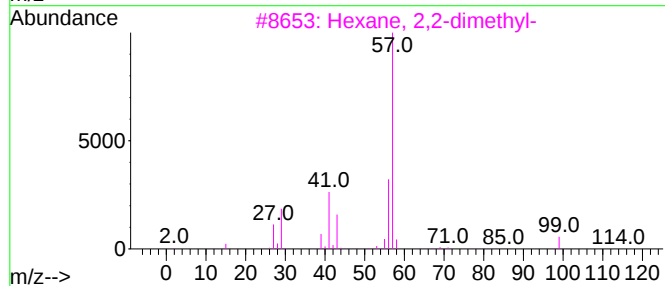
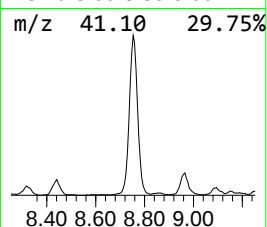
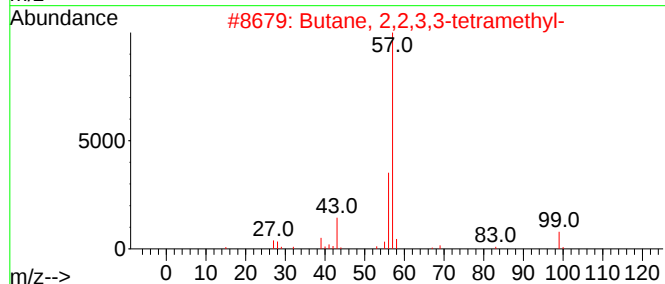
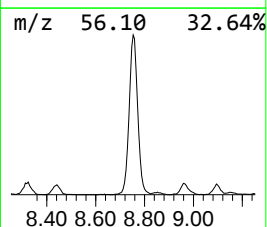
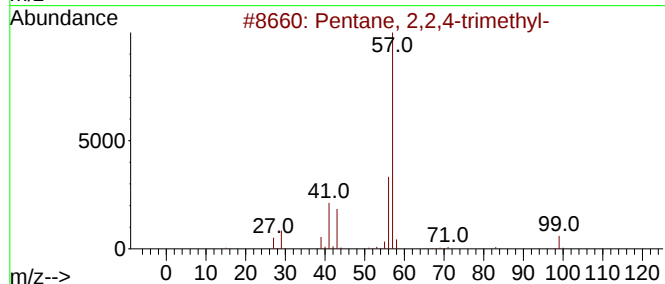
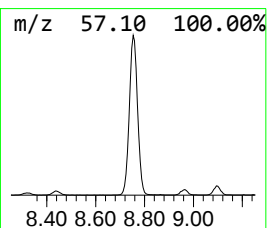
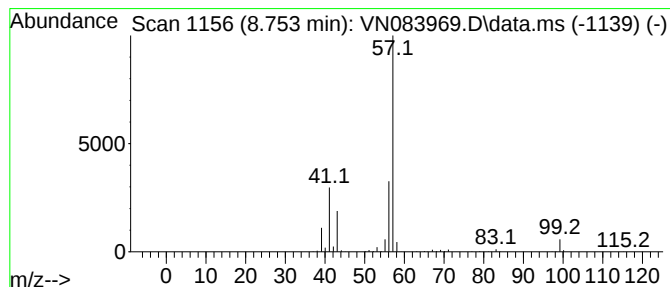
Quant Title :

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

Peak Number 1 Pentane, 2,2,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.753	89.22 ug/l	1596360	1,4-Difluorobenzene	9.094

