

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
 Data File : VN086991.D
 Acq On : 12 Jun 2025 20:26
 Operator : JC\MD
 Sample : Q2268-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-2-20250605

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\82N060625W.M

Title : SW846 8260

Signal : TIC: VN086991.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.283	216	226	243	rBV	371698	913370	5.62%	0.757%
2	3.671	281	292	306	rBV3	109679	303833	1.87%	0.252%
3	4.448	411	424	443	rBV3	65705	237017	1.46%	0.196%
4	5.300	556	569	572	rBV2	154996	457292	2.82%	0.379%
5	5.371	573	581	614	rVB4	334537	1671270	10.29%	1.384%
6	5.836	644	660	681	rBV3	475611	1709715	10.53%	1.416%
7	6.336	733	745	761	rBV	78394	244855	1.51%	0.203%
8	6.677	785	803	815	rBV2	129833	400523	2.47%	0.332%
9	6.812	815	826	836	rBV	84331	268523	1.65%	0.222%
10	7.100	864	875	890	rBV4	106442	335312	2.06%	0.278%
11	7.341	906	916	936	rVV	717065	2204689	13.57%	1.826%
12	8.018	1024	1031	1039	rVB2	147336	361545	2.23%	0.300%
13	8.177	1049	1058	1062	rBV	196144	484341	2.98%	0.401%
14	8.236	1062	1068	1071	rBV	348096	750752	4.62%	0.622%
15	8.336	1080	1085	1096	rVB3	223983	589909	3.63%	0.489%
16	8.453	1096	1105	1112	rBV	156938	361912	2.23%	0.300%
17	8.612	1121	1132	1143	rBV	1272478	3283618	20.21%	2.720%
18	8.736	1143	1153	1156	rBV4	267768	698131	4.30%	0.578%
19	8.788	1157	1162	1170	rVB3	381115	975215	6.00%	0.808%
20	8.865	1170	1175	1183	rVB	133737	300454	1.85%	0.249%
21	8.947	1183	1189	1204	rVB3	64590	194677	1.20%	0.161%
22	9.106	1204	1216	1224	rBV2	774599	1881648	11.58%	1.559%
23	9.341	1249	1256	1260	rBV	107964	215479	1.33%	0.179%
24	9.388	1260	1264	1281	rVB2	91827	197182	1.21%	0.163%
25	9.606	1281	1301	1318	rBV2	483989	1614423	9.94%	1.337%
26	9.782	1325	1331	1337	rVB	126909	239588	1.47%	0.198%
27	9.941	1351	1358	1360	rBV2	102631	185804	1.14%	0.154%
28	10.018	1367	1371	1379	rVB3	95820	202860	1.25%	0.168%
29	10.106	1379	1386	1390	rBV	312729	608542	3.75%	0.504%
30	10.153	1390	1394	1400	rVB2	149648	282104	1.74%	0.234%
31	10.347	1417	1427	1431	rBV7	61024	187211	1.15%	0.155%
32	10.453	1440	1445	1450	rBV	193848	327575	2.02%	0.271%
33	10.571	1457	1465	1471	rBV	902019	1683866	10.37%	1.395%
34	10.629	1471	1475	1482	rVB	145124	285272	1.76%	0.236%
35	10.759	1488	1497	1507	rVV5	103275	276983	1.71%	0.229%
36	10.988	1529	1536	1546	rVB2	171558	462356	2.85%	0.383%

