

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
 Data File : VN083964.D
 Acq On : 18 Sep 2024 05:57
 Operator : JC\MD
 Sample : P3964-03
 Misc : 8.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 FDF-3

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: VN083964.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	rVV2	506278	1232264	2.61%	0.394%
2	8.324	1075	1083	1093	rVB	188586	483175	1.02%	0.154%
3	8.441	1093	1103	1113	rBV	320069	724053	1.53%	0.231%
4	8.753	1140	1156	1168	rBV	1940945	4883717	10.35%	1.560%
5	8.959	1181	1191	1205	rVB	278458	657866	1.39%	0.210%
6	9.094	1205	1214	1221	rBV	482640	1072670	2.27%	0.343%
7	9.588	1285	1298	1303	rBV3	899954	2067259	4.38%	0.660%
8	9.641	1303	1307	1314	rVB	615666	1132360	2.40%	0.362%
9	10.012	1362	1370	1379	rBV	2062494	4114562	8.72%	1.314%
10	10.141	1380	1392	1398	rBV	2840792	5917319	12.54%	1.890%
11	10.200	1398	1402	1406	rBV	475877	717455	1.52%	0.229%
12	10.335	1416	1425	1438	rBV	710237	1771818	3.76%	0.566%
13	10.494	1438	1452	1458	rBV	2532591	4644077	9.84%	1.483%
14	10.565	1458	1464	1470	rBV2	679034	1252167	2.65%	0.400%
15	10.741	1487	1494	1501	rVB	822884	1549963	3.29%	0.495%
16	11.012	1530	1540	1547	rVV2	599730	1343091	2.85%	0.429%
17	11.171	1558	1567	1574	rBV	306917	603257	1.28%	0.193%
18	11.271	1574	1584	1592	rBV	494821	1079148	2.29%	0.345%
19	11.641	1639	1647	1659	rVB2	1206579	2780889	5.90%	0.888%
20	11.741	1659	1664	1674	rBV	957652	1656834	3.51%	0.529%
21	11.841	1674	1681	1682	rBV	759151	1218153	2.58%	0.389%
22	11.859	1682	1684	1689	rVV	876185	1406106	2.98%	0.449%
23	11.929	1689	1696	1698	rVV	640338	1383695	2.93%	0.442%
24	11.965	1698	1702	1708	rVV	1616418	2652186	5.62%	0.847%
25	12.070	1711	1720	1731	rVV	16659855	33110220	70.19%	10.574%
26	12.300	1747	1759	1764	rBV3	418950	949321	2.01%	0.303%
27	12.400	1766	1776	1783	rVV	6555084	11829503	25.08%	3.778%
28	12.476	1784	1789	1795	rVB	442051	806053	1.71%	0.257%
29	12.694	1820	1826	1831	rBV	1760765	2998465	6.36%	0.958%
30	12.823	1841	1848	1855	rVB	2388786	4258885	9.03%	1.360%
31	12.876	1855	1857	1861	rVB	440278	545457	1.16%	0.174%
32	12.929	1861	1866	1871	rVB3	356707	665155	1.41%	0.212%
33	12.988	1871	1876	1879	rBV	762497	1336738	2.83%	0.427%
34	13.035	1879	1884	1889	rVB	2472501	3851432	8.16%	1.230%
35	13.100	1889	1895	1898	rBV	17597513	29251261	62.01%	9.341%
36	13.129	1898	1900	1904	rVV	7584769	11376940	24.12%	3.633%

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

37	13.170	1904	1907	1919	rVB	9521567	15815755	33.53%	5.051%
38	13.335	1926	1935	1942	rBV	6679003	11543728	24.47%	3.686%
39	13.423	1942	1950	1954	rBV	1827183	3255714	6.90%	1.040%
40	13.482	1954	1960	1966	rBV	29522652	47173435	100.00%	15.065%
41	13.535	1966	1969	1974	rVB	773216	1119654	2.37%	0.358%
42	13.641	1974	1987	1996	rBV4	2164008	6963324	14.76%	2.224%
43	13.717	1996	2000	2003	rBV3	325706	472562	1.00%	0.151%
44	13.823	2009	2018	2030	rVB2	7409353	17790620	37.71%	5.681%
45	13.953	2034	2040	2041	rBV2	1399774	2113821	4.48%	0.675%
46	13.988	2041	2046	2049	rBV2	4810831	9197966	19.50%	2.937%
47	14.106	2062	2066	2073	rBV2	456622	808261	1.71%	0.258%
48	14.182	2074	2079	2084	rVB	1552298	2549970	5.41%	0.814%
49	14.241	2084	2089	2092	rBV	2304025	3890489	8.25%	1.242%
50	14.270	2092	2094	2099	rVV	2148837	2907221	6.16%	0.928%
51	14.329	2099	2104	2112	rVB	4275175	6613569	14.02%	2.112%
52	14.441	2118	2123	2128	rVB3	1055284	1800044	3.82%	0.575%
53	14.576	2140	2146	2151	rBV	813831	1319033	2.80%	0.421%
54	14.653	2151	2159	2162	rBV	2495260	4229697	8.97%	1.351%
55	14.694	2162	2166	2170	rVV	3052110	4660623	9.88%	1.488%
56	14.735	2170	2173	2177	rVB3	925249	1249718	2.65%	0.399%
57	14.806	2182	2185	2193	rVB	460812	702630	1.49%	0.224%
58	14.876	2193	2197	2200	rBV2	414113	547226	1.16%	0.175%
59	14.929	2200	2206	2209	rBV	1269510	2251243	4.77%	0.719%
60	15.047	2216	2226	2232	rBV5	1875916	6214036	13.17%	1.984%
61	15.100	2232	2235	2243	rVB2	403348	765477	1.62%	0.244%
62	15.317	2267	2272	2284	rVB2	618410	1569127	3.33%	0.501%
63	15.429	2285	2291	2300	rVB4	395768	954278	2.02%	0.305%
64	15.635	2313	2326	2339	rVB	1992158	4344211	9.21%	1.387%
65	15.823	2350	2358	2370	rVB4	269106	893250	1.89%	0.285%
66	15.941	2370	2378	2385	rBV2	267158	625523	1.33%	0.200%
67	16.782	2513	2521	2522	rBV	838212	1469542	3.12%	0.469%