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	50



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FDF-5

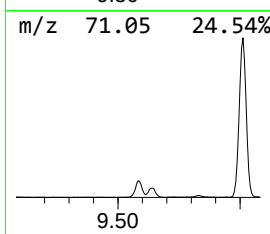
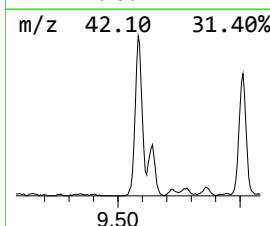
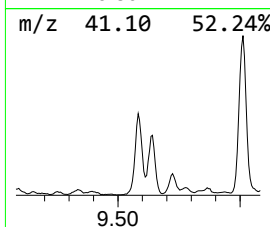
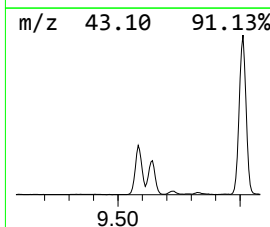
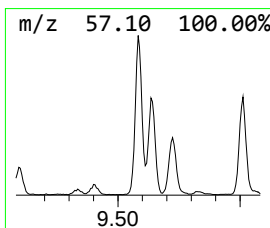
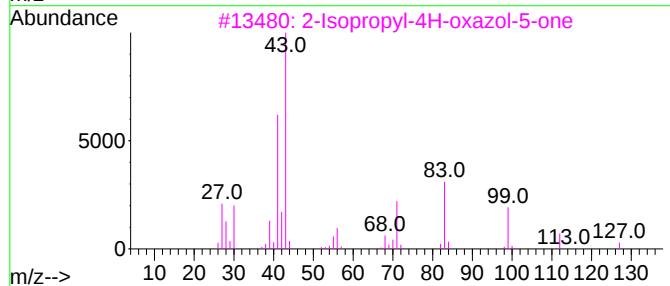
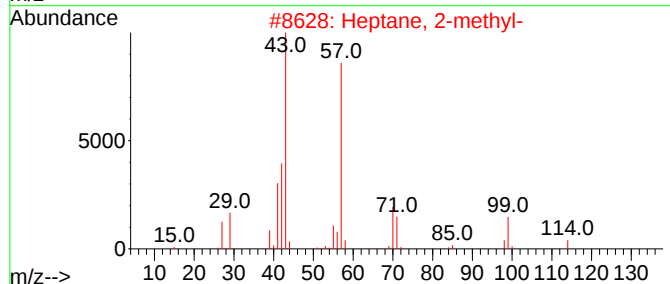
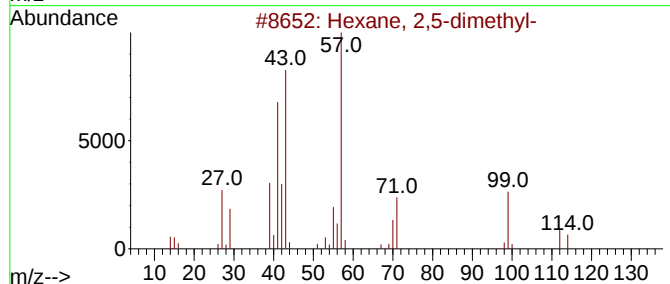
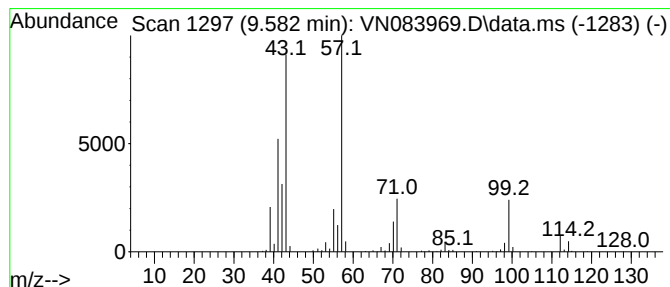
Quant Title :

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

Peak Number 2 Hexane, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.582	50.75 ug/l	907986	1,4-Difluorobenzene	9.094

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	97
2		Heptane, 2-methyl-	114	C8H18	000592-27-8	59
3		2-Isopropyl-4H-oxazol-5-one	127	C6H9NO2	1000190-01-9	50
4		1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	49
5		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	47



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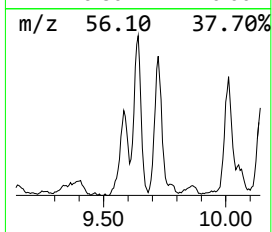
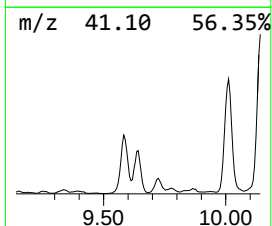
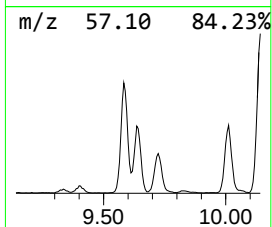
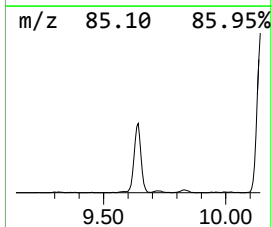
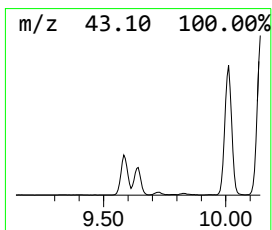
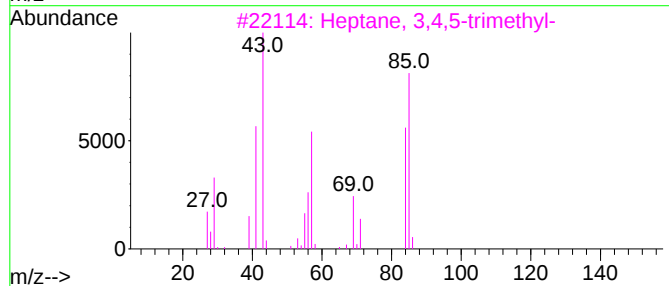
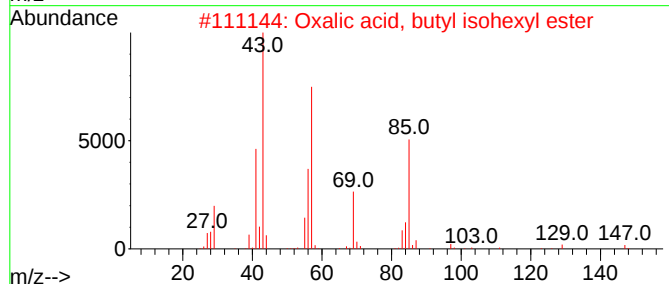
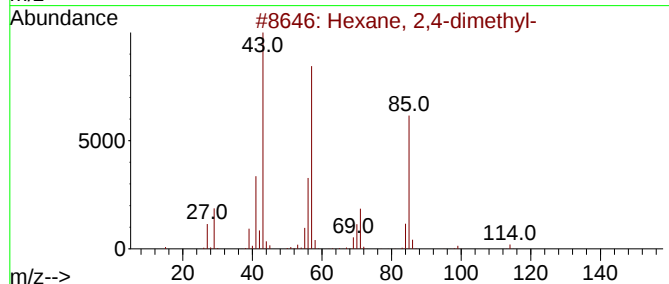
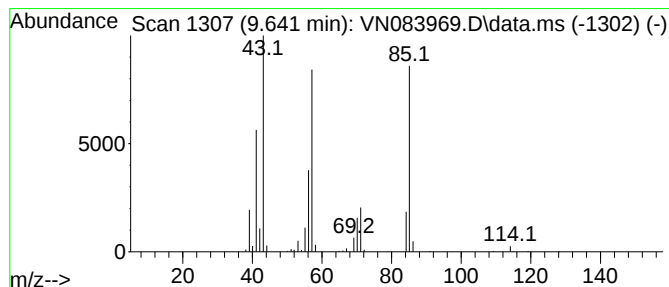
Quant Title :

