

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
 Data File : VN085233.D
 Acq On : 17 Dec 2024 18:46
 Operator : JC\MD
 Sample : P5291-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW2-20241213

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\82N112224W.M

Title : SW846 8260

Signal : TIC: VN085233.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	50	57	68	rBV2	16247	55446	1.20%	0.120%
2	3.242	209	219	232	rVB2	132906	306858	6.63%	0.664%
3	3.647	276	288	301	rVB4	32972	92490	2.00%	0.200%
4	4.147	359	373	382	rBV2	22627	61641	1.33%	0.133%
5	4.424	405	420	431	rBV3	23764	80671	1.74%	0.175%
6	5.277	551	565	568	rBV4	66135	202278	4.37%	0.438%
7	5.341	569	576	592	rVB4	132037	515287	11.13%	1.116%
8	5.812	640	656	673	rBV3	204240	698415	15.09%	1.512%
9	6.306	730	740	752	rVB3	28812	87103	1.88%	0.189%
10	6.659	786	800	810	rBV2	52307	148695	3.21%	0.322%
11	6.794	812	823	834	rBV3	33259	104513	2.26%	0.226%
12	7.083	861	872	888	rBV4	44166	139845	3.02%	0.303%
13	7.224	888	896	903	rVV	24743	66700	1.44%	0.144%
14	7.324	903	913	934	rVB	221187	681897	14.73%	1.476%
15	8.006	1022	1029	1037	rVB2	80716	190132	4.11%	0.412%
16	8.165	1047	1056	1060	rBV2	120812	287899	6.22%	0.623%
17	8.224	1060	1066	1078	rVV4	280904	887874	19.18%	1.922%
18	8.330	1078	1084	1094	rVB3	106043	265608	5.74%	0.575%
19	8.447	1094	1104	1111	rBV	87254	200405	4.33%	0.434%
20	8.600	1119	1130	1140	rBV2	393153	1101437	23.79%	2.385%
21	8.724	1140	1151	1154	rBV3	110892	286788	6.19%	0.621%
22	8.782	1156	1161	1168	rVB5	164428	397837	8.59%	0.861%
23	8.853	1168	1173	1181	rVB2	59657	135918	2.94%	0.294%
24	8.941	1181	1188	1201	rVB4	28592	79792	1.72%	0.173%
25	9.100	1205	1215	1223	rBV3	449549	1044199	22.55%	2.261%
26	9.194	1228	1231	1237	rVV4	32410	61715	1.33%	0.134%
27	9.259	1237	1242	1249	rVV3	36800	69812	1.51%	0.151%
28	9.335	1249	1255	1259	rVV	48804	99960	2.16%	0.216%
29	9.382	1259	1263	1272	rVB	58179	113468	2.45%	0.246%
30	9.600	1281	1300	1307	rBV2	185408	606953	13.11%	1.314%
31	9.777	1323	1330	1336	rVB2	49452	101829	2.20%	0.220%
32	9.941	1351	1358	1359	rBV3	33176	59799	1.29%	0.129%
33	10.012	1365	1370	1378	rVB4	51263	114106	2.46%	0.247%
34	10.100	1378	1385	1389	rBV2	135213	250169	5.40%	0.542%
35	10.147	1389	1393	1401	rVV3	84862	181792	3.93%	0.394%
36	10.335	1416	1425	1431	rBV6	27345	73325	1.58%	0.159%

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Integrator: RTE

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Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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Peak separation: 5

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37	10.447	1439	1444	1450	rBV3	96357	177243	3.83%	0.384%
38	10.565	1457	1464	1470	rBV	515175	953891	20.60%	2.065%
39	10.629	1470	1475	1484	rVV	52837	129004	2.79%	0.279%
40	10.753	1488	1496	1501	rVB6	45040	119548	2.58%	0.259%
41	10.912	1517	1523	1529	rBV4	26050	59295	1.28%	0.128%
42	10.982	1529	1535	1545	rVV3	91061	247094	5.34%	0.535%
43	11.253	1574	1581	1585	rBV5	23453	52293	1.13%	0.113%
44	11.865	1677	1685	1692	rBV	421844	771401	16.66%	1.670%
45	11.965	1693	1702	1712	rVV	2550612	4402654	95.10%	9.532%
46	12.070	1712	1720	1731	rVV	2439262	4629711	100.00%	10.024%
47	12.394	1765	1775	1781	rBV2	37718	76540	1.65%	0.166%
48	12.694	1818	1826	1833	rBV	290003	465692	10.06%	1.008%
49	12.847	1845	1852	1862	rVB	351897	605739	13.08%	1.311%
50	13.035	1874	1884	1890	rBV	586475	950243	20.52%	2.057%
51	13.129	1890	1900	1904	rVV	658948	1162502	25.11%	2.517%
52	13.170	1904	1907	1915	rVB	670394	1009809	21.81%	2.186%
53	13.335	1927	1935	1944	rVB	727459	1164862	25.16%	2.522%
54	13.482	1952	1960	1967	rVB	2143166	3500318	75.61%	7.578%
55	13.612	1974	1982	1988	rVB3	43874	104692	2.26%	0.227%
56	13.817	2006	2017	2026	rBV2	842489	2074693	44.81%	4.492%
57	13.947	2033	2039	2042	rBV	279427	454304	9.81%	0.984%
58	13.994	2042	2047	2062	rVV	1735330	3373333	72.86%	7.303%
59	14.112	2062	2067	2073	rVV	51276	80564	1.74%	0.174%
60	14.182	2073	2079	2084	rVV2	164974	273150	5.90%	0.591%
61	14.241	2084	2089	2092	rVV	153544	260609	5.63%	0.564%
62	14.270	2092	2094	2098	rVV	125639	163458	3.53%	0.354%
63	14.329	2098	2104	2110	rVV	649020	992063	21.43%	2.148%
64	14.394	2110	2115	2118	rVV	145969	235507	5.09%	0.510%
65	14.441	2118	2123	2130	rVB2	545251	940354	20.31%	2.036%
66	14.570	2140	2145	2151	rVB3	68114	114135	2.47%	0.247%
67	14.653	2151	2159	2162	rBV	395738	644769	13.93%	1.396%
68	14.694	2162	2166	2170	rVV	263645	424575	9.17%	0.919%
69	14.729	2170	2172	2176	rVB2	36541	46733	1.01%	0.101%
70	14.923	2200	2205	2211	rBV	409975	688202	14.86%	1.490%
71	15.053	2217	2227	2233	rBV2	686577	1493985	32.27%	3.235%
72	15.111	2233	2237	2246	rVB3	73560	147365	3.18%	0.319%
73	15.206	2246	2253	2261	rBV2	117359	226684	4.90%	0.491%
74	15.311	2261	2271	2276	rBV3	146437	360728	7.79%	0.781%
75	15.435	2284	2292	2303	rVB3	120367	301005	6.50%	0.652%
76	15.635	2318	2326	2335	rVV	871800	1689335	36.49%	3.658%