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Integrator: RTE

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Sampling : 1

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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\82N060625W.M
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37	11.871	1678	1686	1693	rVV	720564	1368369	8.42%	1.134%
38	11.965	1694	1702	1712	rVV	7979810	13515388	83.20%	11.196%
39	12.076	1712	1721	1734	rVB	8746624	16244257	100.00%	13.457%
40	12.400	1765	1776	1786	rBV	184394	345954	2.13%	0.287%
41	12.694	1819	1826	1838	rVB	831173	1372239	8.45%	1.137%
42	12.847	1845	1852	1863	rVB	498849	884833	5.45%	0.733%
43	13.035	1871	1884	1890	rBV	1671229	2759249	16.99%	2.286%
44	13.129	1890	1900	1904	rVV	1594589	2955237	18.19%	2.448%
45	13.171	1904	1907	1915	rVB	1554638	2400911	14.78%	1.989%
46	13.335	1928	1935	1944	rVB	1838051	3006185	18.51%	2.490%
47	13.482	1947	1960	1974	rBV	5340556	8661297	53.32%	7.175%
48	13.612	1974	1982	1987	rBV3	111347	275753	1.70%	0.228%
49	13.818	2006	2017	2033	rVB2	2259201	4991994	30.73%	4.135%
50	13.953	2033	2040	2042	rBV	650034	1063715	6.55%	0.881%
51	13.994	2042	2047	2063	rVV	4923028	9239166	56.88%	7.654%
52	14.118	2063	2068	2073	rVB	121332	196335	1.21%	0.163%
53	14.182	2073	2079	2084	rBV2	386193	634665	3.91%	0.526%
54	14.241	2084	2089	2092	rVV	309357	512778	3.16%	0.425%
55	14.270	2092	2094	2098	rVV	215810	290239	1.79%	0.240%
56	14.329	2098	2104	2110	rVV	1440341	2237361	13.77%	1.853%
57	14.394	2110	2115	2118	rVV	354877	568236	3.50%	0.471%
58	14.441	2118	2123	2131	rVB2	1328012	2308590	14.21%	1.912%
59	14.570	2140	2145	2151	rVB2	150333	257275	1.58%	0.213%
60	14.653	2151	2159	2163	rBV	900426	1523492	9.38%	1.262%
61	14.694	2163	2166	2170	rVV	478179	688486	4.24%	0.570%
62	14.923	2200	2205	2211	rBV	1011543	1691744	10.41%	1.401%
63	15.053	2217	2227	2233	rBV2	1653504	3583927	22.06%	2.969%
64	15.117	2233	2238	2247	rVV3	158365	326974	2.01%	0.271%
65	15.206	2247	2253	2261	rVV2	291876	554137	3.41%	0.459%
66	15.317	2261	2272	2277	rVV3	289735	796783	4.91%	0.660%
67	15.359	2277	2279	2284	rVV2	124963	191716	1.18%	0.159%
68	15.435	2284	2292	2302	rVB2	230050	592803	3.65%	0.491%
69	15.635	2312	2326	2338	rBV	3486683	6941827	42.73%	5.751%
70	15.747	2338	2345	2350	rVV	240521	507527	3.12%	0.420%
71	15.941	2371	2378	2387	rBV	106977	213795	1.32%	0.177%
72	16.123	2400	2409	2420	rBV	63128	198290	1.22%	0.164%
73	16.776	2512	2520	2522	rBV	793897	1415990	8.72%	1.173%

