

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082223.D
Acq On : 20 May 2024 20:36
Operator : JC\MD
Sample : P2541-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
50322

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M

Title : SW846 8260

Signal : TIC: VN082223.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.483	84	90	95	rBV	25867	45458	1.95%	0.119%
2	2.665	115	121	127	rBV	48911	85284	3.66%	0.224%
3	3.248	212	220	235	rVB	119328	286740	12.29%	0.752%
4	3.642	275	287	298	rBV	80571	199341	8.55%	0.523%
5	4.424	409	420	447	rBV	376867	1127232	48.32%	2.958%
6	5.277	552	565	566	rBV	66049	149666	6.42%	0.393%
7	5.342	568	576	590	rVV2	227493	795691	34.11%	2.088%
8	5.518	592	606	624	rVB3	73872	281554	12.07%	0.739%
9	5.818	640	657	672	rVB	156378	531968	22.81%	1.396%
10	6.312	727	741	757	rVB2	145146	438852	18.81%	1.152%
11	6.471	757	768	776	rBV6	9519	29391	1.26%	0.077%
12	6.659	794	800	809	rVB3	11406	32286	1.38%	0.085%
13	7.083	861	872	884	rBV6	17608	60629	2.60%	0.159%
14	7.224	886	896	905	rVV4	59377	165067	7.08%	0.433%
15	7.330	905	914	922	rVV	88599	250960	10.76%	0.659%
16	7.436	922	932	956	rVB	825999	2332672	100.00%	6.121%
17	7.936	1009	1017	1024	rBV5	20823	54736	2.35%	0.144%
18	8.165	1047	1056	1061	rBV	144917	360595	15.46%	0.946%
19	8.224	1061	1066	1077	rVV	374685	896562	38.43%	2.353%
20	8.330	1077	1084	1094	rVB2	96807	238677	10.23%	0.626%
21	8.447	1094	1104	1112	rBV	146912	326622	14.00%	0.857%
22	8.583	1119	1127	1134	rBV	163216	367827	15.77%	0.965%
23	8.665	1134	1141	1142	rVV5	26938	58002	2.49%	0.152%
24	8.765	1144	1158	1169	rVV3	168908	742260	31.82%	1.948%
25	8.859	1169	1174	1183	rVB3	42377	101363	4.35%	0.266%
26	8.971	1183	1193	1202	rBV2	88493	210423	9.02%	0.552%
27	9.100	1207	1215	1223	rBV	436519	946242	40.56%	2.483%
28	9.265	1237	1243	1250	rVB3	31275	62171	2.67%	0.163%
29	9.400	1260	1266	1280	rVB3	19599	57726	2.47%	0.151%
30	9.600	1282	1300	1305	rBV6	138600	433189	18.57%	1.137%
31	9.647	1305	1308	1316	rVB3	45004	91368	3.92%	0.240%
32	9.777	1325	1330	1336	rVB2	35705	67602	2.90%	0.177%
33	9.871	1336	1346	1350	rBV5	21846	51966	2.23%	0.136%
34	10.012	1363	1370	1381	rVB	104655	227407	9.75%	0.597%
35	10.147	1381	1393	1399	rBV	172200	377680	16.19%	0.991%
36	10.206	1399	1403	1407	rBV2	35293	60070	2.58%	0.158%

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37	10.341	1417	1426	1438	rBV4	56795	151153	6.48%	0.397%
38	10.447	1438	1444	1448	rBV4	33503	63986	2.74%	0.168%
39	10.494	1448	1452	1457	rVB2	29087	49606	2.13%	0.130%
40	10.571	1457	1465	1472	rBV	628918	1189456	50.99%	3.121%
41	10.747	1488	1495	1502	rVB4	48731	104724	4.49%	0.275%
42	10.918	1518	1524	1530	rBV8	16912	38955	1.67%	0.102%
43	11.000	1530	1538	1545	rVV6	37976	100660	4.32%	0.264%
44	11.082	1550	1552	1559	rVB4	18530	29965	1.28%	0.079%
45	11.194	1559	1571	1575	rBV5	24556	70341	3.02%	0.185%
46	11.300	1575	1589	1594	rVV3	62798	140795	6.04%	0.369%
47	11.576	1631	1636	1640	rBV3	21990	38106	1.63%	0.100%
48	11.641	1640	1647	1652	rBV3	34110	70451	3.02%	0.185%
49	11.747	1660	1665	1676	rVB2	28269	50575	2.17%	0.133%
50	11.865	1676	1685	1694	rBV	549221	986586	42.29%	2.589%
51	11.965	1696	1702	1712	rVB	134487	242081	10.38%	0.635%
52	12.071	1712	1720	1731	rBV	395986	808342	34.65%	2.121%
53	12.400	1765	1776	1783	rBV	153083	303507	13.01%	0.796%
54	12.459	1783	1786	1795	rVB5	20607	37229	1.60%	0.098%
55	12.582	1796	1807	1811	rBV7	26043	83593	3.58%	0.219%
56	12.700	1820	1827	1832	rBV	87347	159132	6.82%	0.418%
57	12.847	1846	1852	1863	rVB	421371	768210	32.93%	2.016%
58	12.953	1863	1870	1878	rBV	208079	389336	16.69%	1.022%
59	13.035	1879	1884	1889	rVV	282180	470051	20.15%	1.233%
60	13.100	1889	1895	1898	rVV	607409	1041880	44.66%	2.734%
61	13.129	1898	1900	1904	rVV	384440	586554	25.15%	1.539%
62	13.176	1904	1908	1918	rVB	456251	741278	31.78%	1.945%
63	13.335	1928	1935	1945	rVB	305111	508163	21.78%	1.333%
64	13.482	1954	1960	1974	rVB	1258943	2052198	87.98%	5.385%
65	13.617	1974	1983	1988	rBV3	68125	172541	7.40%	0.453%
66	13.670	1988	1992	1997	rBV	79225	120821	5.18%	0.317%
67	13.729	1997	2002	2006	rVB	29579	49993	2.14%	0.131%
68	13.794	2006	2013	2016	rBV	536890	999800	42.86%	2.624%
69	13.859	2020	2024	2034	rVB3	394821	818651	35.09%	2.148%
70	13.953	2034	2040	2042	rBV2	172962	288639	12.37%	0.757%
71	13.988	2042	2046	2049	rBV2	221257	358841	15.38%	0.942%
72	14.023	2049	2052	2063	rVB4	432824	968260	41.51%	2.541%
73	14.117	2063	2068	2074	rVB2	41516	73049	3.13%	0.192%
74	14.182	2074	2079	2084	rBV	139633	223615	9.59%	0.587%
75	14.247	2084	2090	2093	rBV	458629	791422	33.93%	2.077%
76	14.329	2099	2104	2110	rVB	453586	682291	29.25%	1.790%