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ClientSampleId :
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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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Title : SW846 8260

77	15.747	2338	2345	2350	rVV2	68046	136892	2.96%	0.296%
78	15.806	2350	2355	2363	rVB	33419	70828	1.53%	0.153%
79	15.941	2369	2378	2388	rBV2	56370	116052	2.51%	0.251%
80	16.129	2398	2410	2420	rBV2	31463	111671	2.41%	0.242%
81	16.341	2438	2446	2454	rVB4	21391	57273	1.24%	0.124%
82	16.782	2512	2521	2522	rBV	165030	274466	5.93%	0.594%

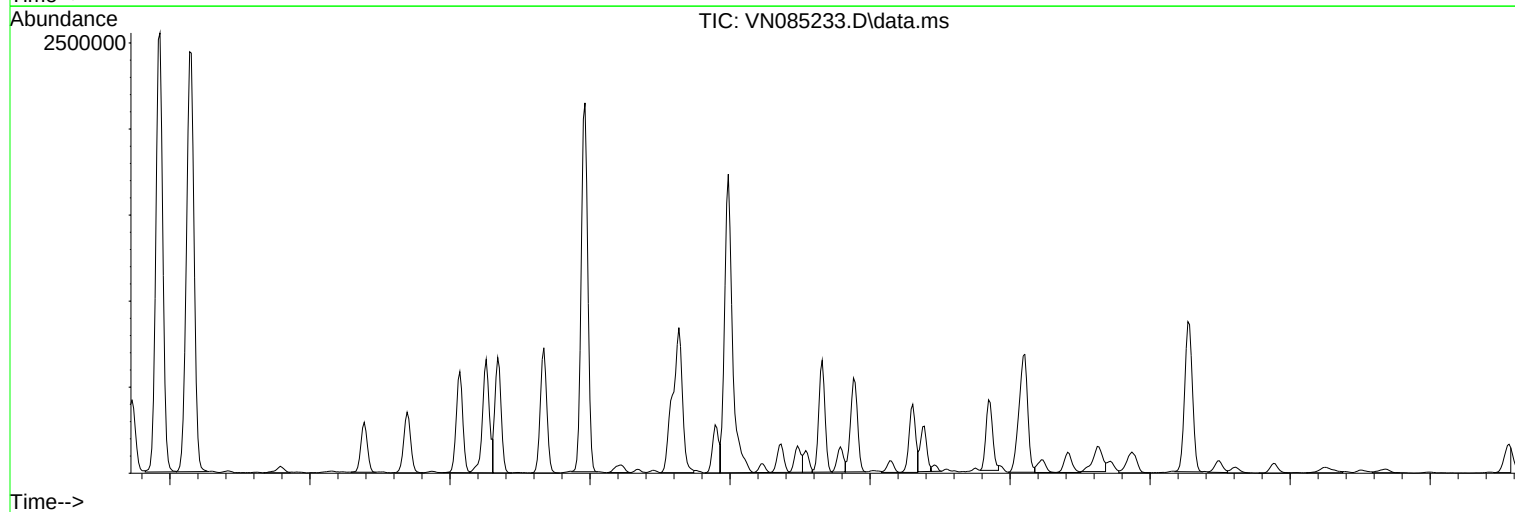
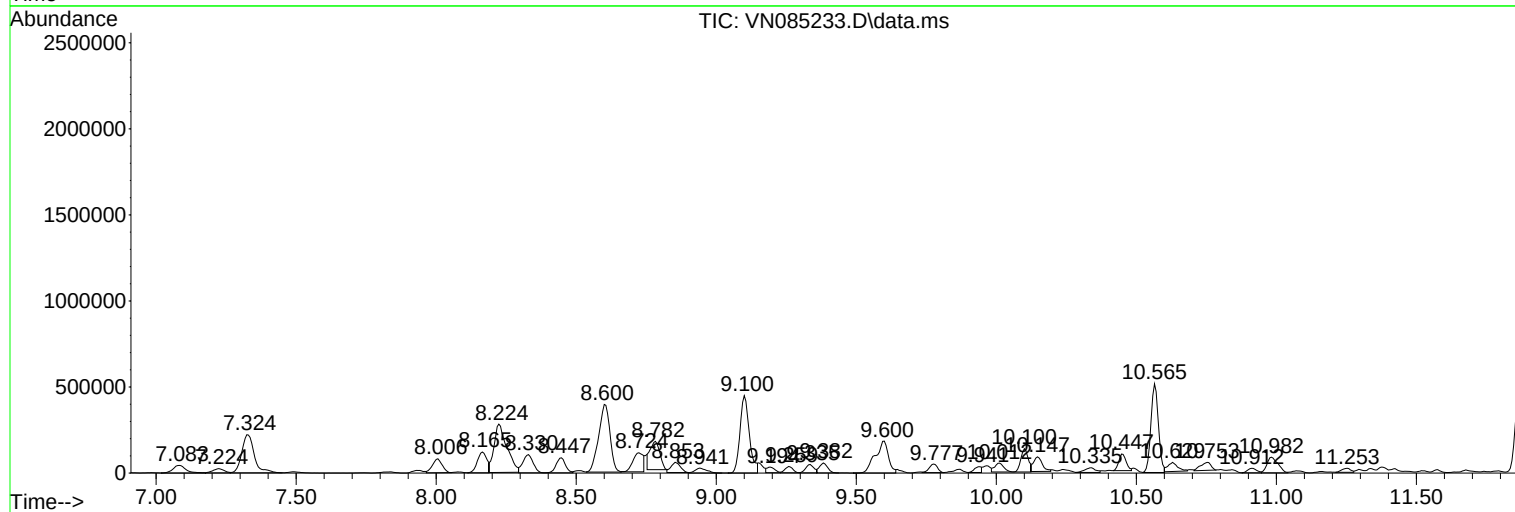
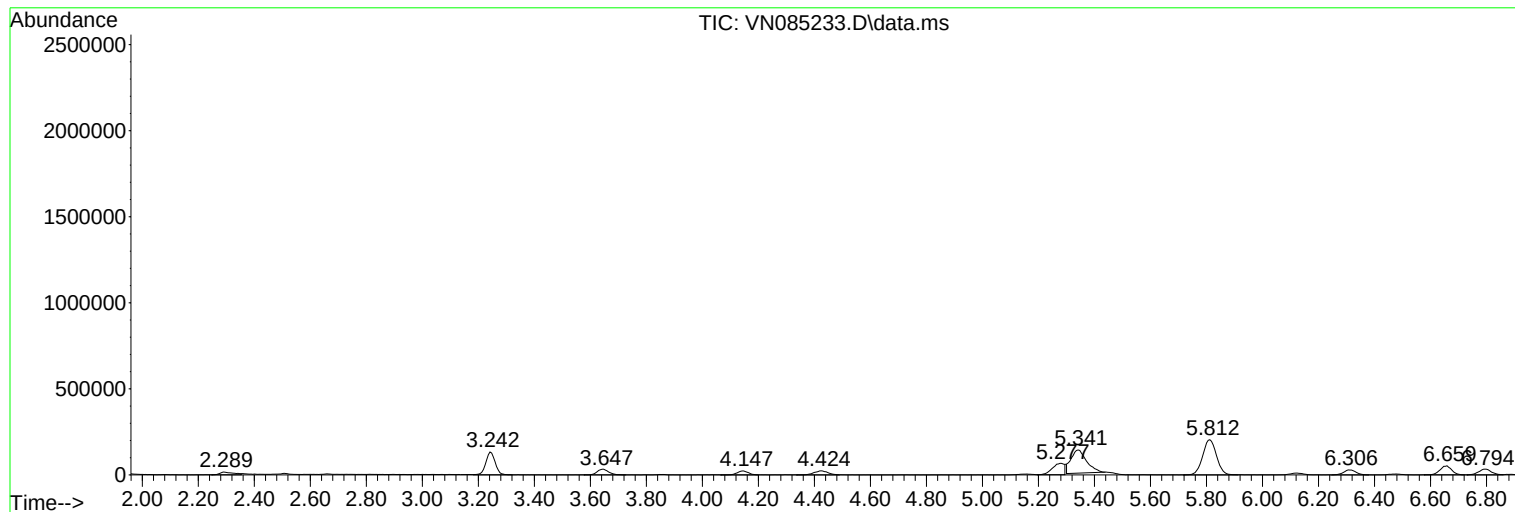
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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