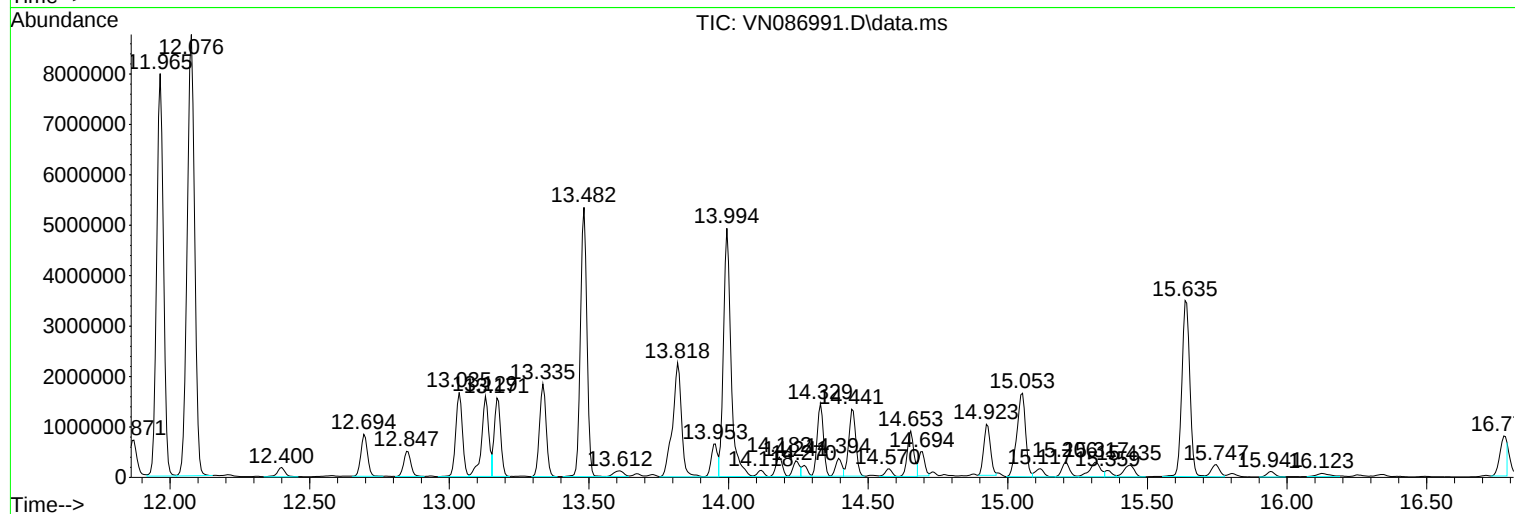
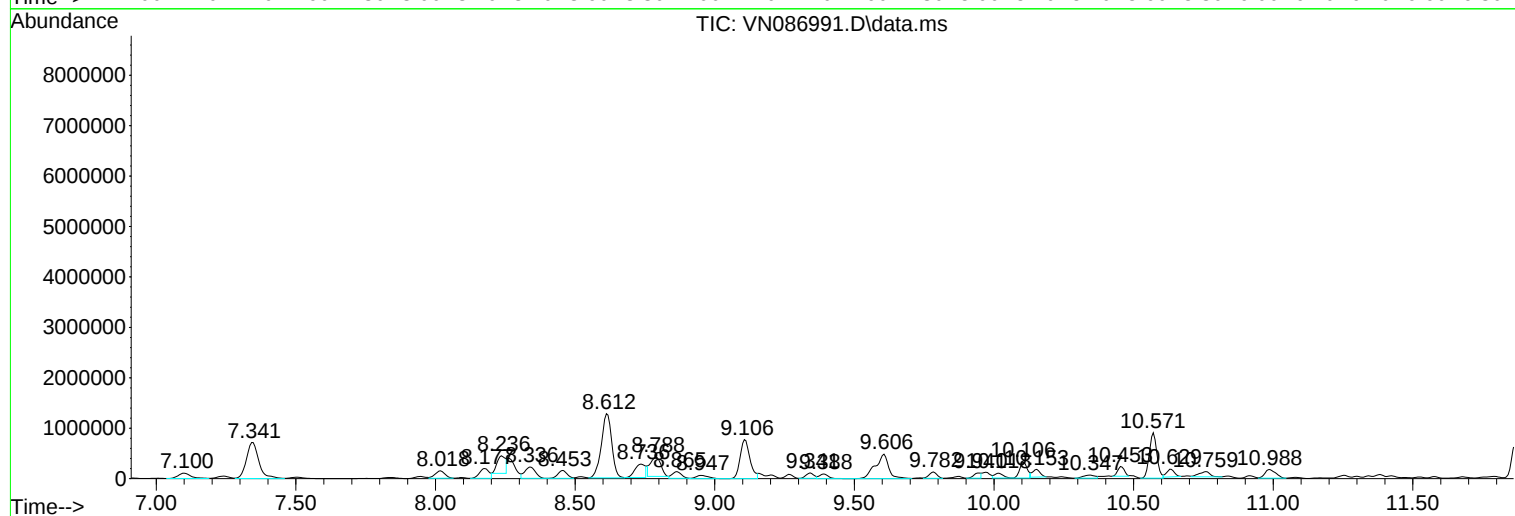
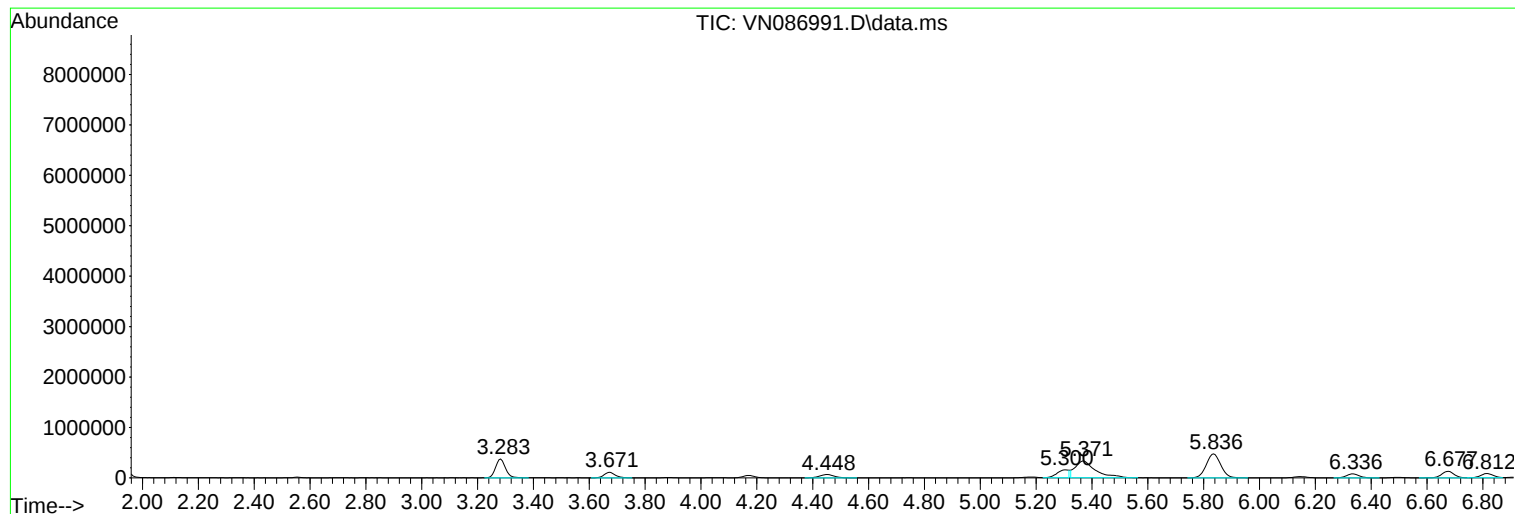
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ClientSampleId :
MW-2-20250605