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77	14.394	2110	2115	2118	rBV	67356	108409	4.65%	0.284%
78	14.447	2118	2124	2132	rVB3	292272	560438	24.03%	1.471%
79	14.529	2132	2138	2142	rBV3	120717	200273	8.59%	0.526%
80	14.576	2142	2146	2151	rVB	100950	163603	7.01%	0.429%
81	14.653	2151	2159	2163	rBV2	261620	560682	24.04%	1.471%
82	14.694	2163	2166	2170	rVV	249618	347862	14.91%	0.913%
83	14.735	2170	2173	2176	rVV3	140433	207869	8.91%	0.545%
84	14.770	2176	2179	2193	rVB	294336	639674	27.42%	1.679%
85	14.882	2193	2198	2202	rBV4	79546	140561	6.03%	0.369%
86	14.929	2202	2206	2211	rBV3	162909	244344	10.47%	0.641%
87	15.053	2217	2227	2232	rBV3	281113	735706	31.54%	1.931%
88	15.106	2232	2236	2249	rVB3	320690	734486	31.49%	1.927%
89	15.212	2249	2254	2259	rBV4	31425	62338	2.67%	0.164%
90	15.323	2263	2273	2285	rVB3	197394	526328	22.56%	1.381%
91	15.464	2286	2297	2311	rVV2	1186973	2175321	93.25%	5.708%
92	15.641	2322	2327	2340	rVB2	202461	440953	18.90%	1.157%
93	15.753	2340	2346	2351	rBV3	30146	55098	2.36%	0.145%
94	15.806	2353	2355	2368	rVB4	28264	57186	2.45%	0.150%
95	15.947	2371	2379	2384	rBV3	36541	72472	3.11%	0.190%
96	16.017	2384	2391	2404	rBV	184147	415028	17.79%	1.089%
97	16.253	2426	2431	2438	rVB4	18563	37044	1.59%	0.097%
98	16.347	2438	2447	2452	rBV5	24157	55639	2.39%	0.146%
99	16.506	2466	2474	2481	rBV8	18579	51985	2.23%	0.136%
100	16.782	2514	2521	2522	rBV	95164	144769	6.21%	0.380%