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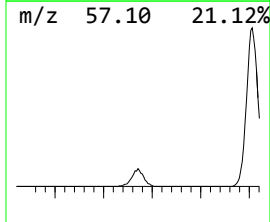
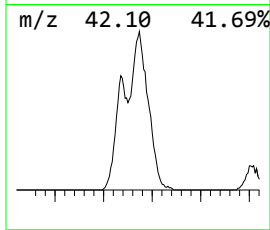
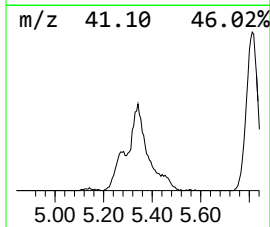
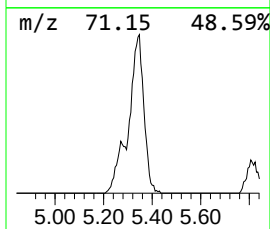
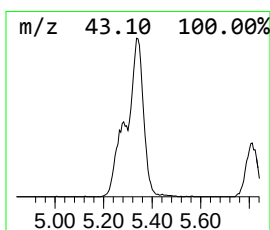
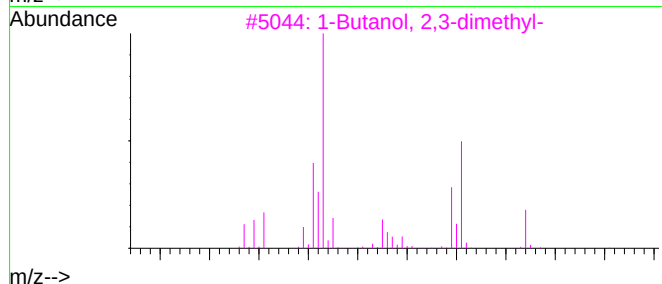
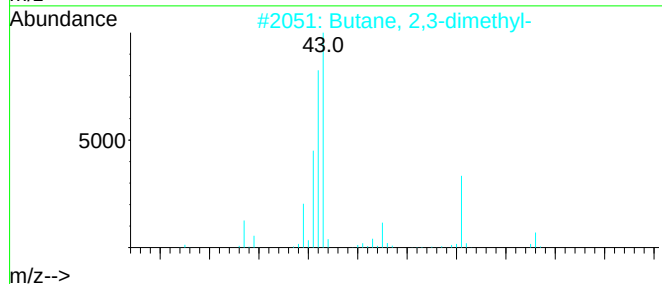
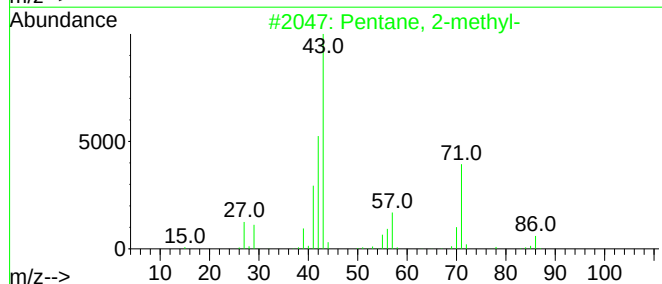
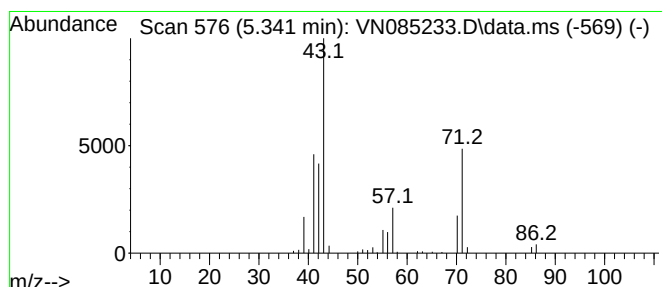
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.341	29.02 ug/l	515287	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	47
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	39
4	Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	38
5	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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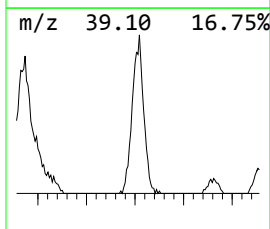
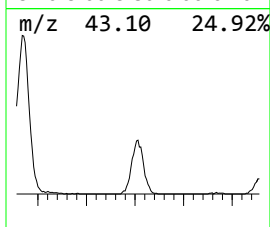
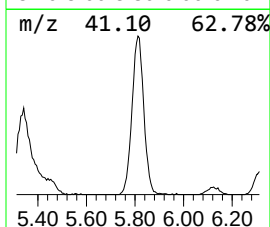
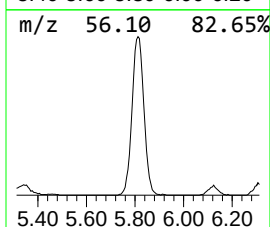
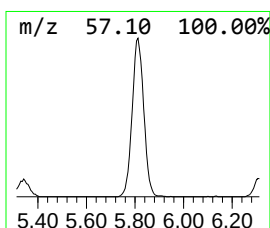
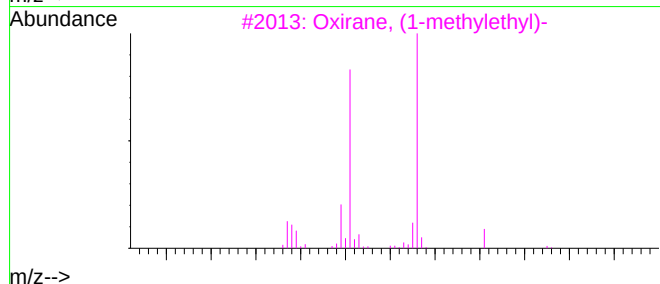
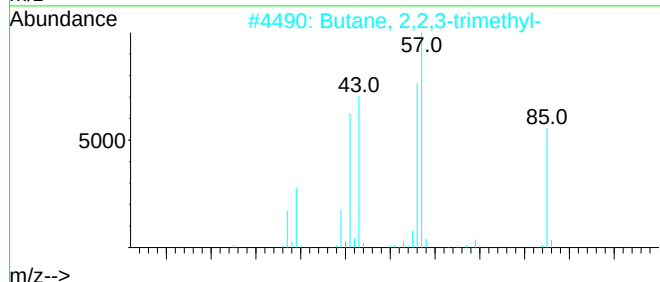
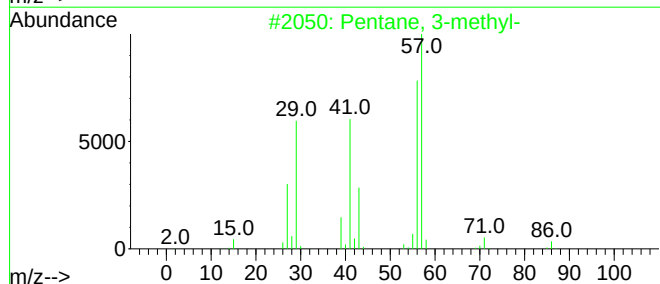
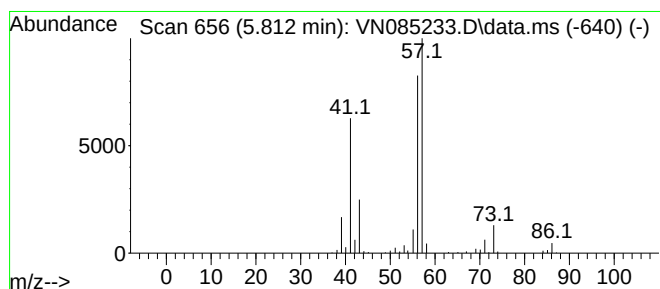
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.812	39.33 ug/l	698415	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	83
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	72
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	53
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50
5	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50