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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



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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

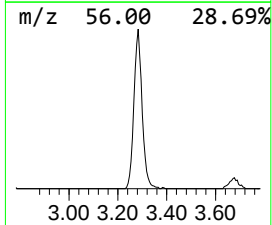
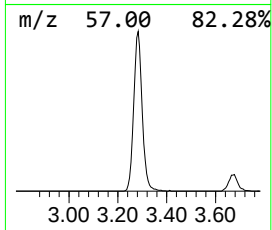
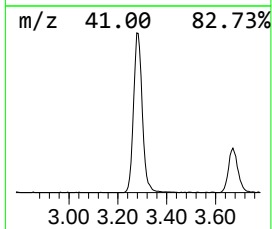
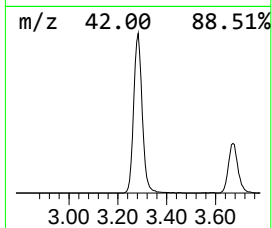
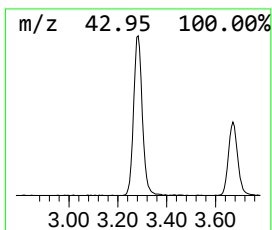
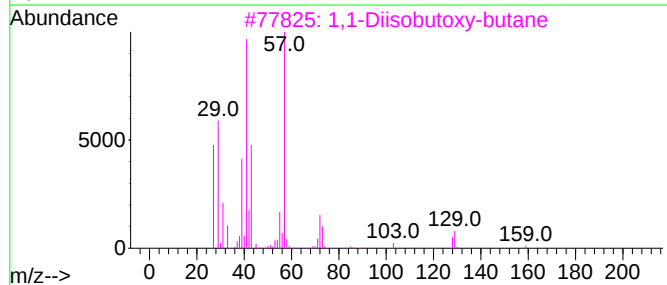
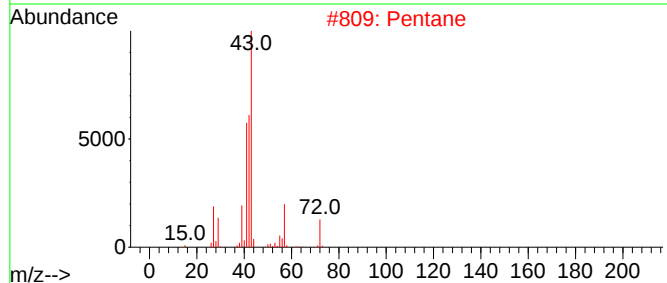
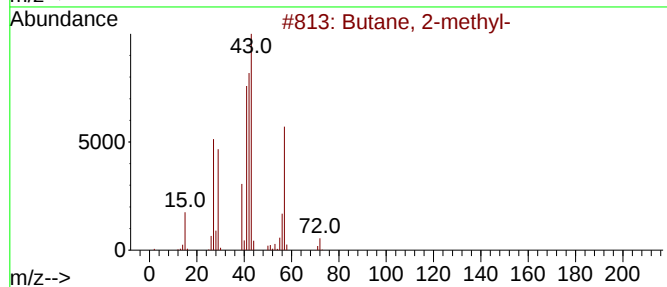
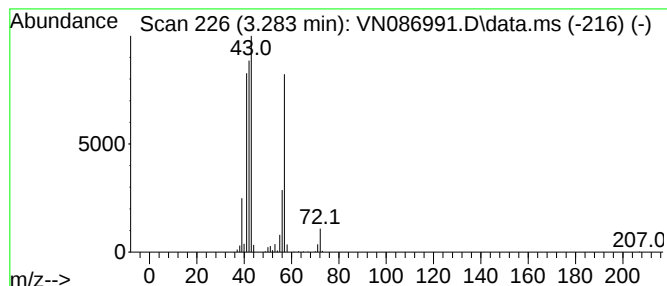
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.283	60.83 ug/l	913370	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Pentane	72	C5H12	000109-66-0	43
3			1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	27
4			3-Buten-1-ol	72	C4H8O	000627-27-0	25
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	17