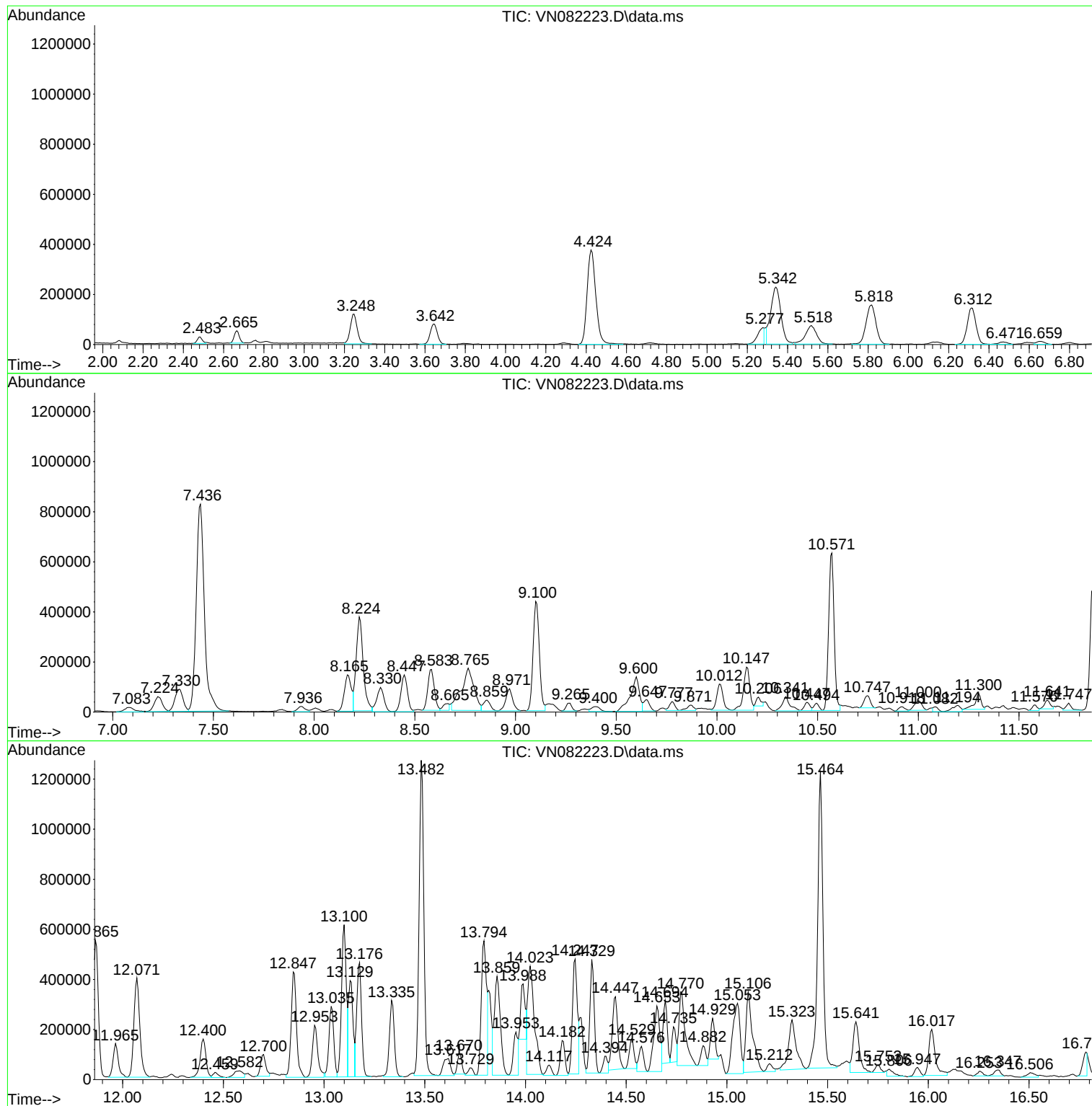
Sum of corrected areas: 38108183

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



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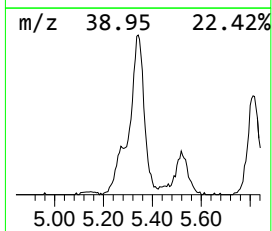
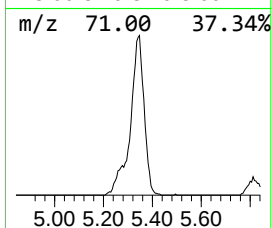
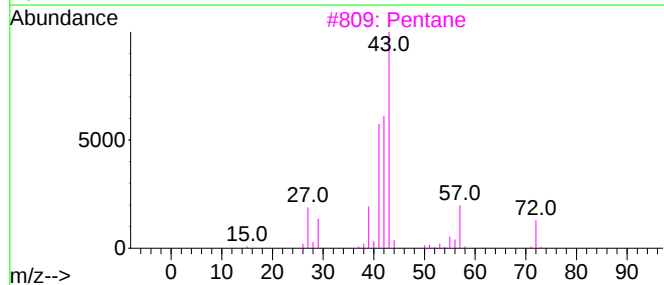
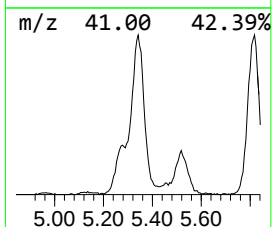
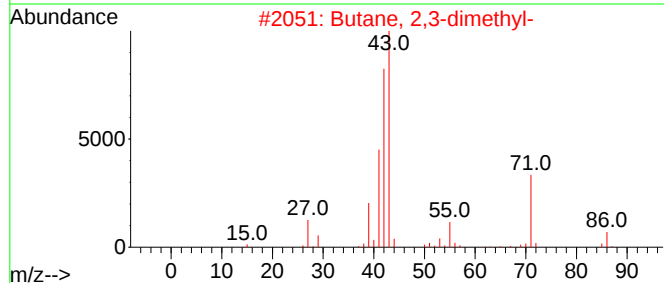
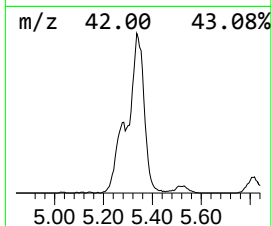
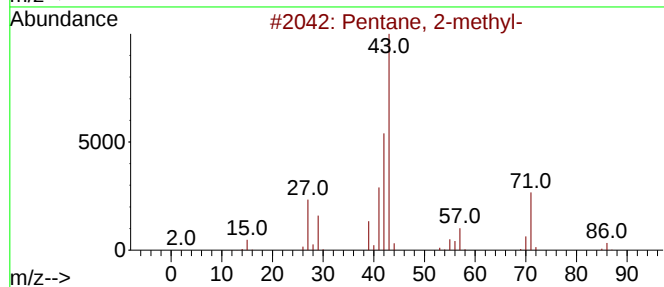
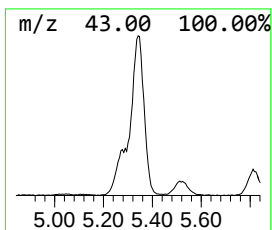
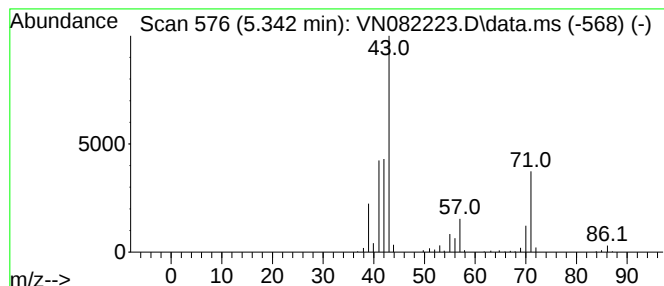
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.342	44.37 ug/l	795691	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	59
3			Pentane	72	C5H12	000109-66-0	47