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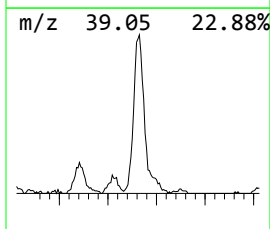
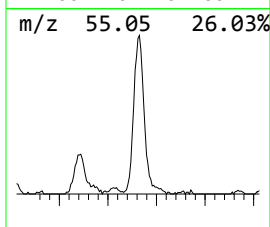
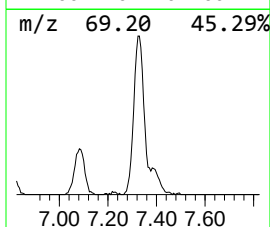
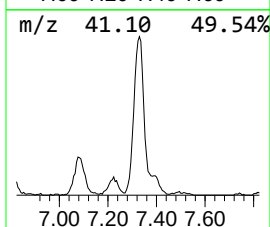
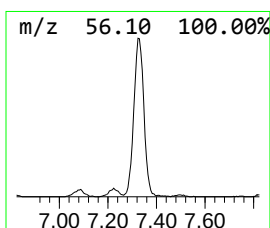
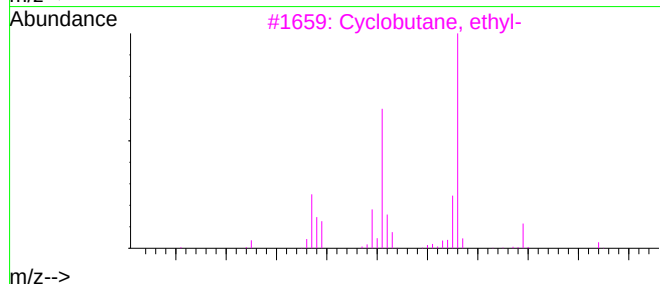
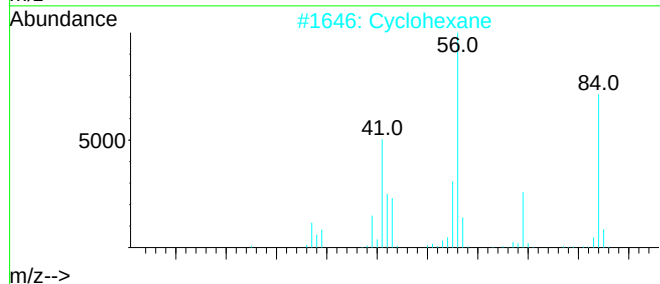
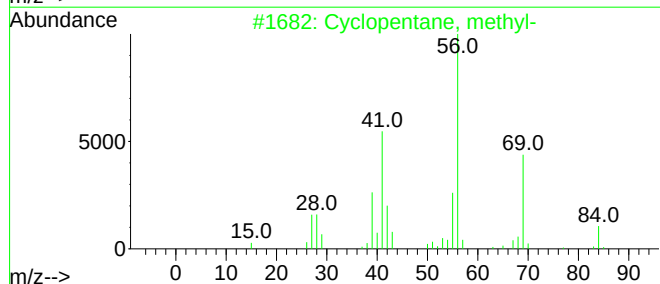
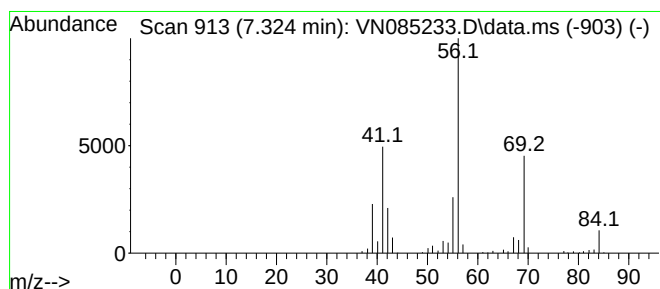
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.324	38.40 ug/l	681897	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50