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

Peak Number 3 Hexane, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.641	33.77 ug/l	604233	1,4-Difluorobenzene	9.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	91
2			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	72
3			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	72
4			Nonane, 5-methyl-	142	C10H22	015869-85-9	72
5			Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	59



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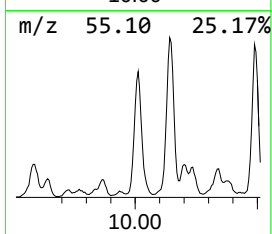
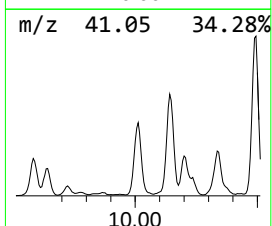
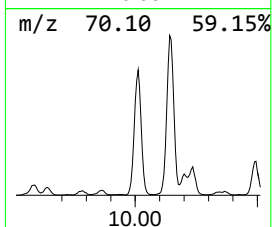
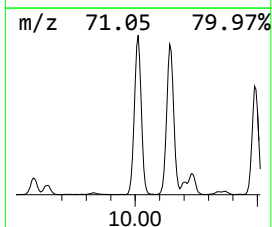
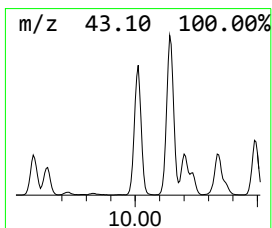
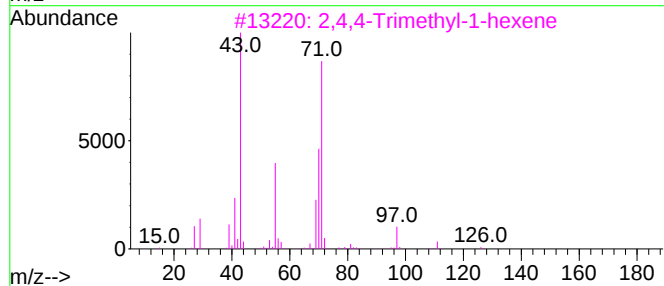
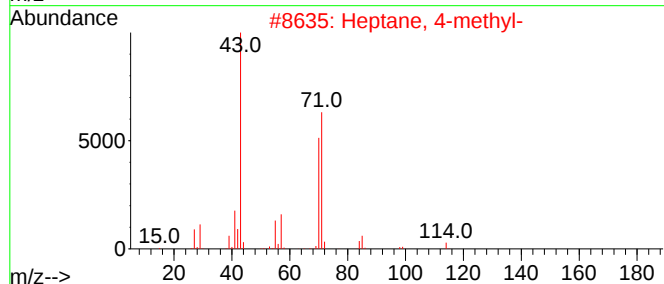
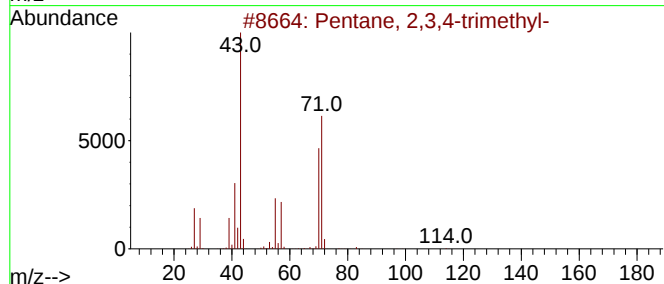
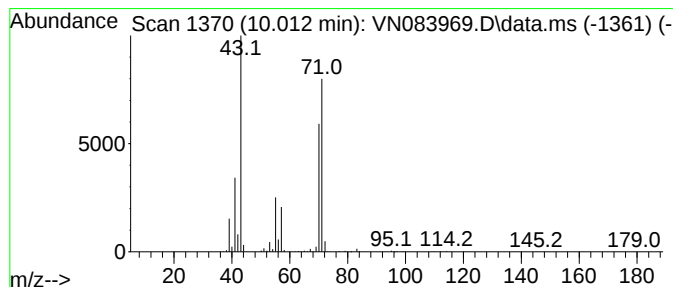
Quant Title :

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

Peak Number 4 Pentane, 2,3,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.012	120.58 ug/l	2157580	1,4-Difluorobenzene	9.094