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	33



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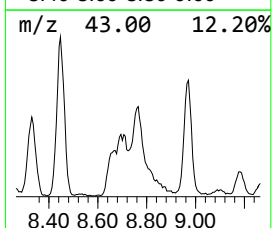
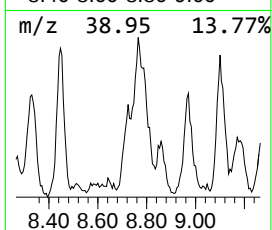
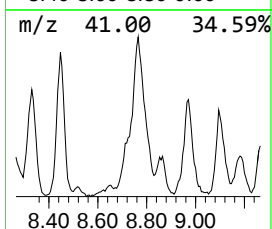
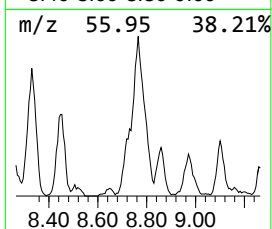
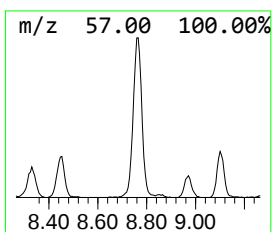
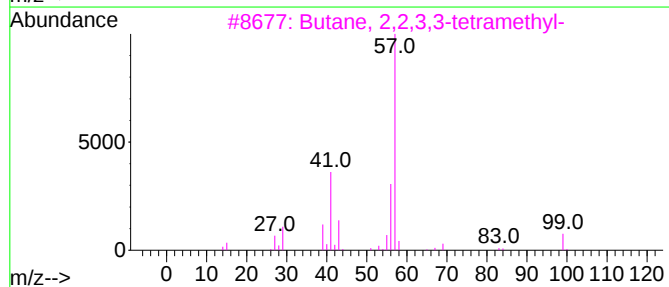
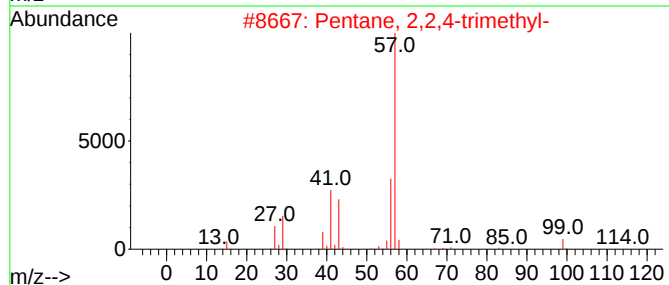
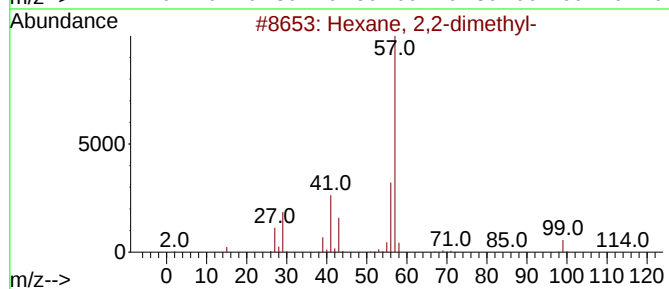
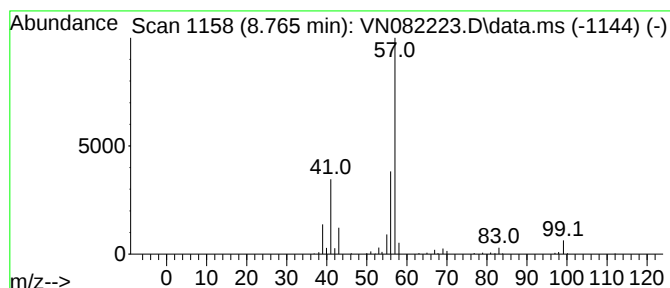
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexane, 2,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.765	39.22 ug/l	742260	1,4-Difluorobenzene	9.100	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
5	2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	50