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

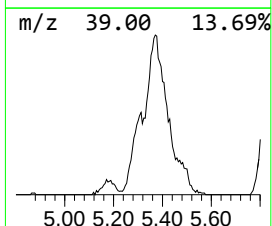
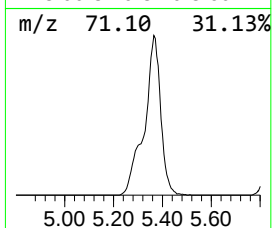
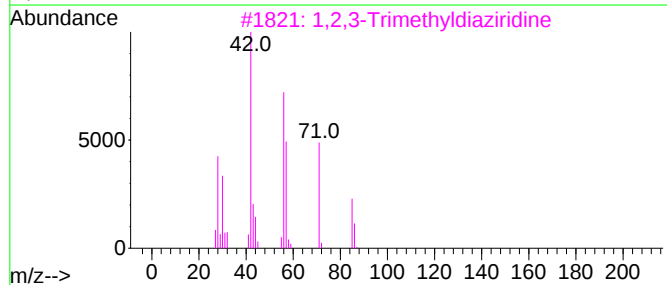
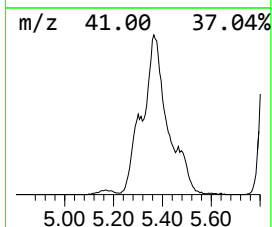
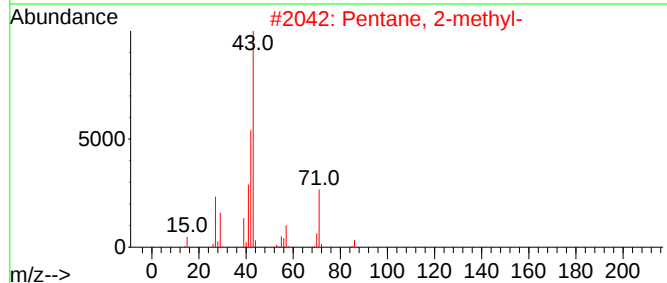
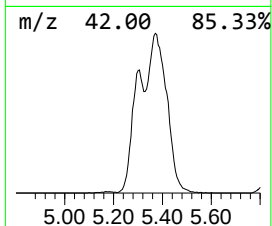
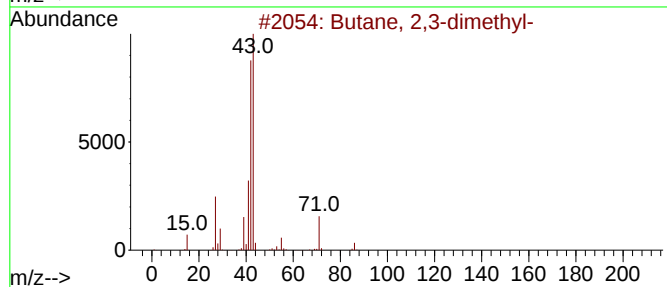
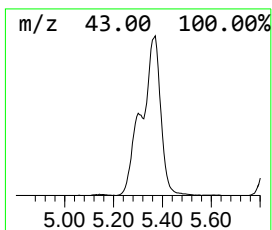
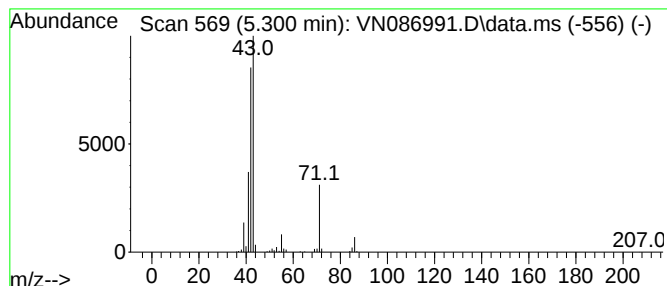
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.300	30.46 ug/l	457292	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	38
4			Pentane	72	C5H12	000109-66-0	36
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	12