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3		2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083969.D
Acq On : 18 Sep 2024 07:56
Operator : JC\MD
Sample : P3964-08
Misc : 2.91g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-5

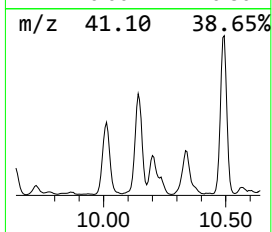
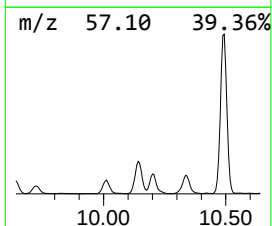
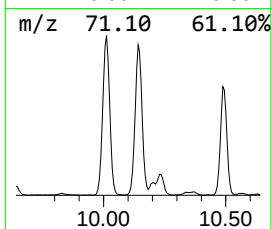
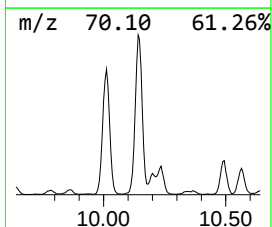
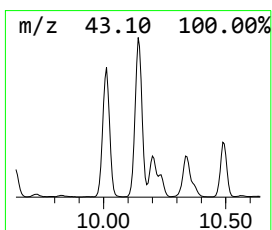
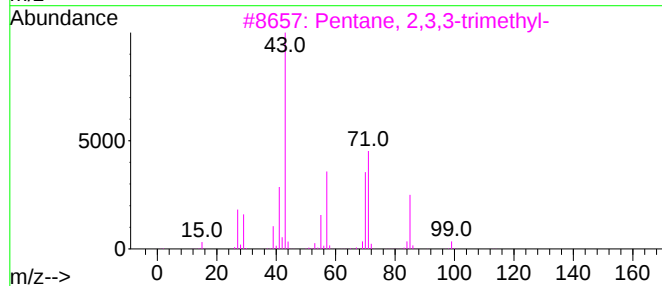
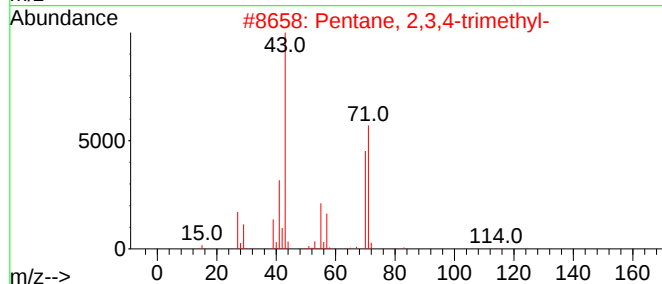
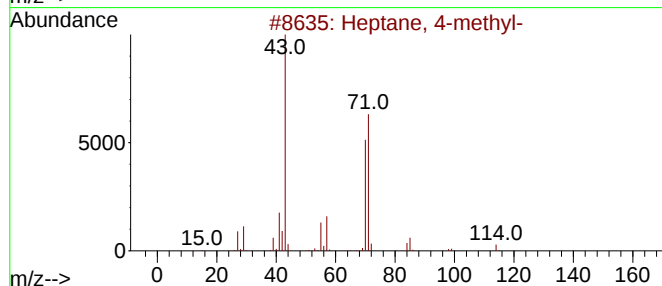
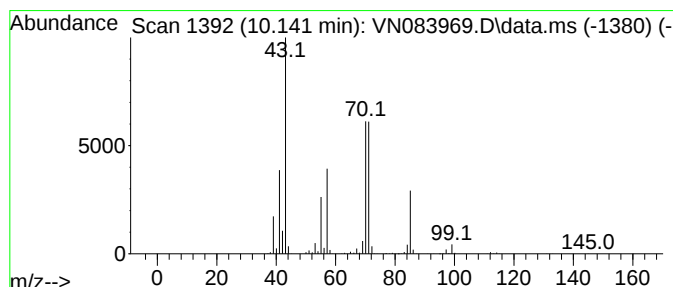
Quant Title :

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

Peak Number 5 Heptane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.141	174.04 ug/l	3114080	1,4-Difluorobenzene	9.094

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 4-methyl-	114	C8H18	000589-53-7	72
2		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	72
3		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	72
5		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083969.D
Acq On : 18 Sep 2024 07:56
Operator : JC\MD
Sample : P3964-08
Misc : 2.91g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-5