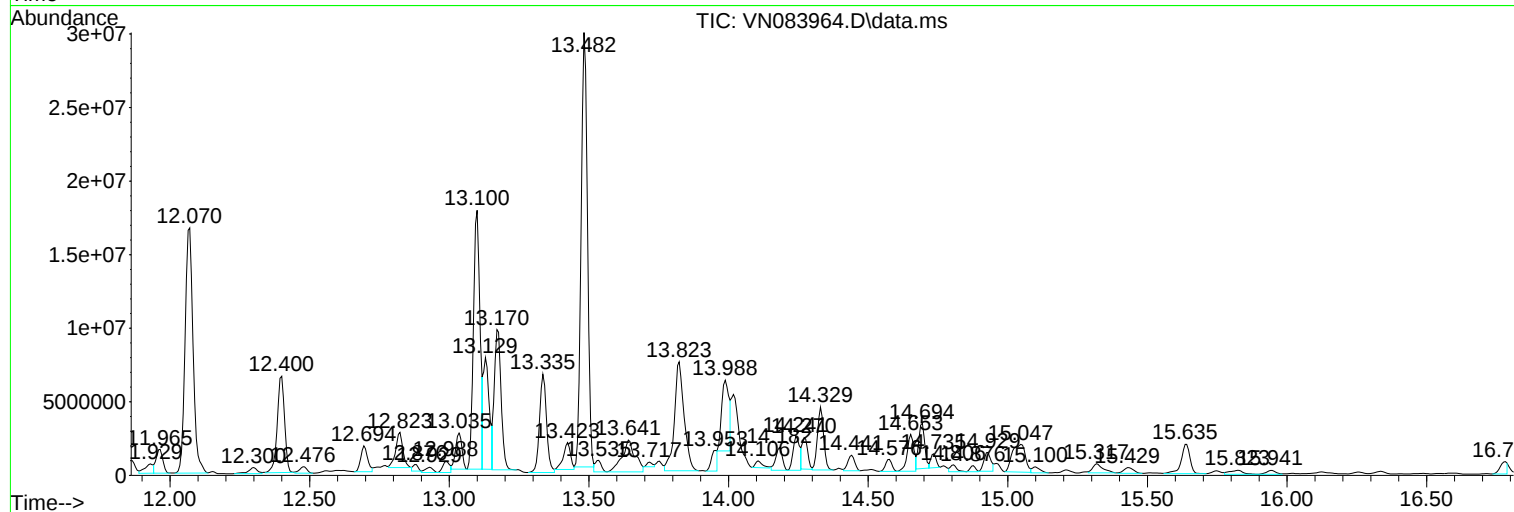
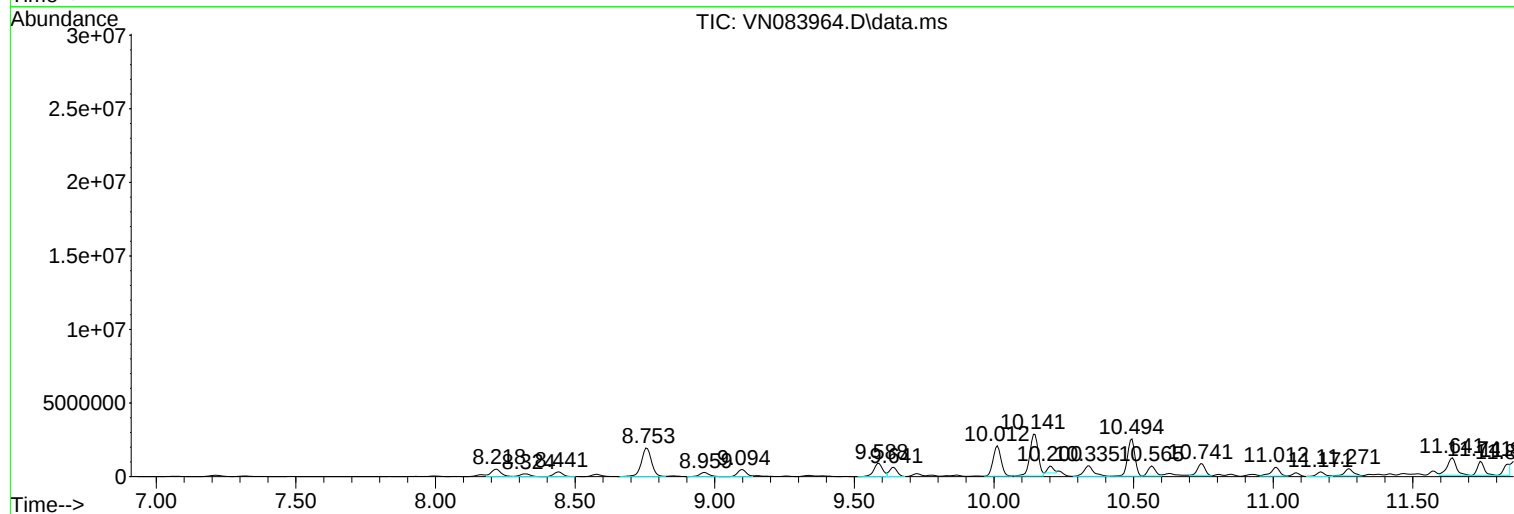
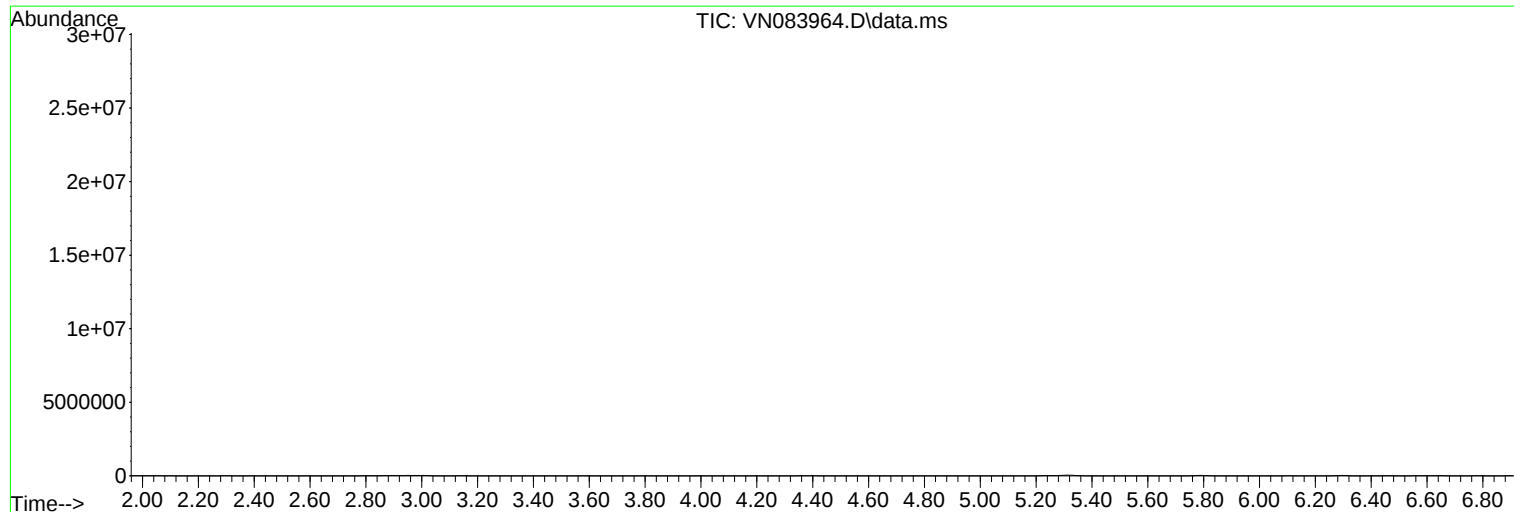
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Instrument :
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ClientSampleId :
FDF-3