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Instrument :
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ClientSampleId :
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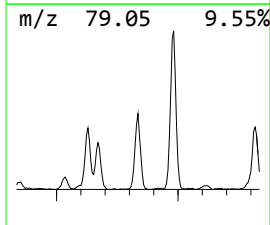
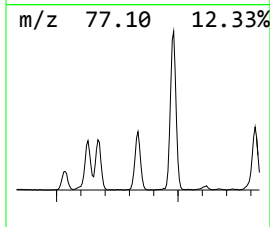
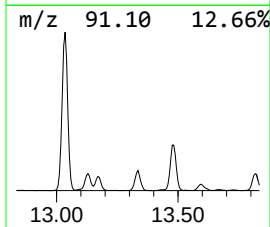
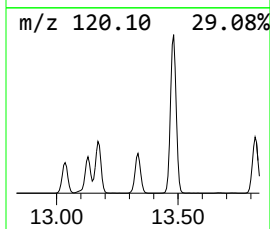
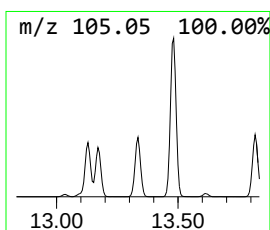
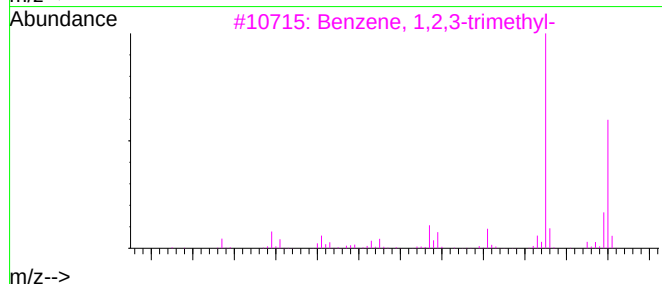
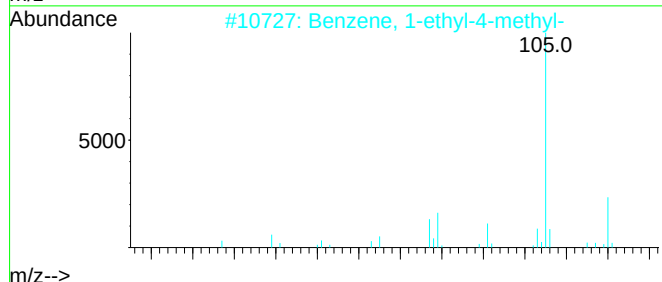
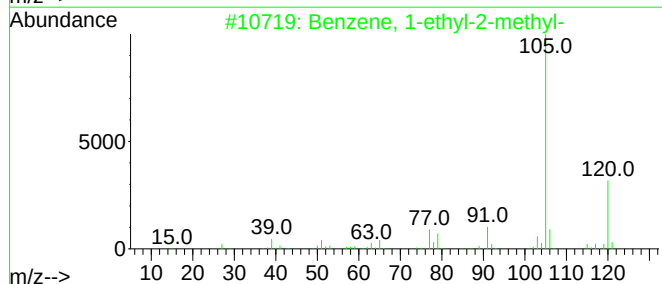
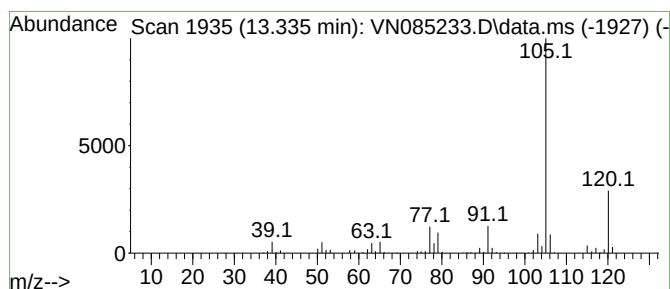
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	28.07 ug/l	1164860	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	93
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085233.D
Acq On : 17 Dec 2024 18:46
Operator : JC\MD
Sample : P5291-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW2-20241213