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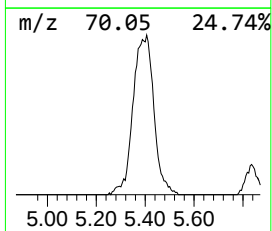
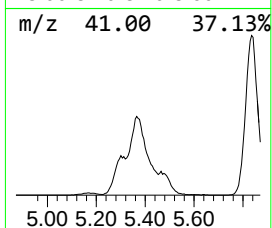
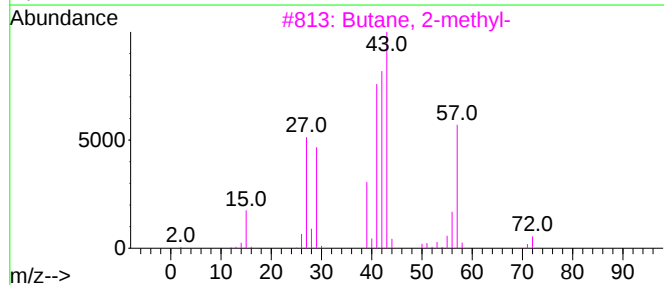
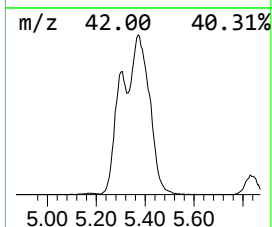
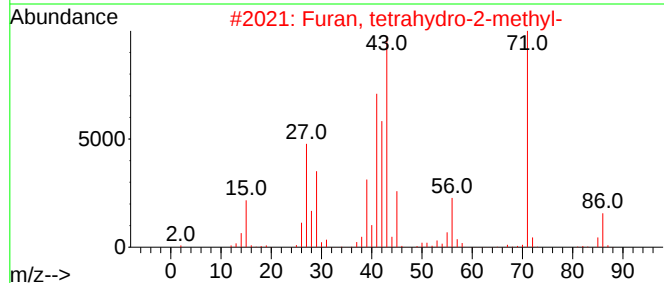
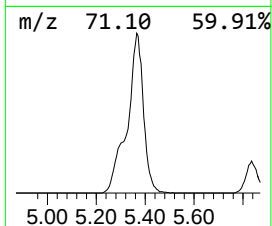
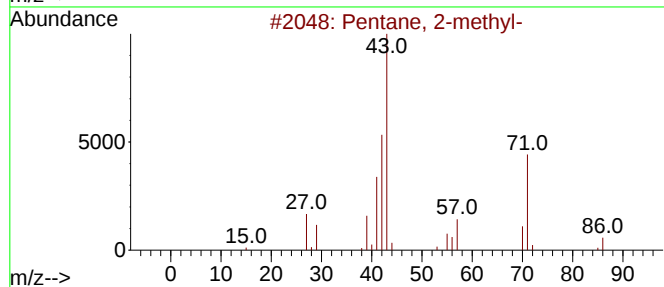
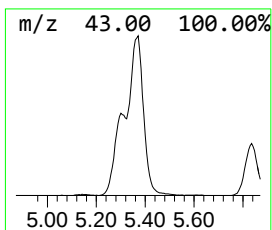
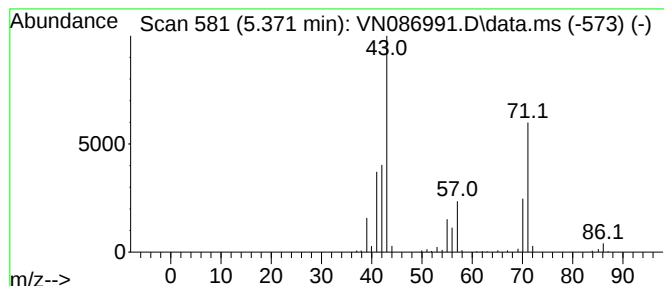
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.371	111.31 ug/l	1671270	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	87
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	36
3			Butane, 2-methyl-	72	C5H12	000078-78-4	27
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	25
5			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	25