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

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



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ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-3

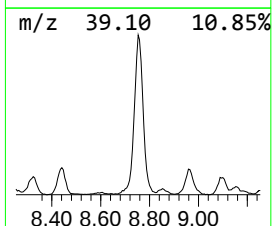
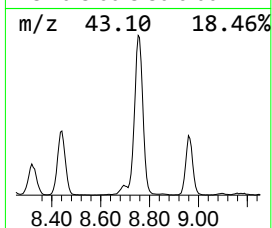
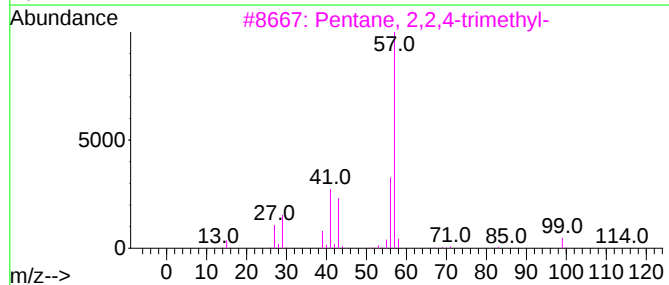
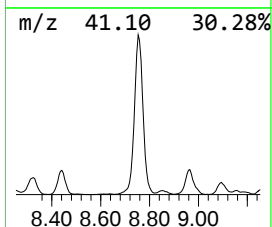
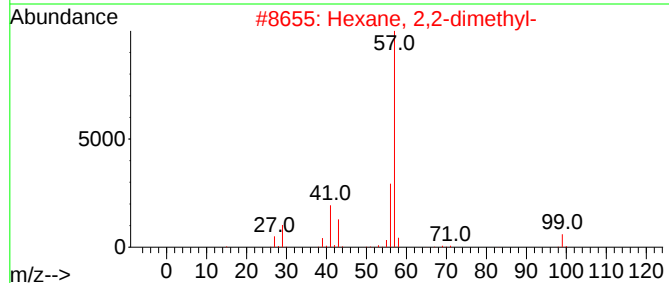
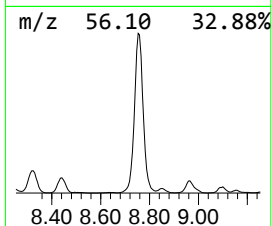
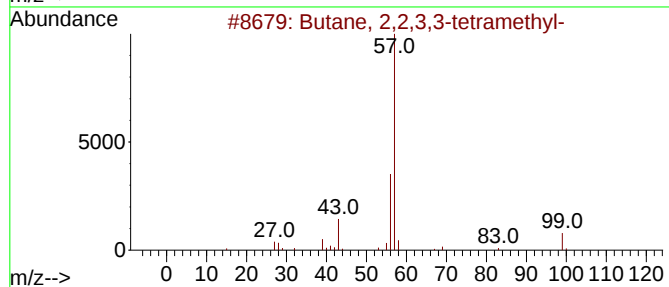
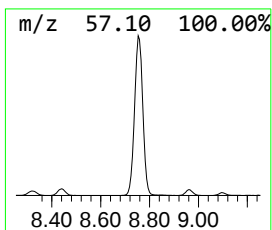
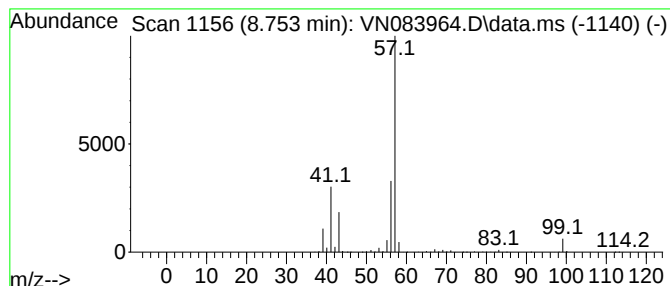
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.753	227.64 ug/l	4883720	1,4-Difluorobenzene	9.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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Instrument :
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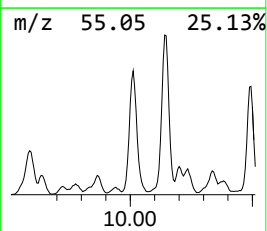
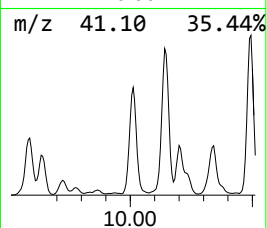
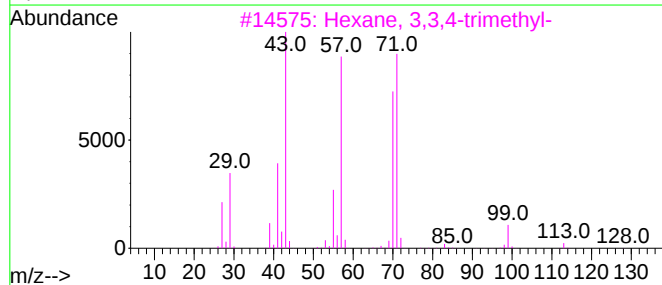
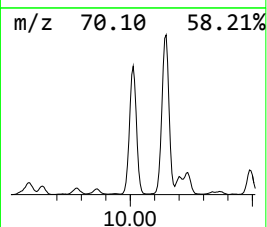
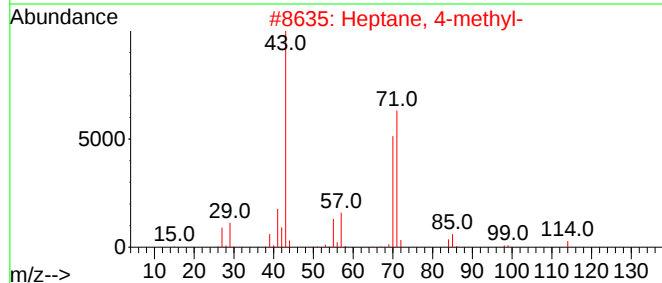
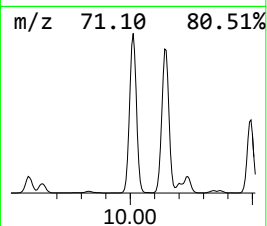
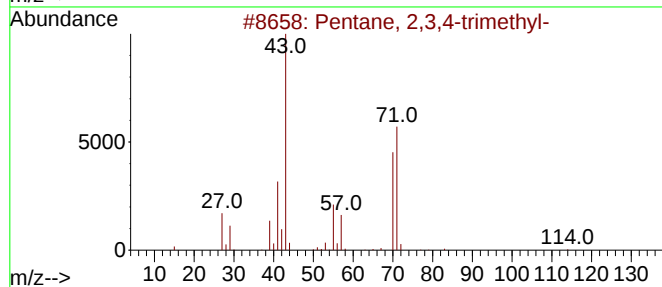
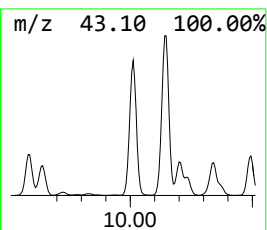
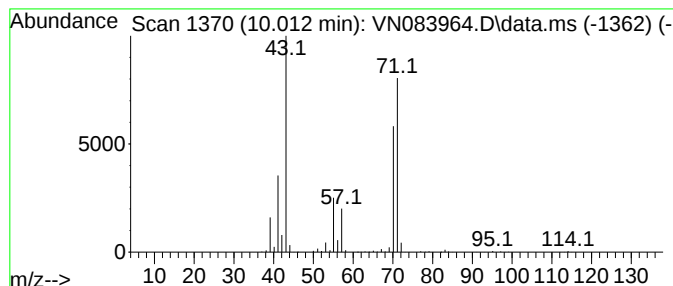
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.012	191.79 ug/l	4114560	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			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	83
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	74