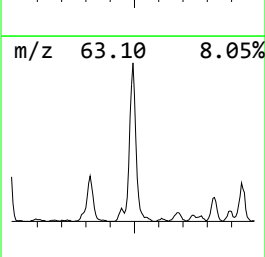
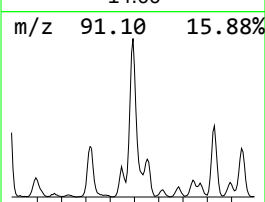
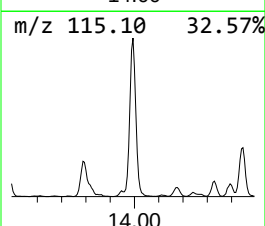
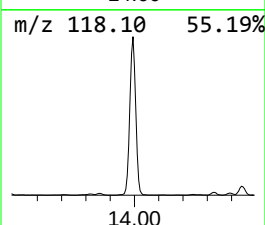
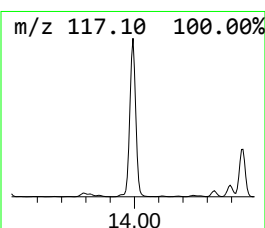
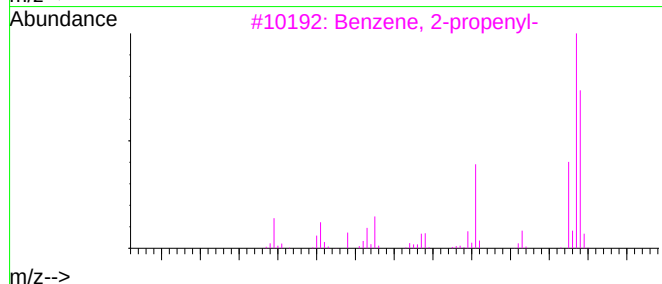
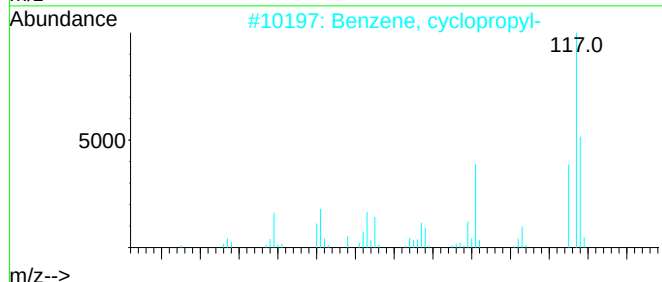
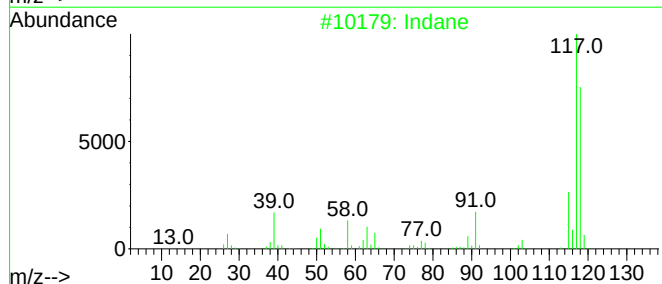
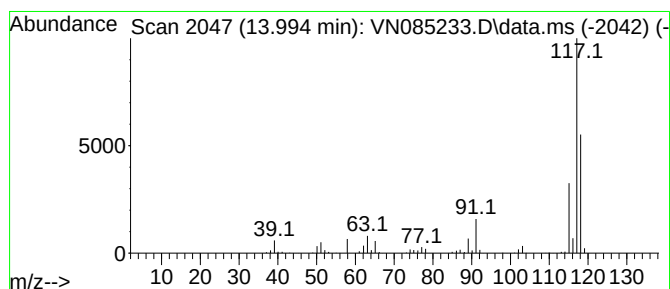
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Quant Title : SW846 8260