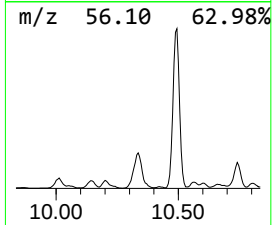
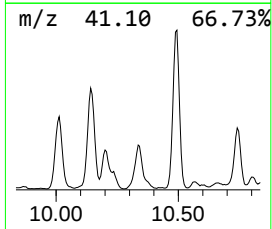
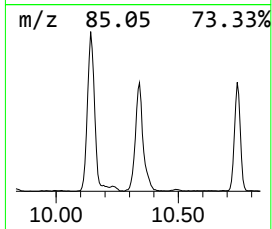
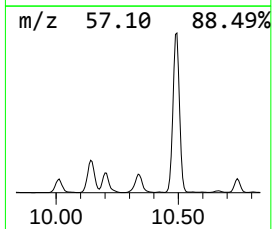
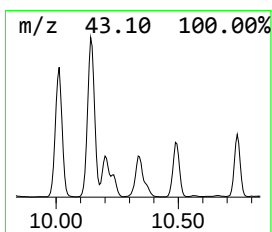
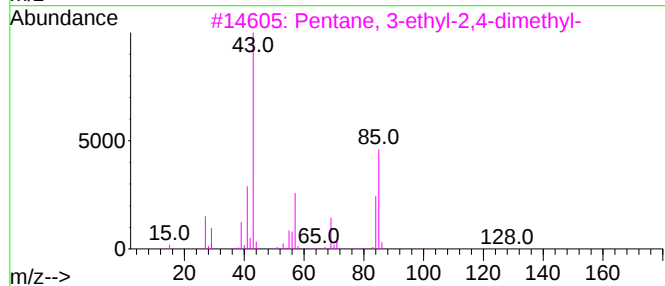
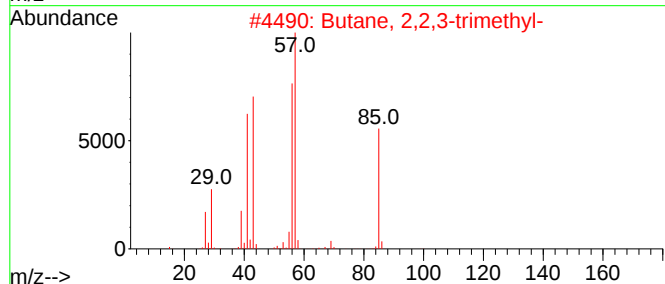
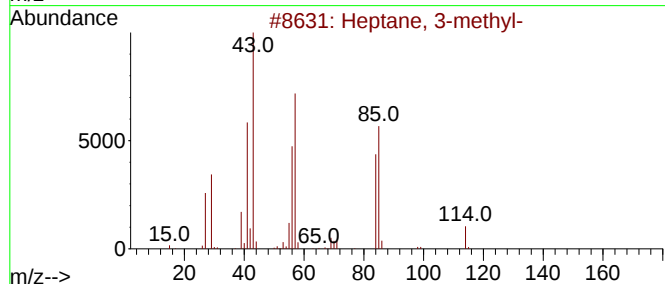
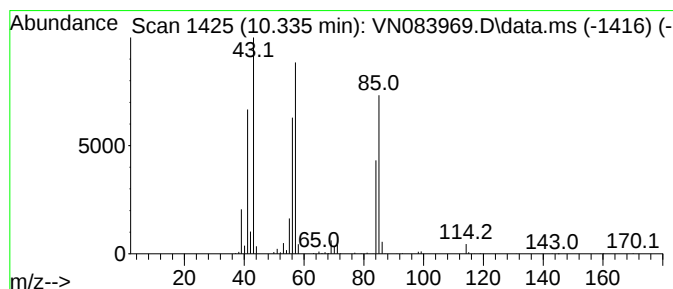
Quant Title :

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.335	64.47 ug/l	1153620	1,4-Difluorobenzene	9.094

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 3-methyl-	114	C8H18	000589-81-1	90
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
3		Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	59
4		Hexane, 3-ethyl-	114	C8H18	000619-99-8	59
5		Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083969.D
Acq On : 18 Sep 2024 07:56
Operator : JC\MD
Sample : P3964-08
Misc : 2.91g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-5