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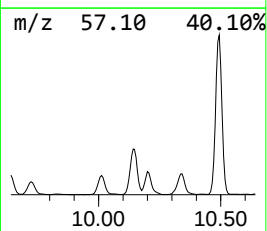
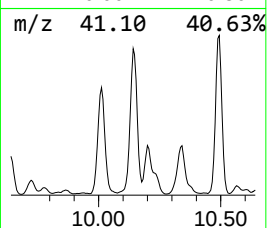
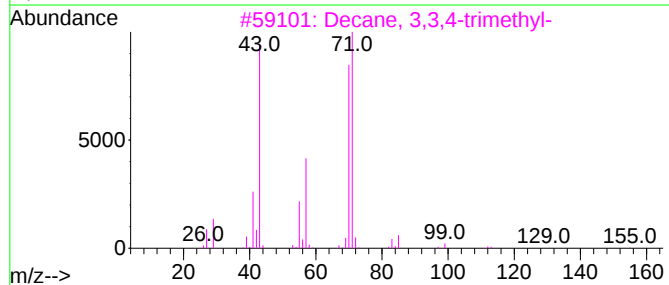
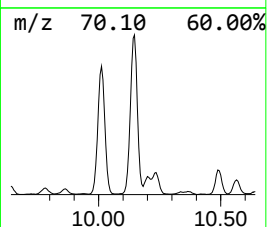
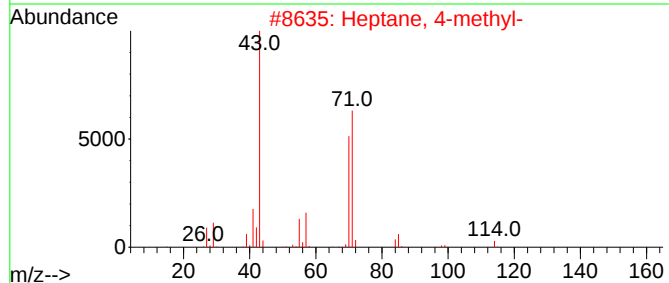
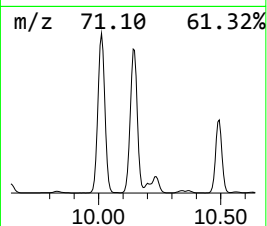
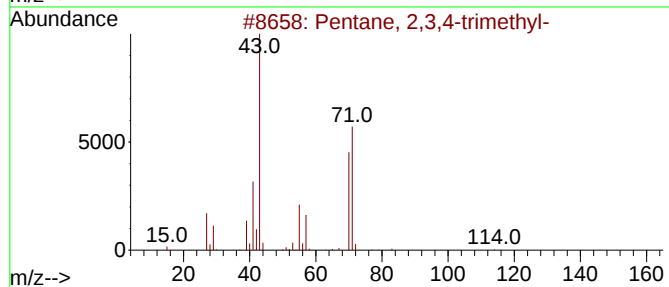
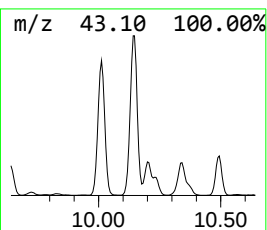
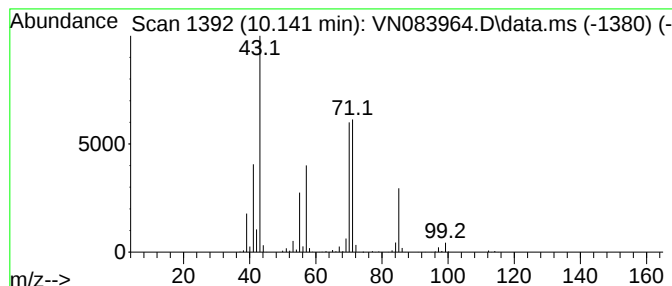
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.141	275.82 ug/l	5917320	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	74
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	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		3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	59



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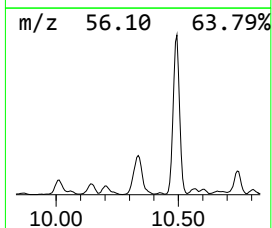
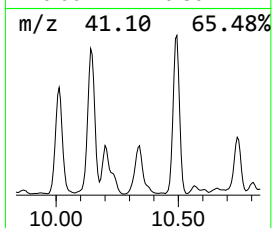
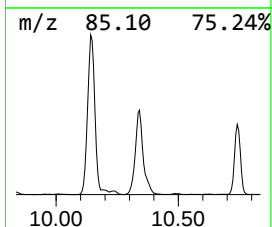
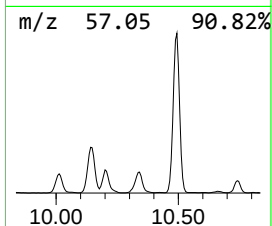
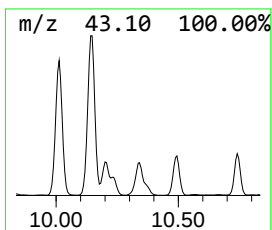
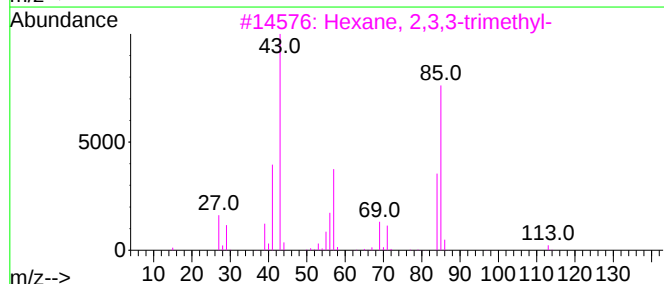
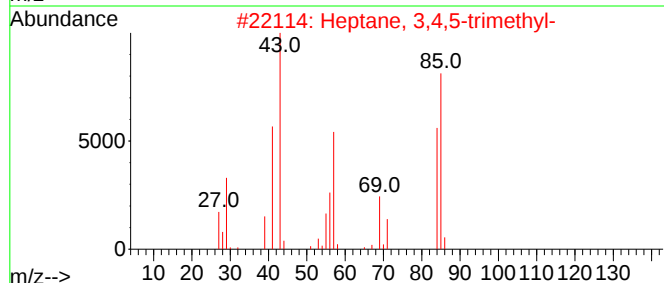
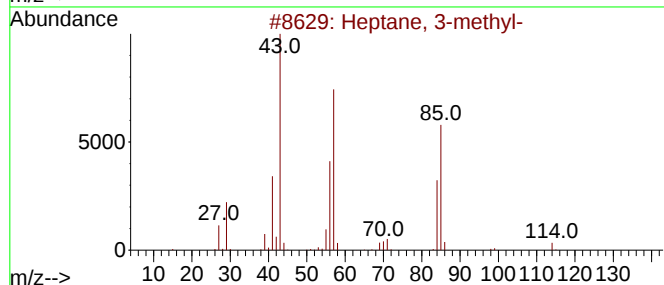
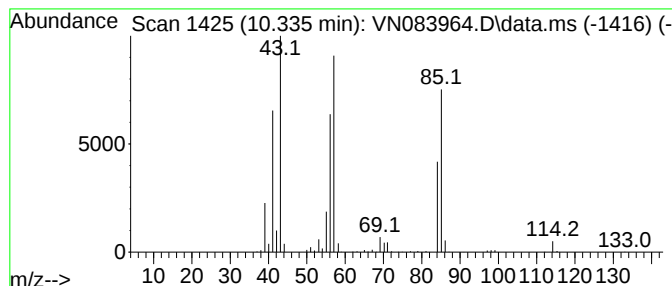
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.335	82.59 ug/l	1771820	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			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	64
3			Hexane, 2,3,3-trimethyl-	128	C9H20	016747-28-7	64
4			Hexane, 1-(hexyloxy)-2-methyl-	200	C13H28O	074421-17-3	64
5			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083964.D
Acq On : 18 Sep 2024 05:57
Operator : JC\MD
Sample : P3964-03
Misc : 8.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-3