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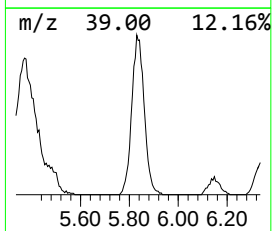
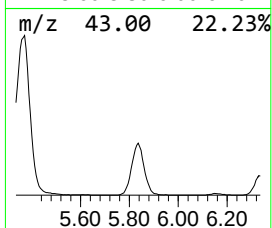
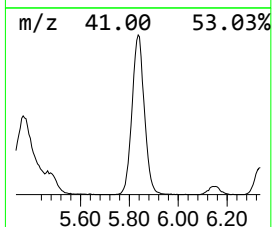
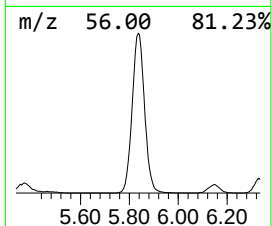
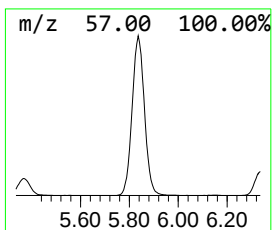
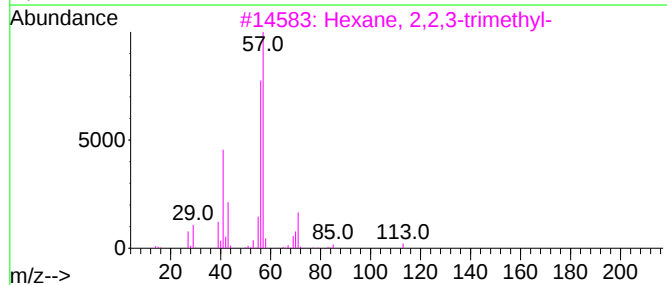
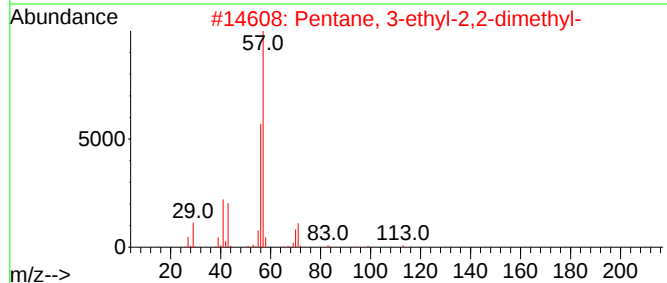
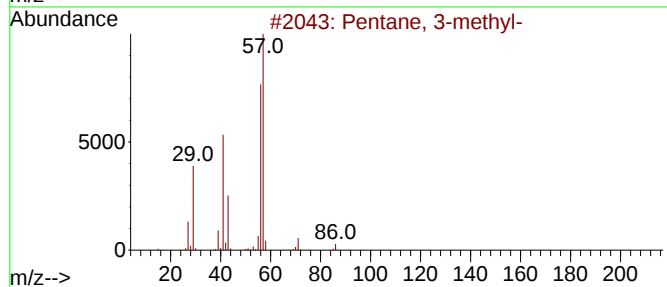
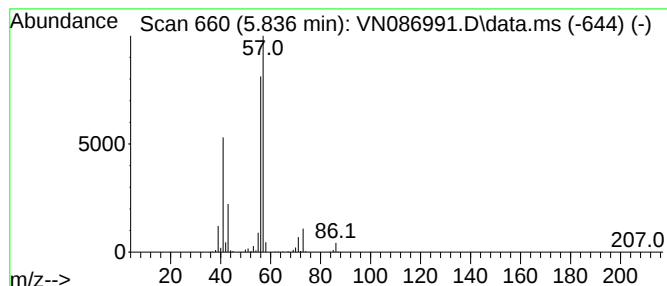
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.836	113.87 ug/l	1709720	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	72
3			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	56
4			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	50
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086991.D
Acq On : 12 Jun 2025 20:26
Operator : JC\MD
Sample : Q2268-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