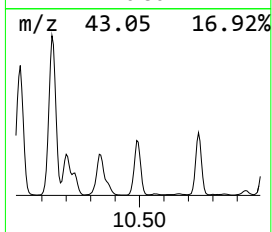
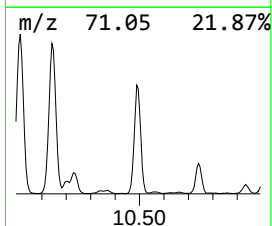
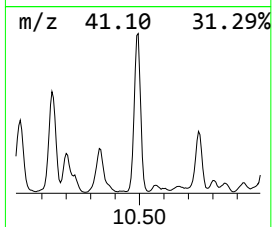
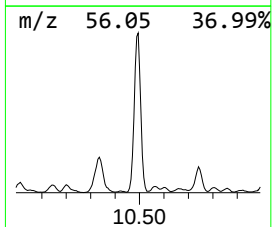
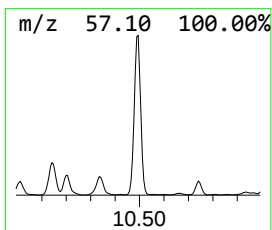
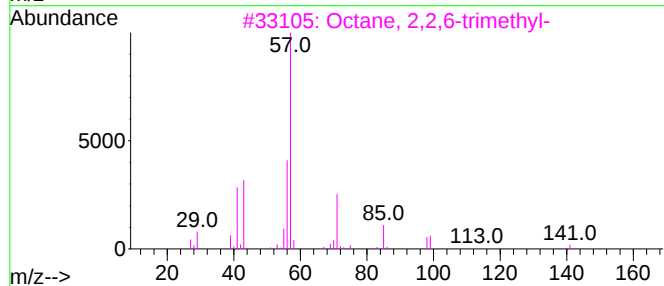
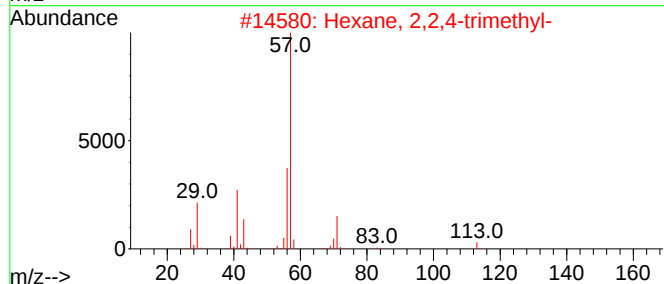
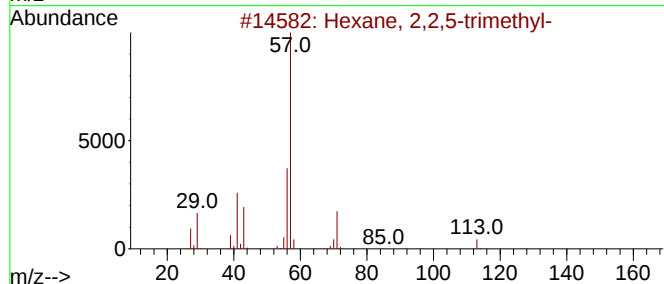
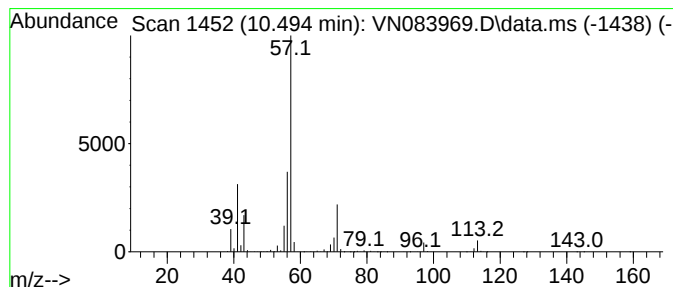
Quant Title :

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

Peak Number 7 Hexane, 2,2,5-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.494	68.96 ug/l	3486780	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	72
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	72
3			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	64
4			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	53
5			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083969.D
Acq On : 18 Sep 2024 07:56
Operator : JC\MD
Sample : P3964-08
Misc : 2.91g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-5

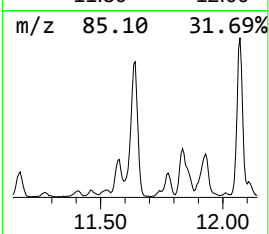
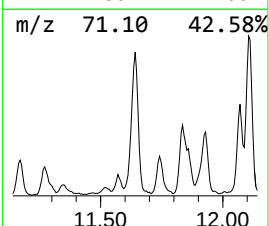
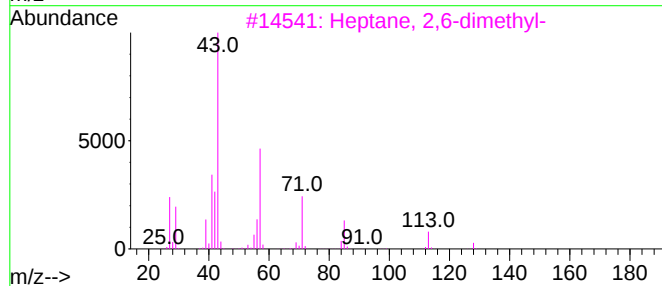
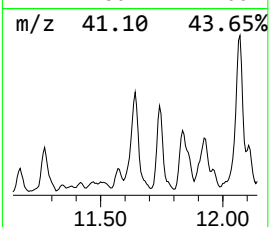
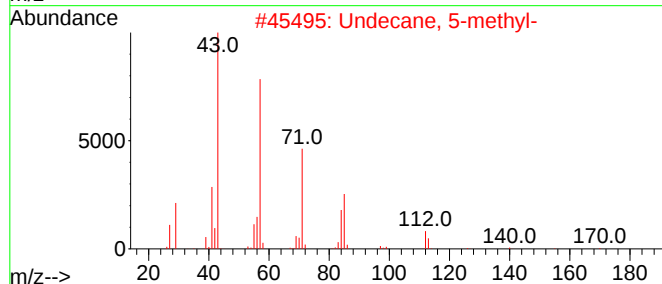
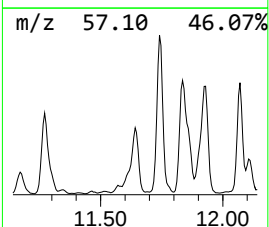
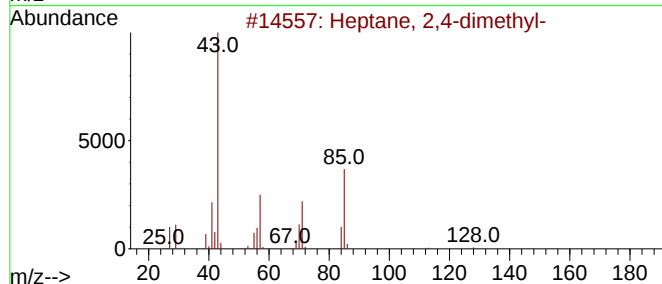
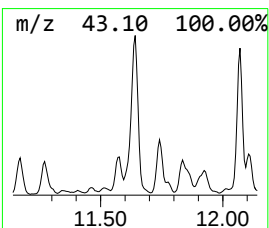
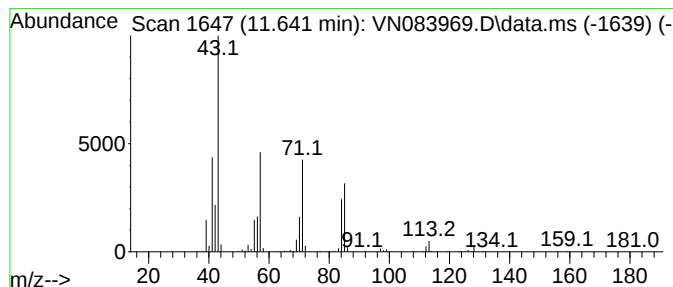
Quant Title :