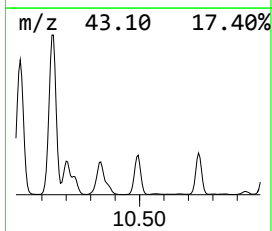
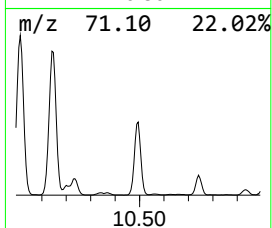
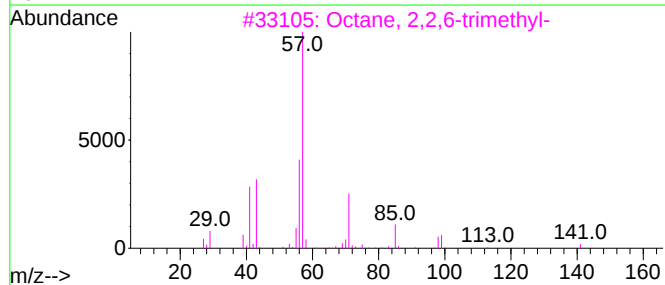
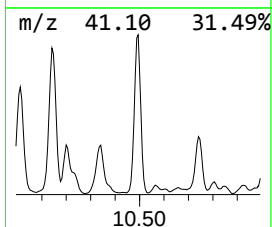
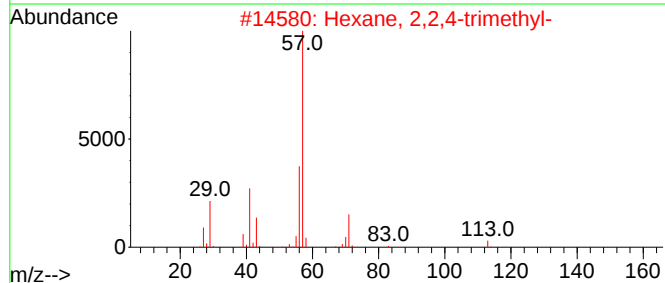
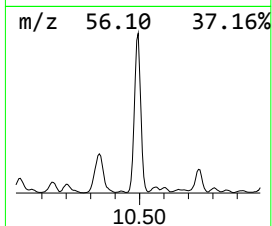
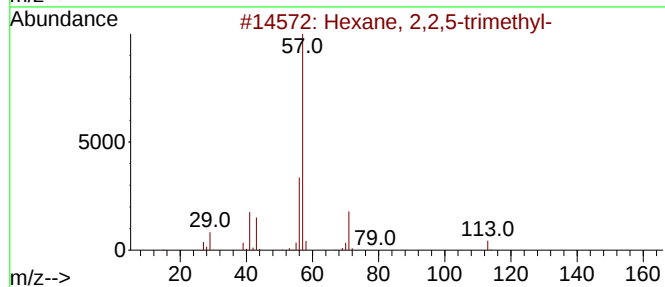
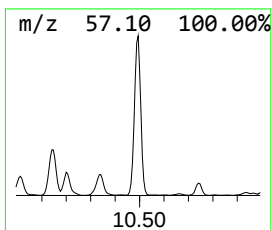
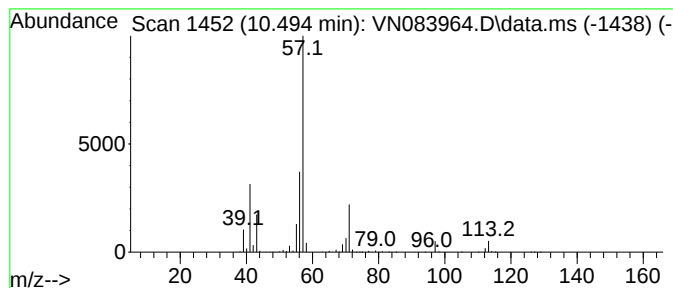
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Quant Title : SW846 8260

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

Peak Number 5 Hexane, 2,2,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.494	165.14 ug/l	4644080	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 : VN083964.D
Acq On : 18 Sep 2024 05:57
Operator : JC\MD
Sample : P3964-03
Misc : 8.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-3