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

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	81.30 ug/l	3373330	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	68
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085233.D
Acq On : 17 Dec 2024 18:46
Operator : JC\MD
Sample : P5291-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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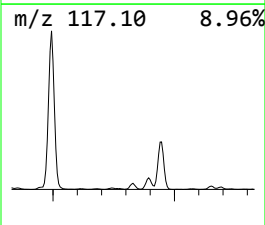
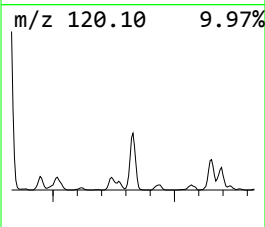
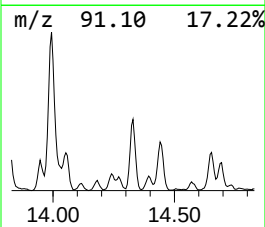
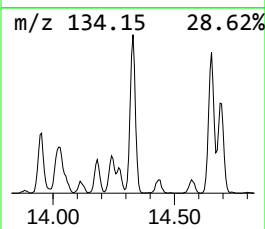
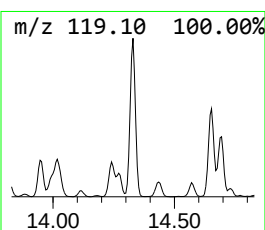
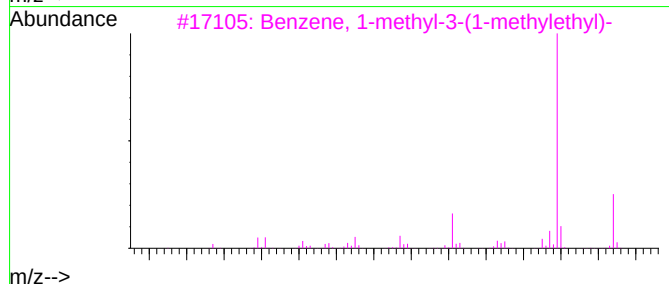
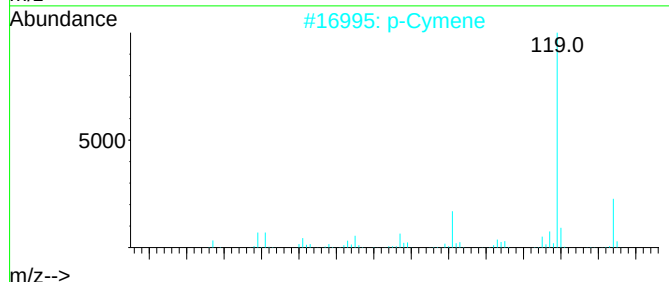
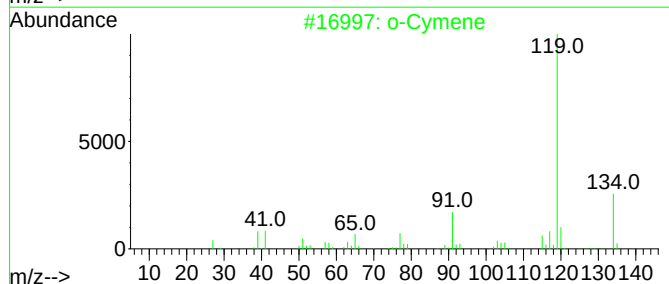
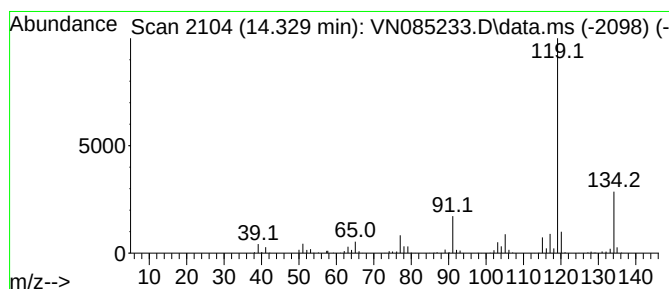
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Quant Title : SW846 8260

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

Peak Number 7 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	23.91 ug/l	992063	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	p-Cymene	134	C10H14	000099-87-6	95
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085233.D
Acq On : 17 Dec 2024 18:46
Operator : JC\MD
Sample : P5291-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

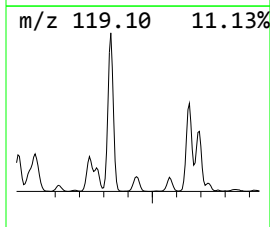
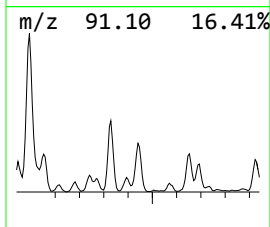
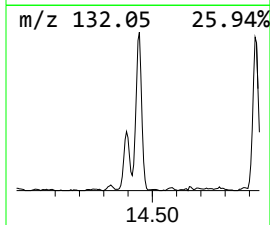
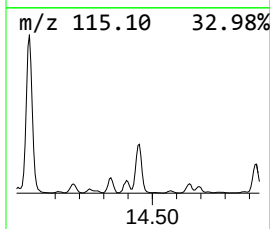
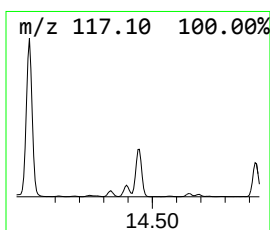
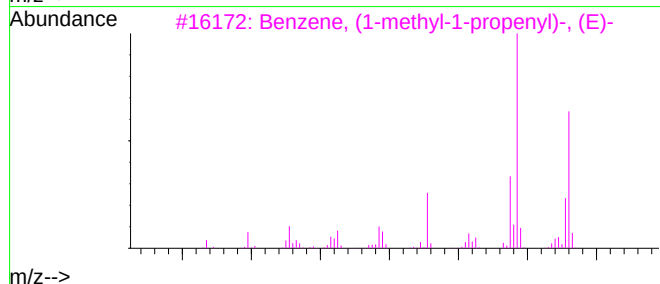
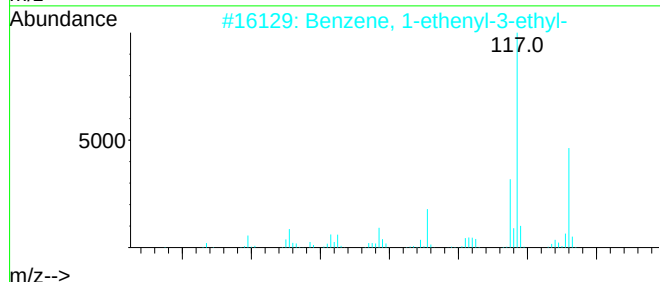
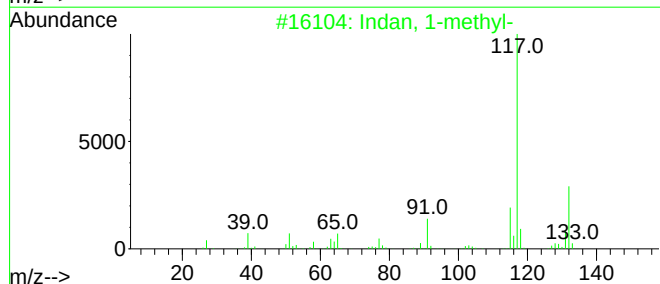
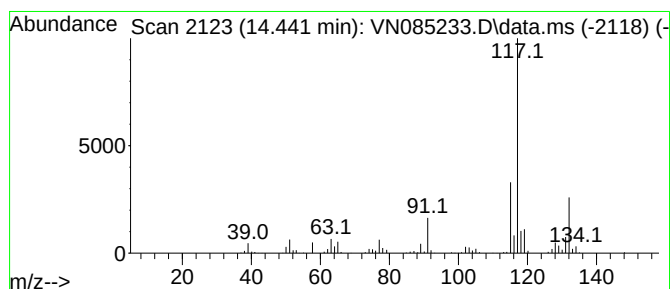
Instrument :
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ClientSampleId :
MW2-20241213