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

Peak Number 8 Heptane, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.641	46.22 ug/l	2336910	Chlorobenzene-d5	11.865

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
2		Undecane, 5-methyl-	170	C12H26	001632-70-8	59
3		Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	59
4		Octane, 2-methyl-	128	C9H20	003221-61-2	58
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083969.D
Acq On : 18 Sep 2024 07:56
Operator : JC\MD
Sample : P3964-08
Misc : 2.91g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-5

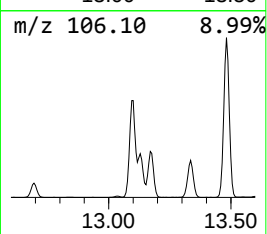
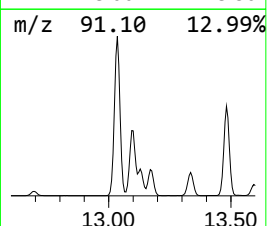
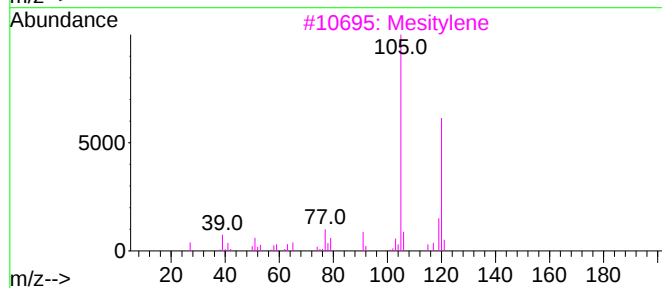
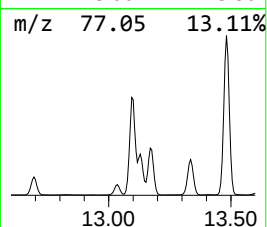
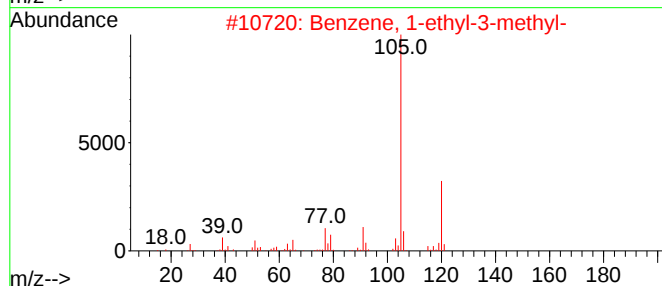
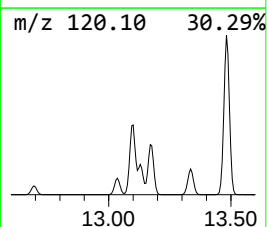
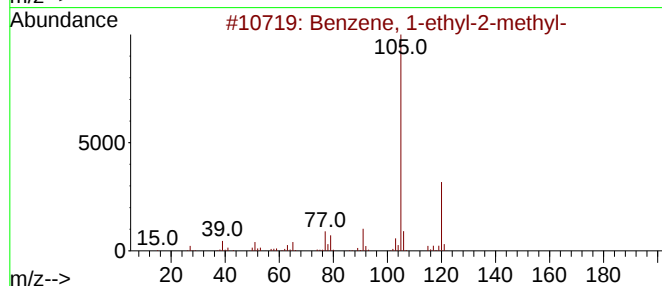
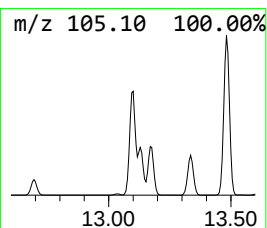
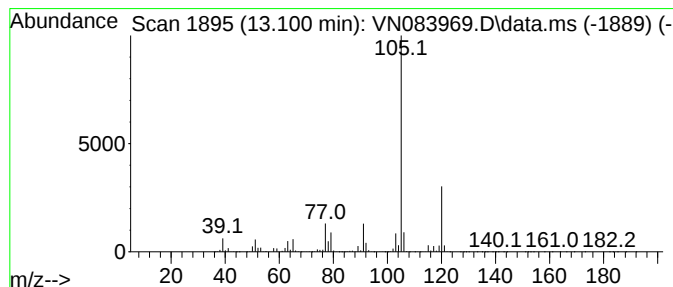
Quant Title :

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

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	80.27 ug/l	22970900	1,4-Dichlorobenzene-d4	13.788