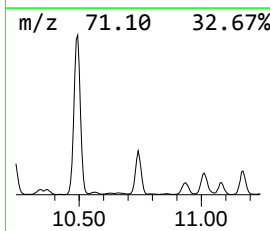
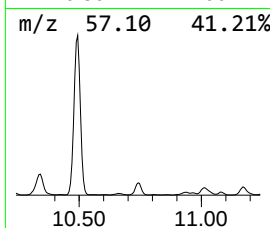
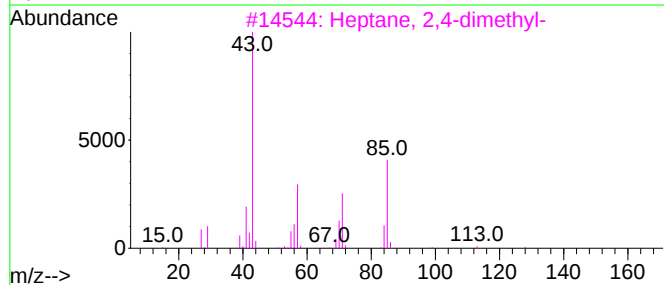
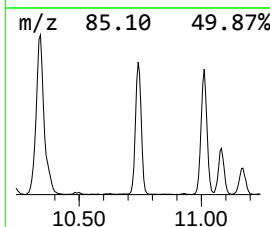
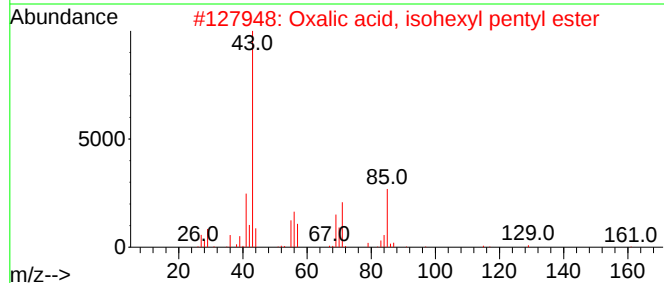
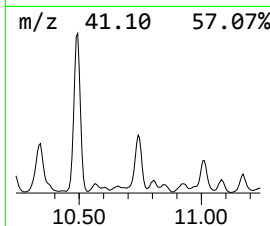
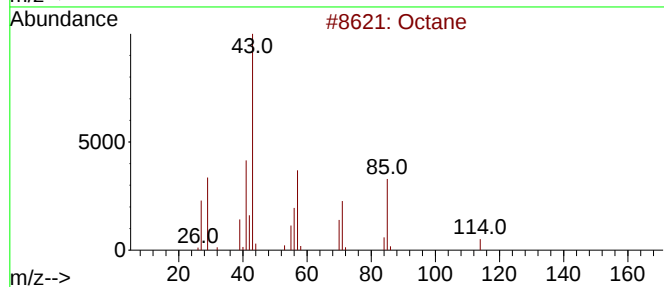
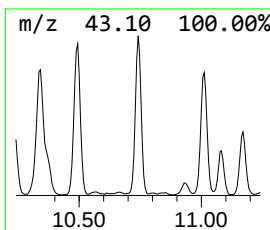
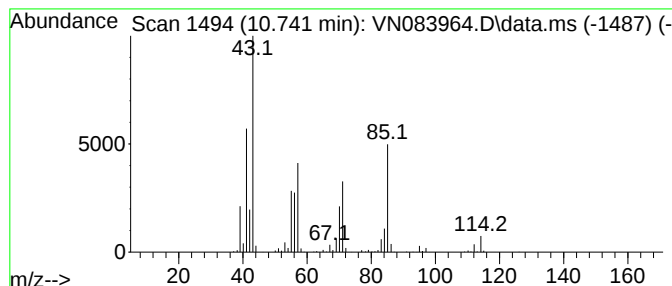
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Quant Title : SW846 8260

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

Peak Number 6 Octane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.741	55.12 ug/l	1549960	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	91
2			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	78
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
4			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	64
5			Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083964.D
Acq On : 18 Sep 2024 05:57
Operator : JC\MD
Sample : P3964-03
Misc : 8.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-3

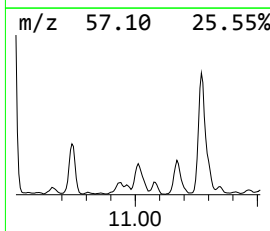
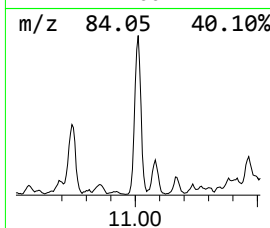
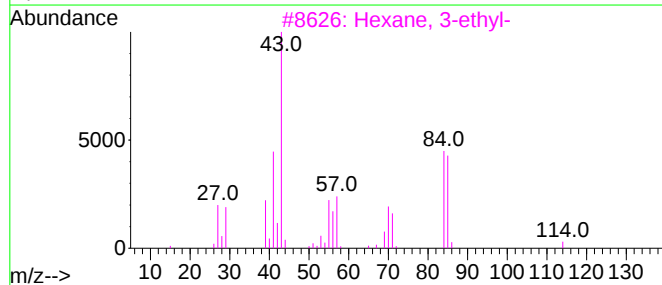
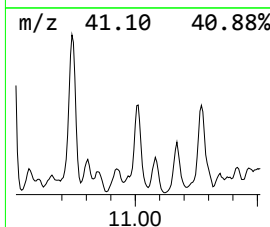
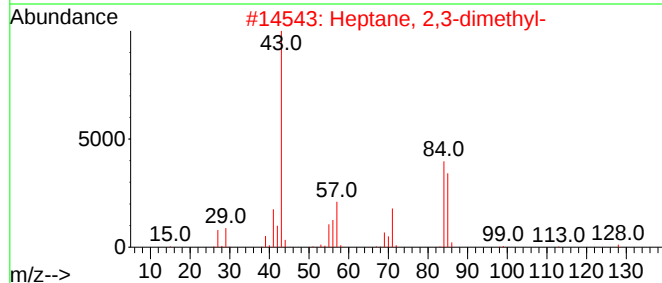
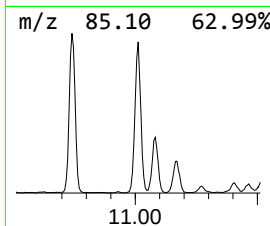
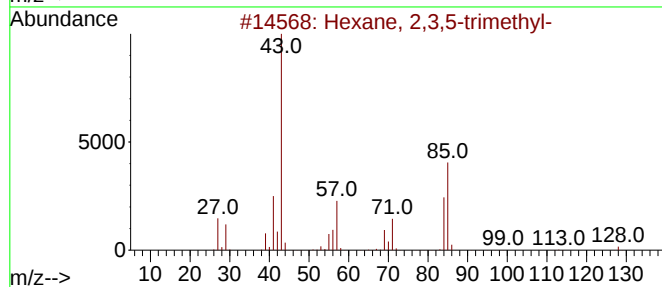
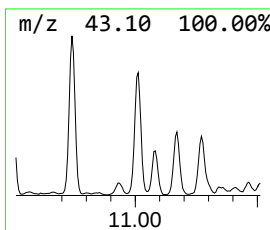
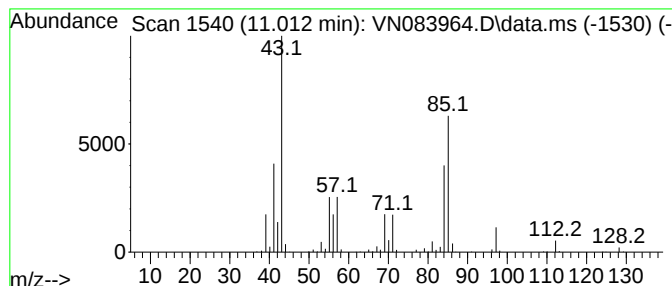
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Quant Title : SW846 8260