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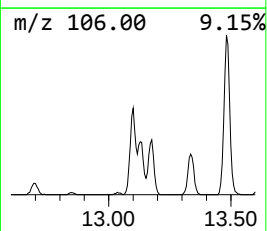
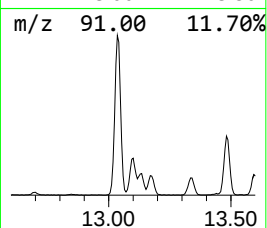
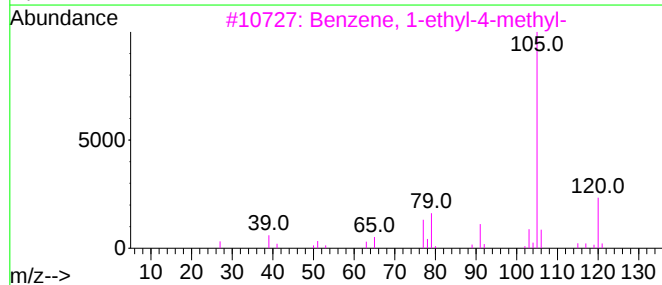
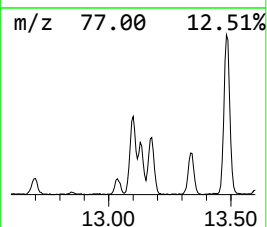
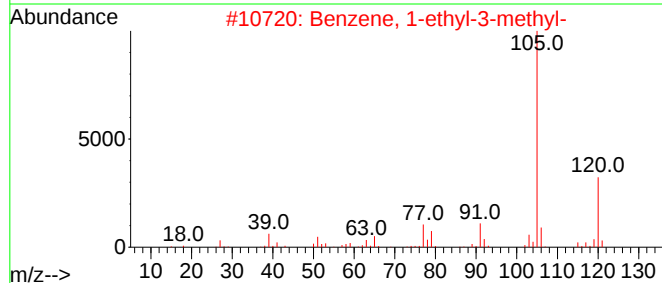
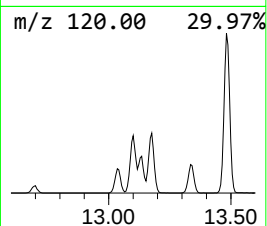
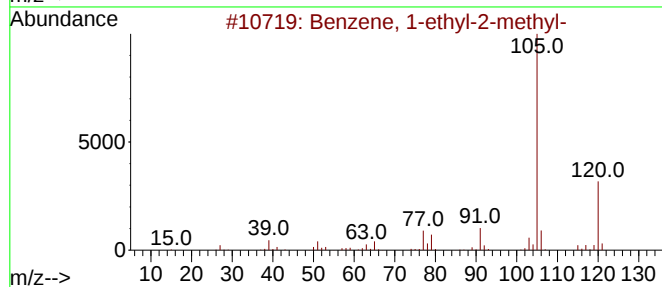
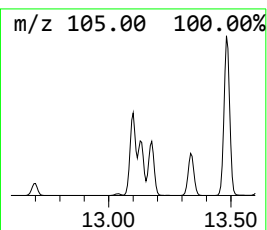
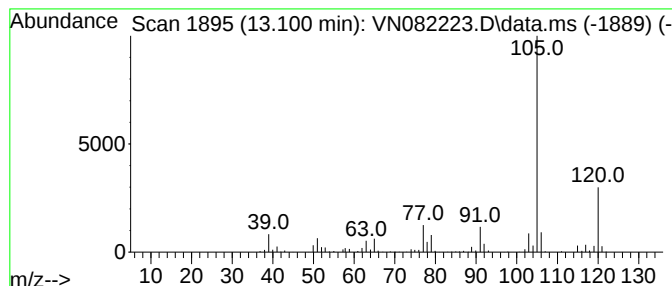
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	52.10 ug/l	1041880	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	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082223.D
Acq On : 20 May 2024 20:36
Operator : JC\MD
Sample : P2541-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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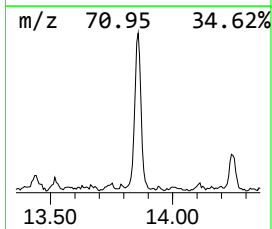
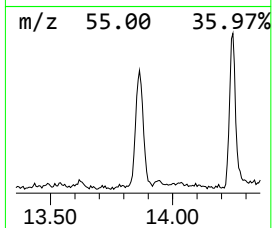
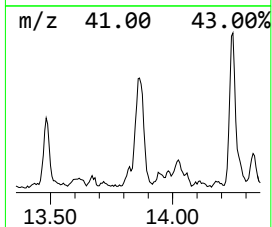
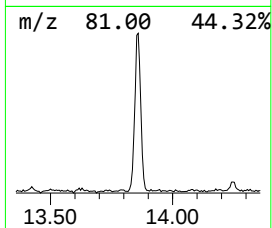
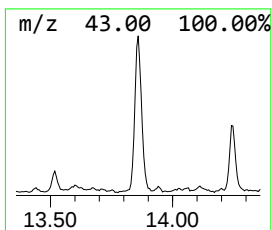
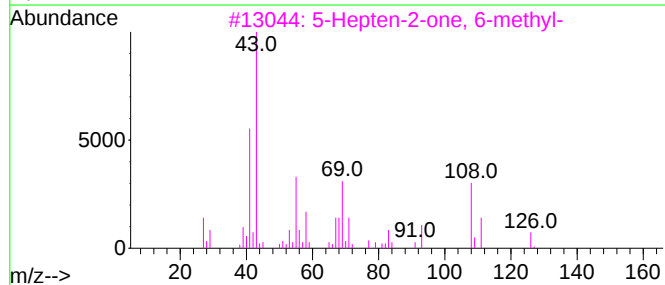
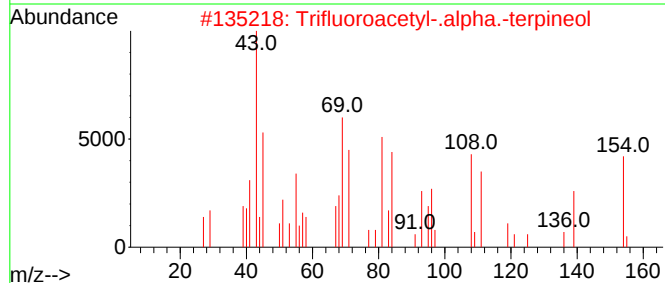
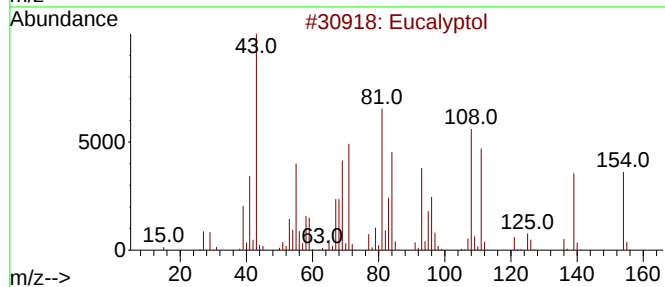
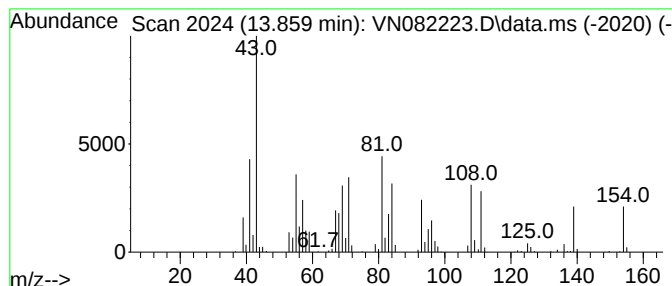
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Quant Title : SW846 8260