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083969.D
Acq On : 18 Sep 2024 07:56
Operator : JC\MD
Sample : P3964-08
Misc : 2.91g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-5

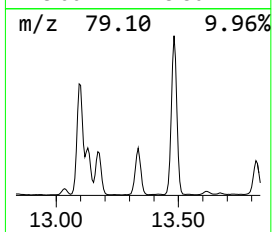
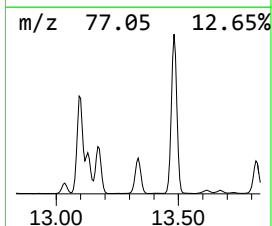
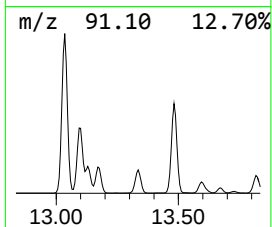
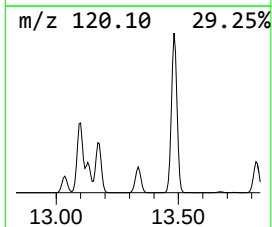
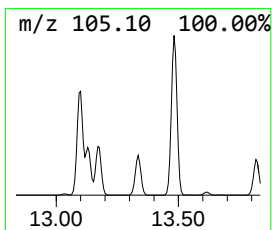
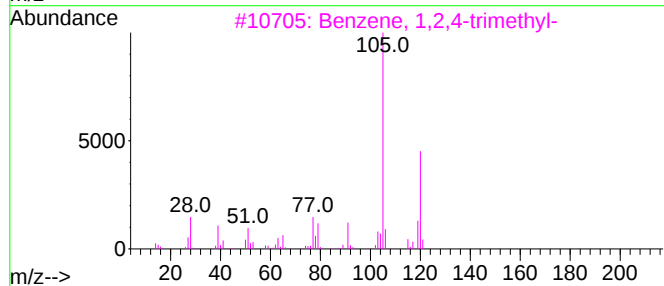
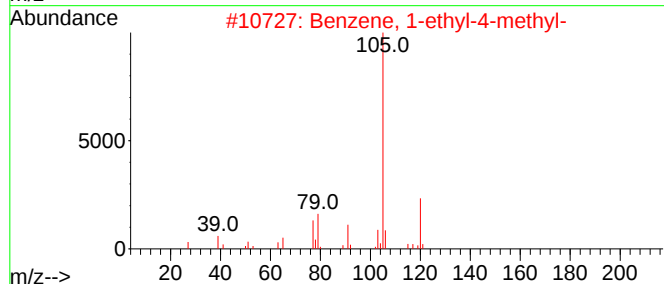
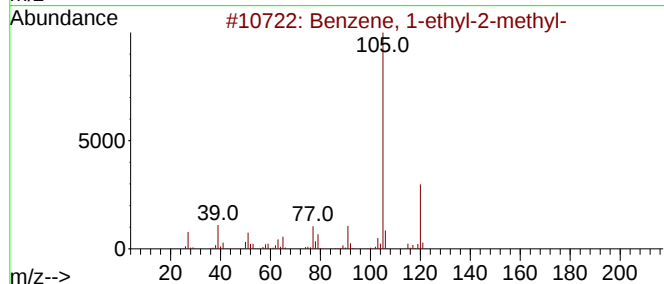
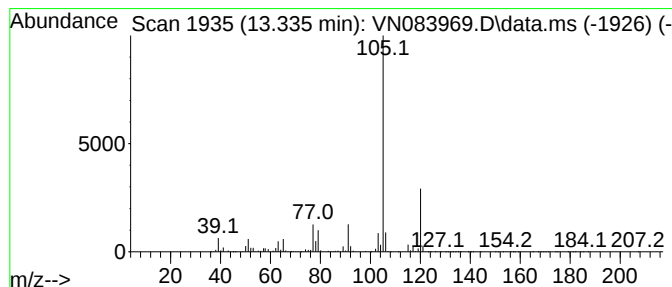
Quant Title :

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

Peak Number 10 Benzene, 1-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	31.42 ug/l	8991250	1,4-Dichlorobenzene-d4	13.788

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083969.D
Acq On : 18 Sep 2024 07:56
Operator : JC\MD
Sample : P3964-08
Misc : 2.91g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-5

Quant Title :

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Hexane, 2,5-dim...	9.582	50.8	ug/l	907986	2	9.094	894632	50.0
Hexane, 2,4-dim...	9.641	33.8	ug/l	604233	2	9.094	894632	50.0
Pentane, 2,3,4-...	10.012	120.6	ug/l	2157580	2	9.094	894632	50.0
Heptane, 4-methyl-	10.141	174.0	ug/l	3114080	2	9.094	894632	50.0
Heptane, 3-methyl-	10.335	64.5	ug/l	1153620	2	9.094	894632	50.0
Hexane, 2,2,5-t...	10.494	69.0	ug/l	3486780	3	11.865	2528160	50.0
Heptane, 2,4-di...	11.641	46.2	ug/l	2336910	3	11.865	2528160	50.0
Benzene, 1-ethy...	13.100	80.3	ug/l	22970900	4	13.788	14309100	50.0
Benzene, 1-ethy...	13.335	31.4	ug/l	8991250	4	13.788	14309100	50.0