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

Peak Number 7 Hexane, 2,3,5-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.012	47.76 ug/l	1343090	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	72
2			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	68
3			Hexane, 3-ethyl-	114	C8H18	000619-99-8	59
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5			Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083964.D
Acq On : 18 Sep 2024 05:57
Operator : JC\MD
Sample : P3964-03
Misc : 8.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-3

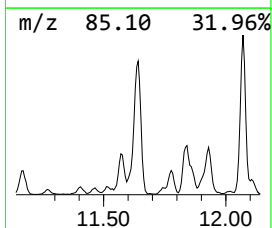
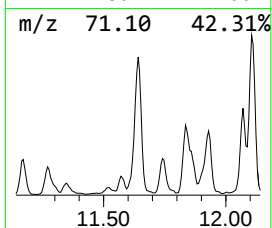
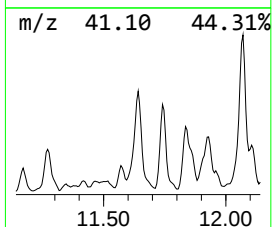
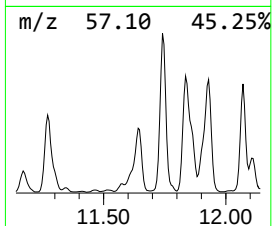
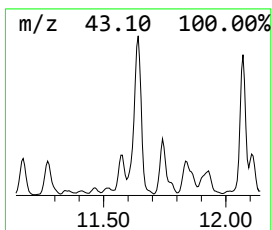
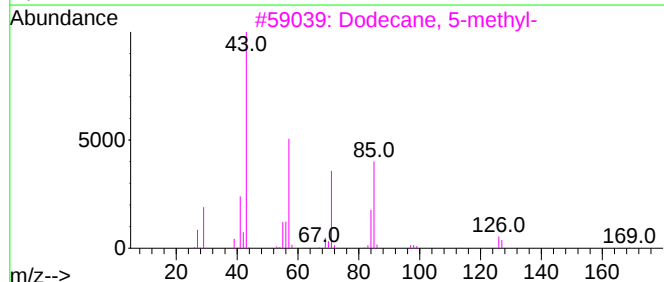
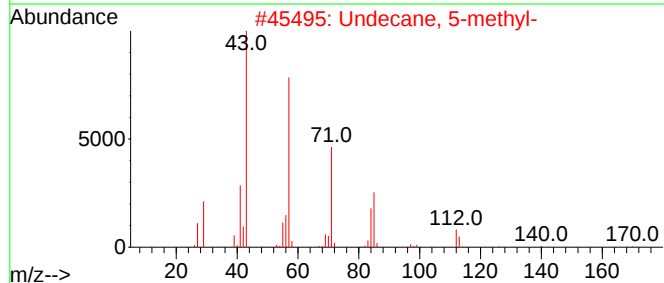
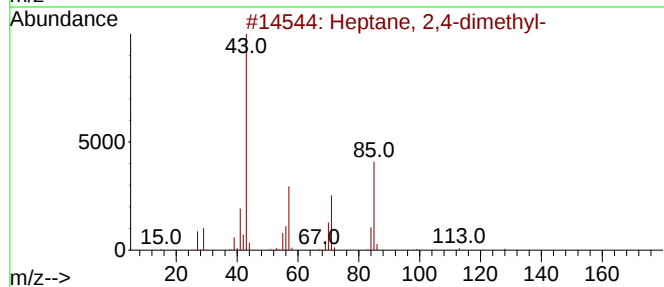
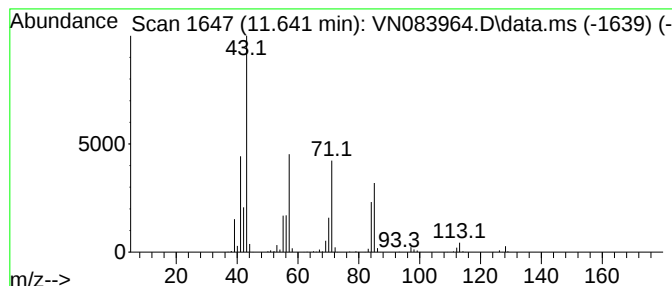
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Quant Title : SW846 8260

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

Peak Number 8 Heptane, 2,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.641	98.89 ug/l	2780890	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			Dodecane, 5-methyl-	184	C13H28	017453-93-9	59
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5			Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083964.D
Acq On : 18 Sep 2024 05:57
Operator : JC\MD
Sample : P3964-03
Misc : 8.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-3

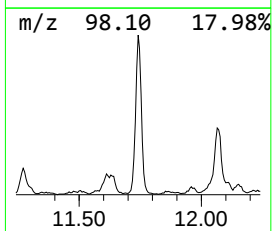
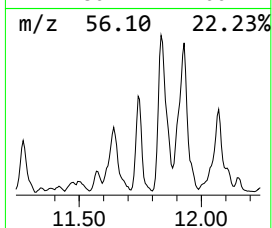
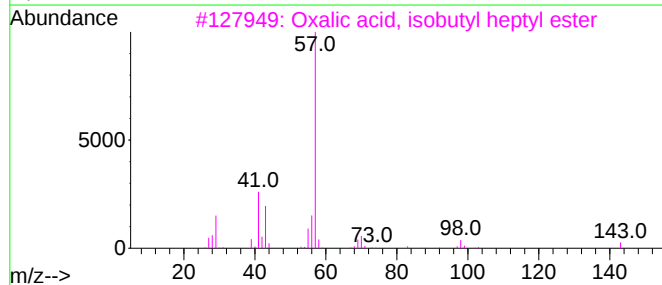
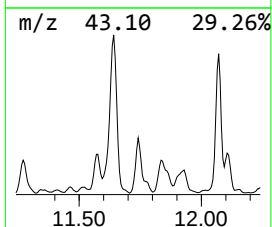
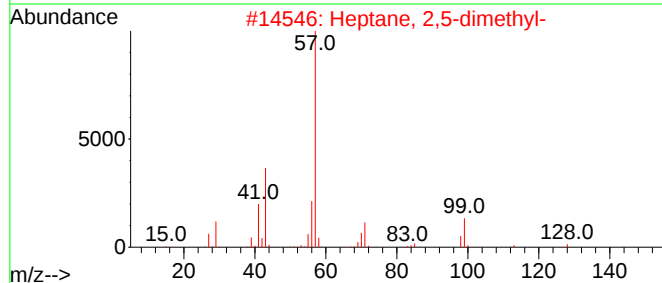
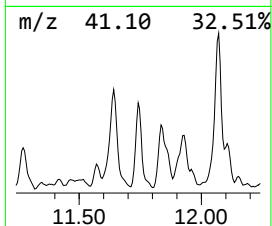
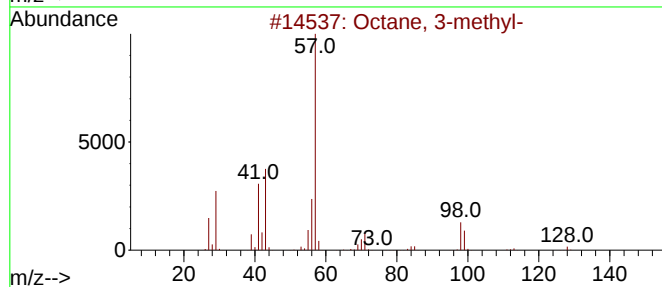
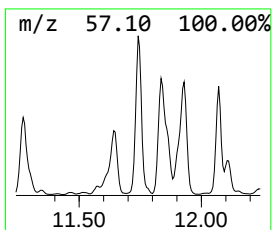
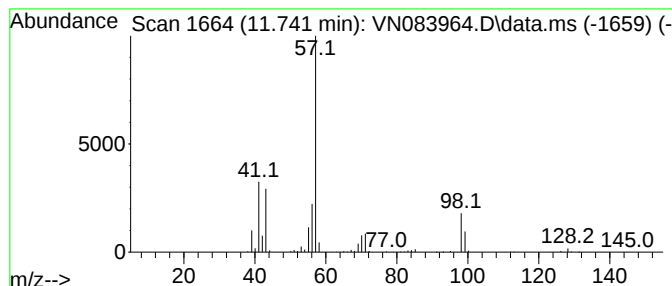
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Quant Title : SW846 8260