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

Peak Number 5 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.859	40.94 ug/l	818651	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	98
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	58
3			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	27
4			2-(3'-Oxo-butyl)-cyclopentanone	154	C9H14O2	1010143-37-2	22
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082223.D
Acq On : 20 May 2024 20:36
Operator : JC\MD
Sample : P2541-01
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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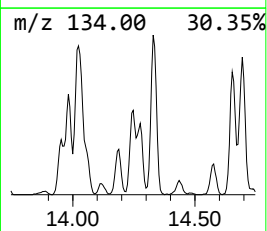
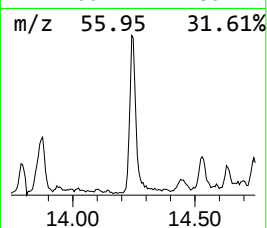
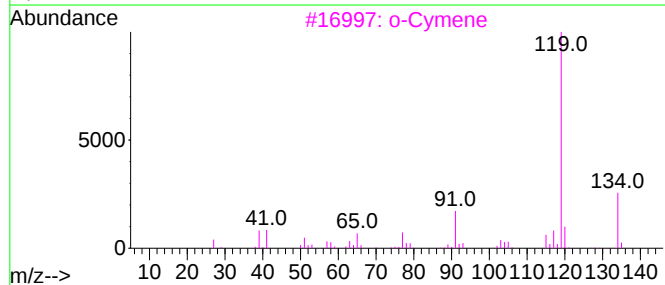
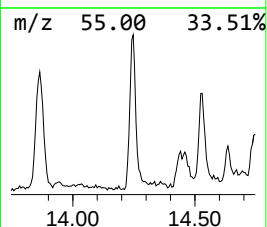
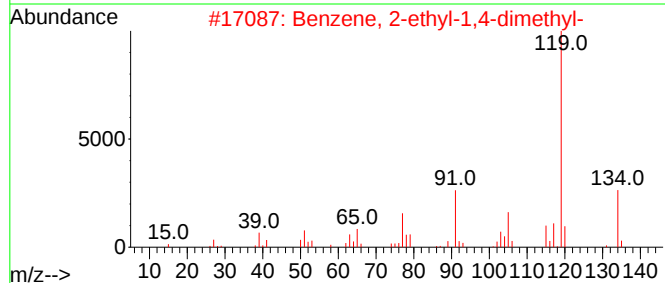
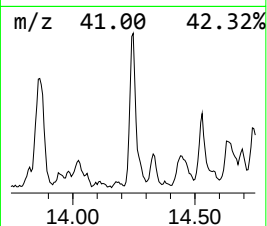
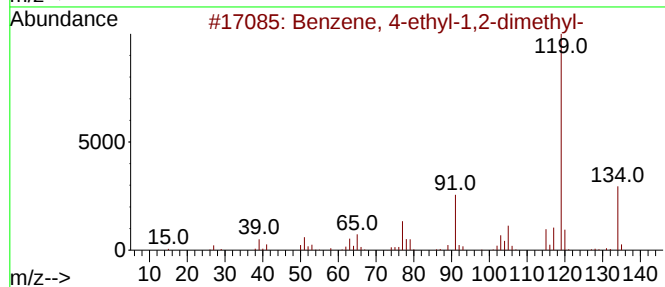
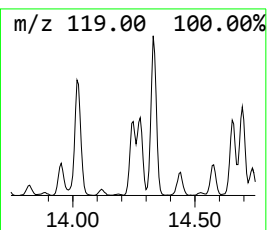
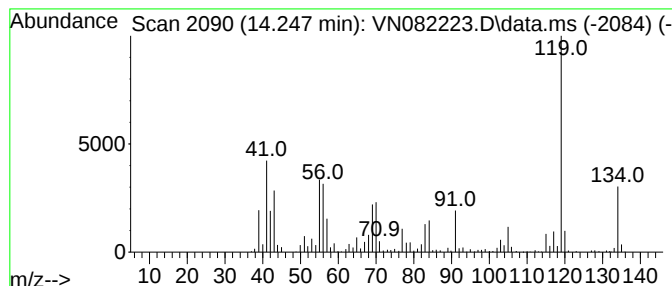
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.247	39.58 ug/l	791422	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93
3			o-Cymene	134	C10H14	000527-84-4	92
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082223.D
Acq On : 20 May 2024 20:36
Operator : JC\MD
Sample : P2541-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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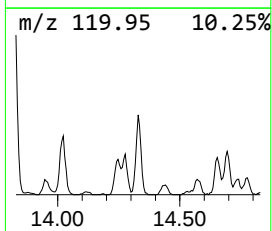
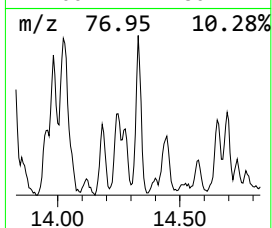
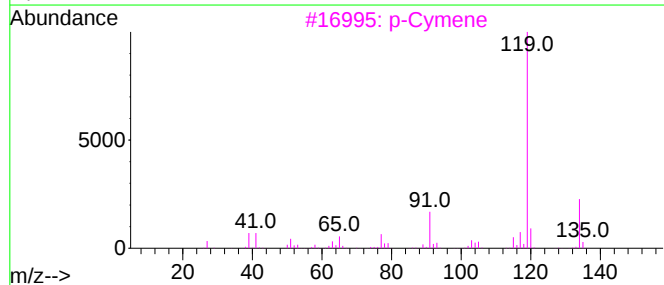
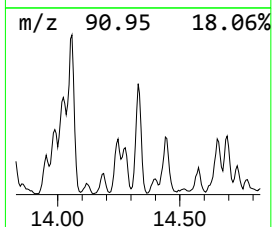
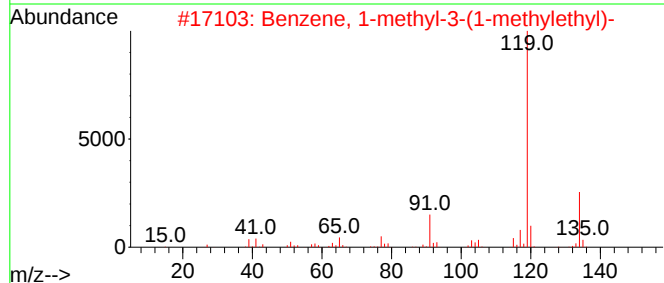
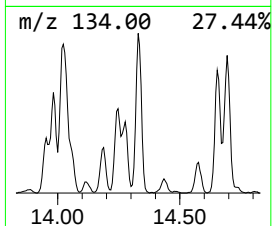
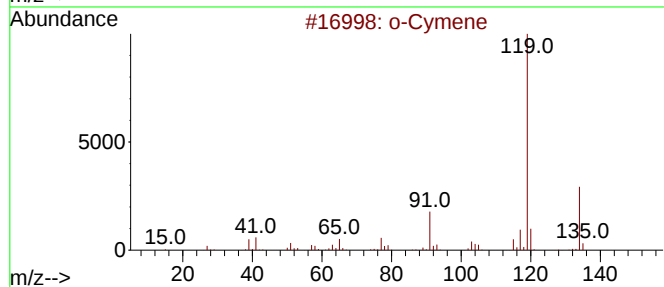
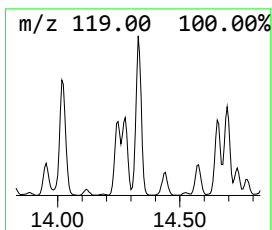
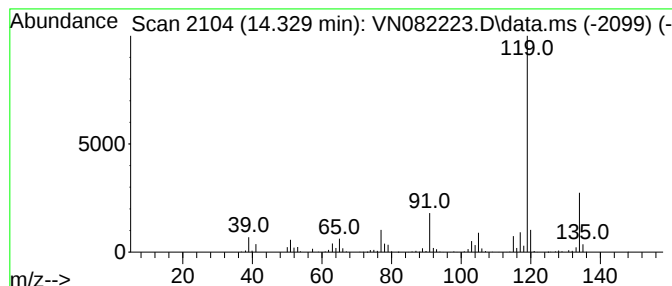
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Quant Title : SW846 8260