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

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

Peak Number 8 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.441	22.66 ug/l	940354	1,4-Dichlorobenzene-d4	13.788	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	90
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	86
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085233.D
Acq On : 17 Dec 2024 18:46
Operator : JC\MD
Sample : P5291-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW2-20241213

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.M
Quant Title : SW846 8260

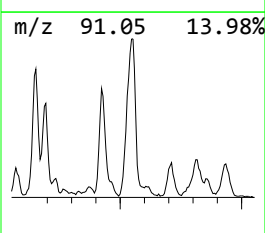
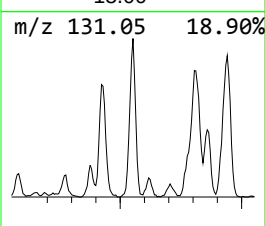
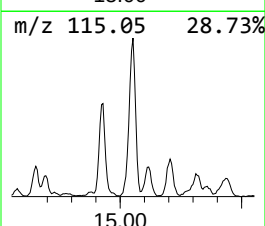
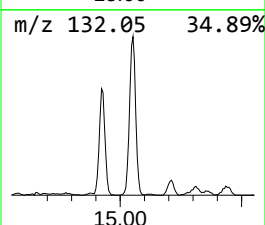
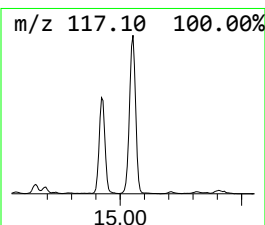
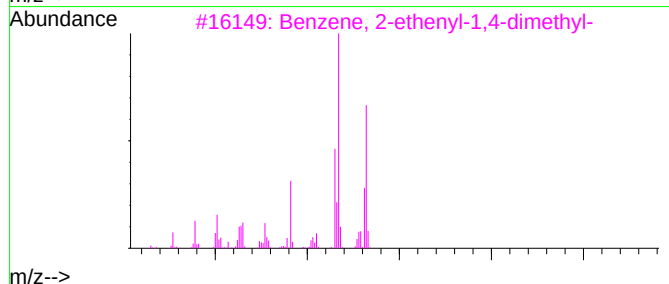
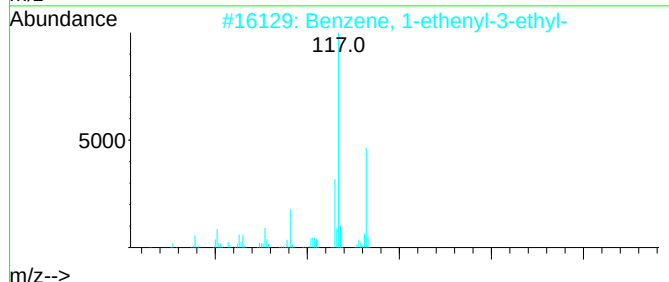
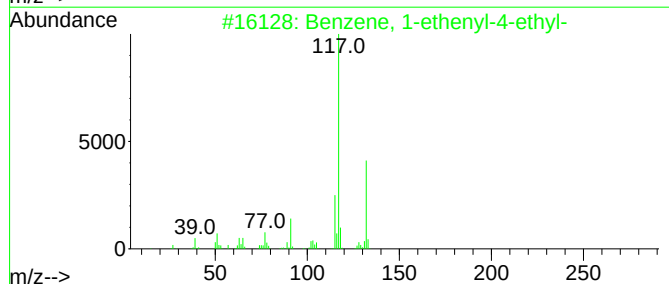
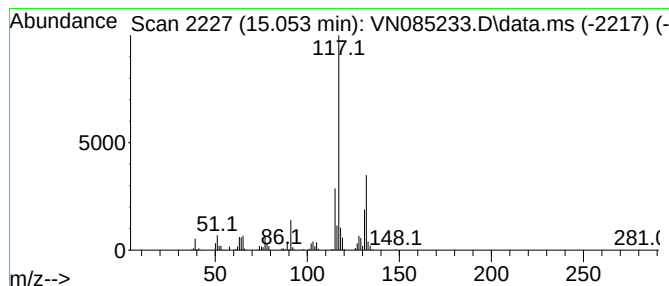
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	36.01 ug/l	1493990	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	93
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121724\
Data File : VN085233.D
Acq On : 17 Dec 2024 18:46
Operator : JC\MD
Sample : P5291-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW2-20241213

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112224W.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
Pentane, 2-methyl-	5.341	29.0	ug/l	515287	1	8.224	887874	50.0
Pentane, 3-methyl-	5.812	39.3	ug/l	698415	1	8.224	887874	50.0
Cyclopentane, m...	7.324	38.4	ug/l	681897	1	8.224	887874	50.0
Benzene, 1-ethy...	13.335	28.1	ug/l	1164860	4	13.788	2074690	50.0
Indane	13.994	81.3	ug/l	3373330	4	13.788	2074690	50.0
o-Cymene	14.329	23.9	ug/l	992063	4	13.788	2074690	50.0
Indan, 1-methyl-	14.441	22.7	ug/l	940354	4	13.788	2074690	50.0
Benzene, 1-ethe...	15.053	36.0	ug/l	1493990	4	13.788	2074690	50.0