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

Peak Number 9 Octane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.741	58.92 ug/l	1656830	Chlorobenzene-d5	11.865

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	86
3			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	59
4			Undecane, 6-methyl-	170	C12H26	017302-33-9	59
5			Heptane, 3-ethyl-	128	C9H20	015869-80-4	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083964.D
Acq On : 18 Sep 2024 05:57
Operator : JC\MD
Sample : P3964-03
Misc : 8.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-3

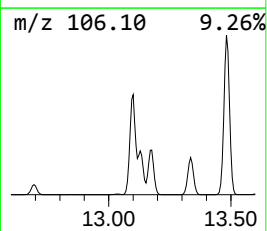
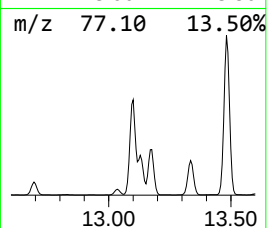
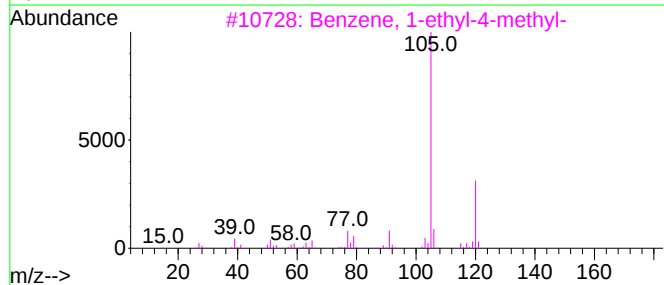
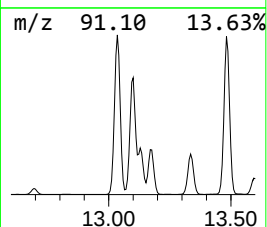
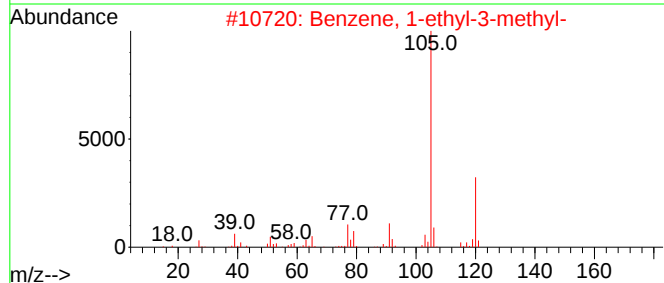
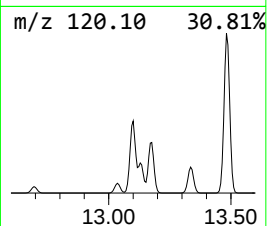
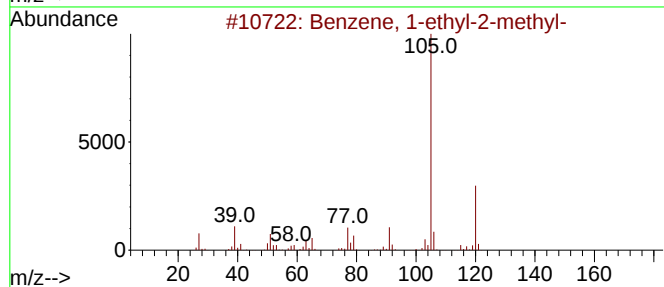
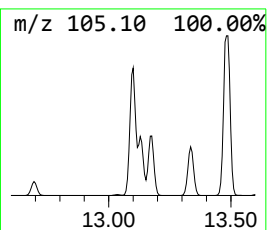
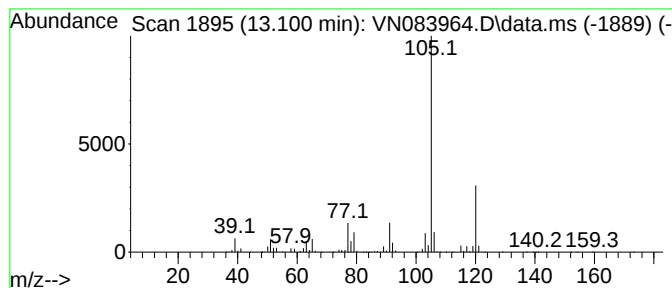
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Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	82.21 ug/l	29251300	1,4-Dichlorobenzene-d4	13.794

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			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091724\
Data File : VN083964.D
Acq On : 18 Sep 2024 05:57
Operator : JC\MD
Sample : P3964-03
Misc : 8.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FDF-3

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2,2,3,3...	8.753	227.6	ug/l	4883720	2	9.094	1072670	50.0
Pentane, 2,3,4-...	10.012	191.8	ug/l	4114560	2	9.094	1072670	50.0
Heptane, 4-methyl-	10.141	275.8	ug/l	5917320	2	9.094	1072670	50.0
Heptane, 3-methyl-	10.335	82.6	ug/l	1771820	2	9.094	1072670	50.0
Hexane, 2,2,5-t...	10.494	165.1	ug/l	4644080	3	11.865	1406110	50.0
Octane	10.741	55.1	ug/l	1549960	3	11.865	1406110	50.0
Hexane, 2,3,5-t...	11.012	47.8	ug/l	1343090	3	11.865	1406110	50.0
Heptane, 2,4-di...	11.641	98.9	ug/l	2780890	3	11.865	1406110	50.0
Octane, 3-methyl-	11.741	58.9	ug/l	1656830	3	11.865	1406110	50.0
Benzene, 1-ethy...	13.100	82.2	ug/l	29251300	4	13.794	17790600	50.0