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

Peak Number 7 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	34.12 ug/l	682291	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	97
3			p-Cymene	134	C10H14	000099-87-6	97
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082223.D
Acq On : 20 May 2024 20:36
Operator : JC\MD
Sample : P2541-01
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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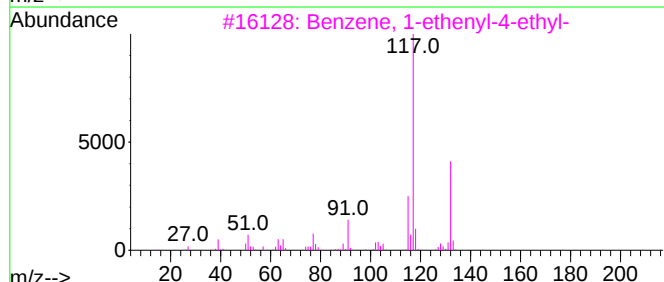
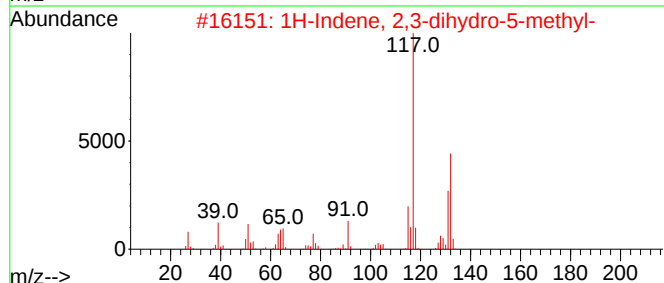
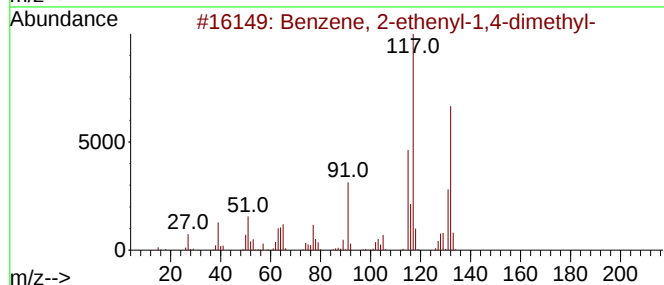
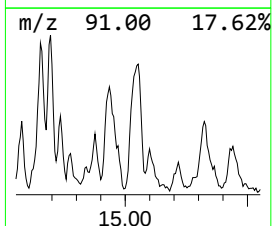
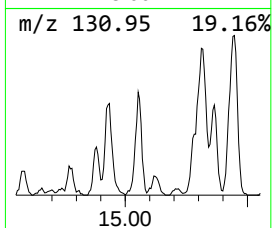
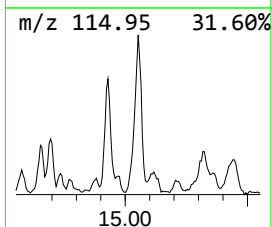
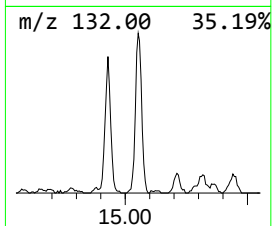
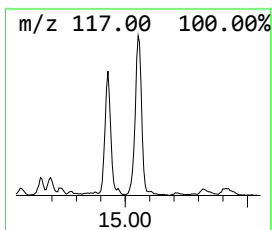
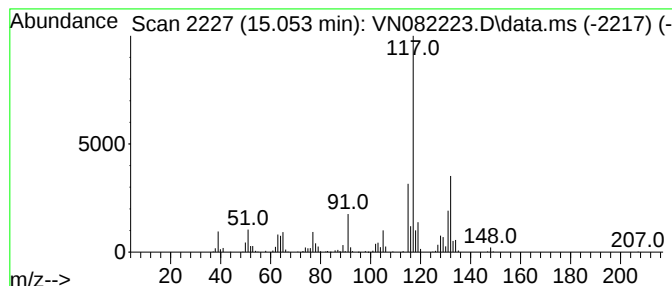
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	36.79 ug/l	735706	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
4			2,4-Dimethylstyrene	132	C10H12	002234-20-0	92
5			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082223.D
Acq On : 20 May 2024 20:36
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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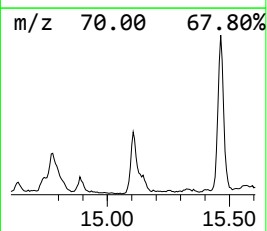
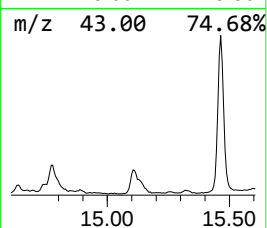
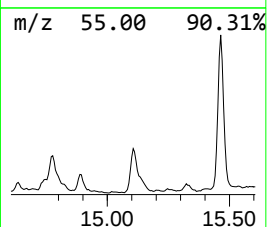
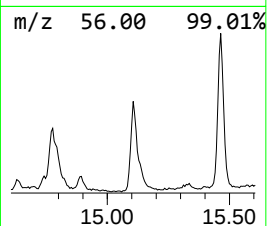
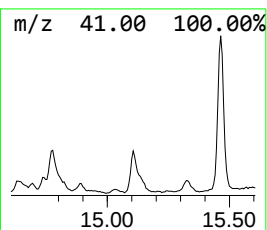
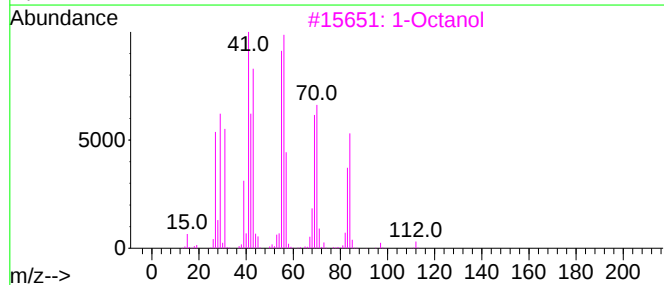
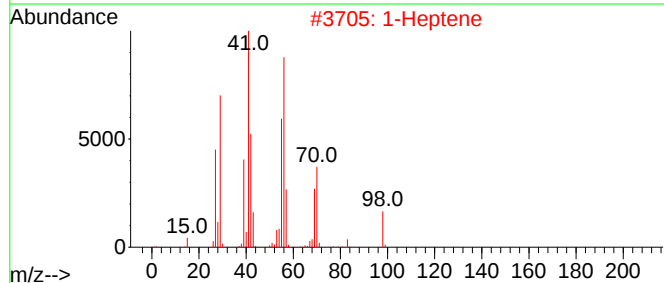
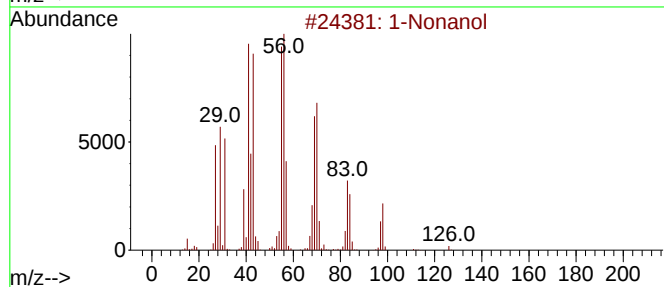
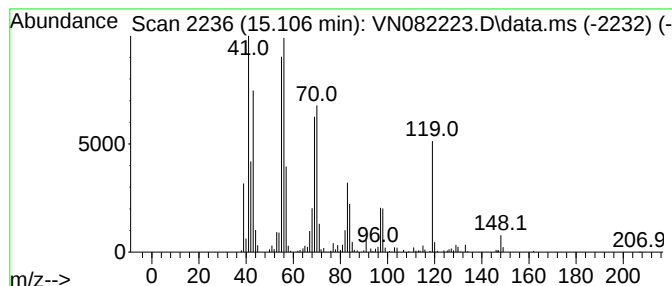
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Quant Title : SW846 8260

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

Peak Number 9 1-Nonanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.106	36.73 ug/l	734486	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol			144	C9H20O	000143-08-8	83
2	1-Heptene			98	C7H14	000592-76-7	64
3	1-Octanol			130	C8H18O	000111-87-5	58
4	Cycloheptane			98	C7H14	000291-64-5	53
5	Cyclopentane, 1,2-dimethyl-			98	C7H14	002452-99-5	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082223.D
Acq On : 20 May 2024 20:36
Operator : JC\MD
Sample : P2541-01
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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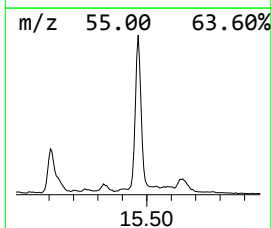
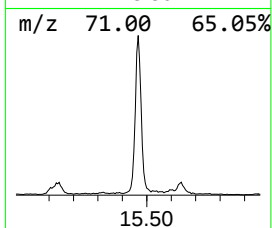
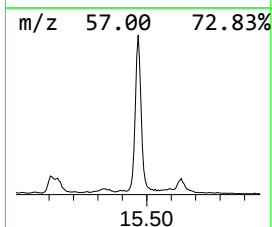
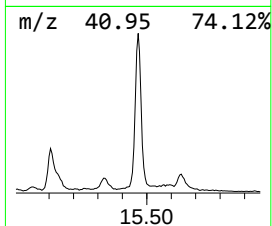
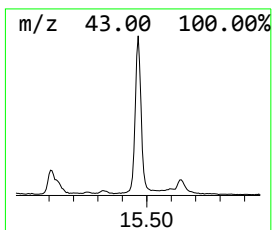
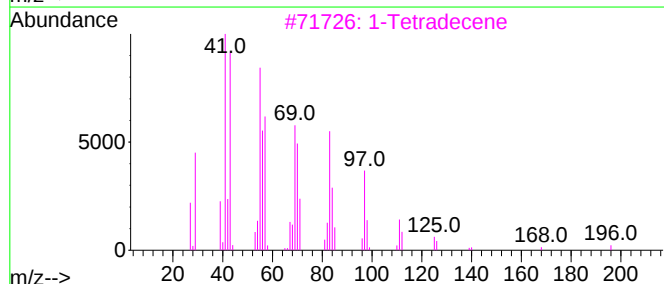
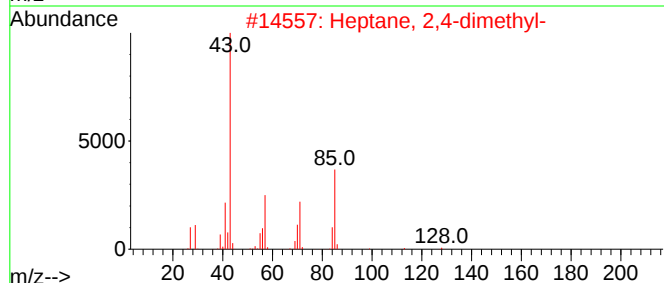
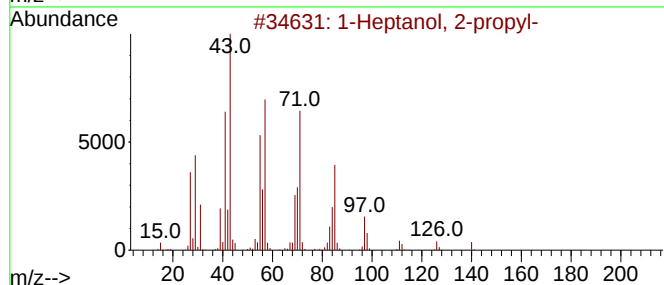
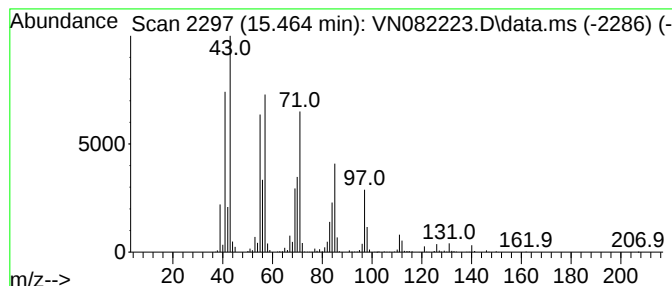
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Quant Title : SW846 8260

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

Peak Number 10 1-Heptanol, 2-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.464	108.79 ug/l	2175320	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	72
2		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	50
3		1-Tetradecene	196	C14H28	001120-36-1	47
4		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
5		Cyclodecane	140	C10H20	000293-96-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052024\
Data File : VN082223.D
Acq On : 20 May 2024 20:36
Operator : JC\MD
Sample : P2541-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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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
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Hexane, 2,2-dim...	8.765	39.2	ug/l	742260	2	9.100	946242	50.0
Benzene, 1-ethy...	13.100	52.1	ug/l	1041880	4	13.794	999800	50.0
Eucalyptol	13.859	40.9	ug/l	818651	4	13.794	999800	50.0
Benzene, 4-ethy...	14.247	39.6	ug/l	791422	4	13.794	999800	50.0
o-Cymene	14.329	34.1	ug/l	682291	4	13.794	999800	50.0
Benzene, 2-ethe...	15.053	36.8	ug/l	735706	4	13.794	999800	50.0
1-Nonanol	15.106	36.7	ug/l	734486	4	13.794	999800	50.0
1-Heptanol, 2-p...	15.464	108.8	ug/l	2175320	4	13.794	999800	50.0