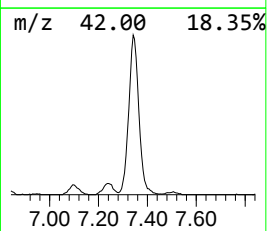
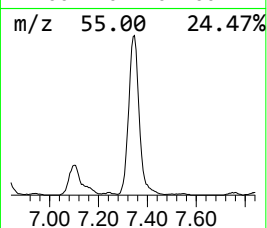
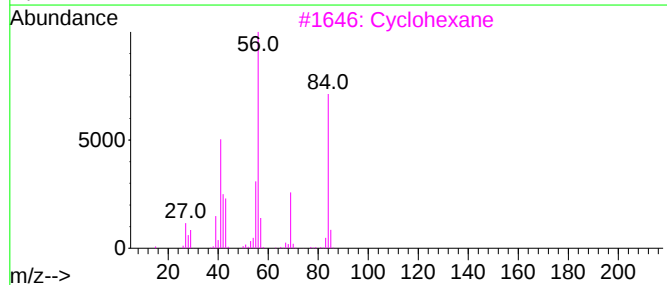
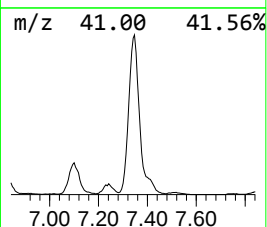
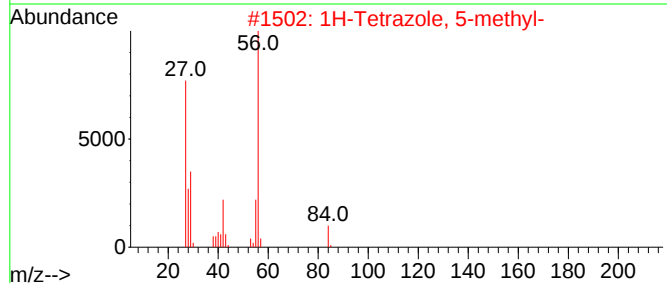
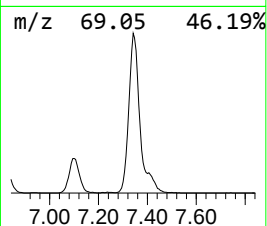
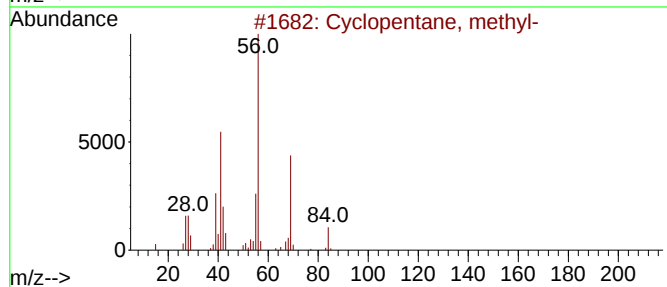
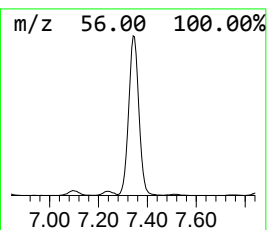
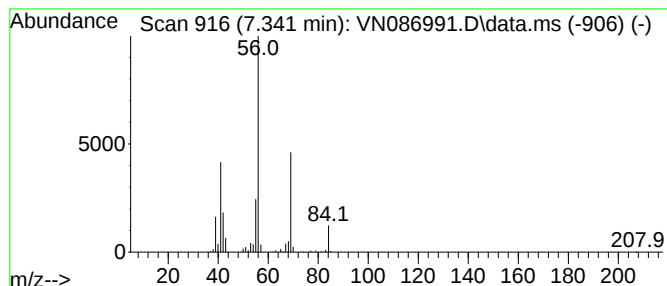
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.341	146.83 ug/l	2204690	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclohexane	84	C6H12	000110-82-7	78
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086991.D
Acq On : 12 Jun 2025 20:26
Operator : JC\MD
Sample : Q2268-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

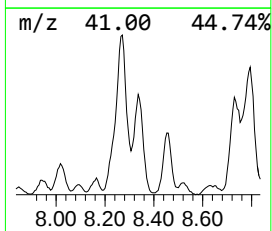
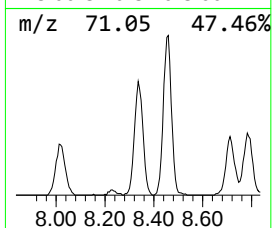
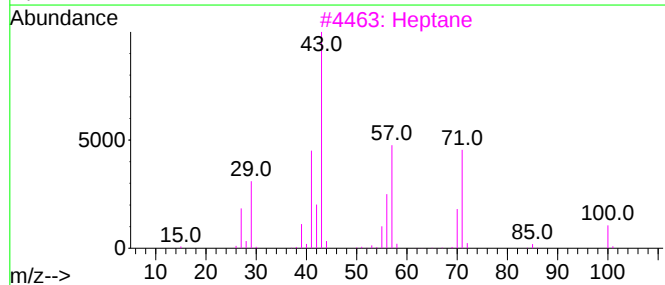
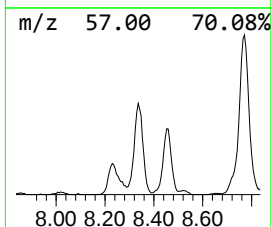
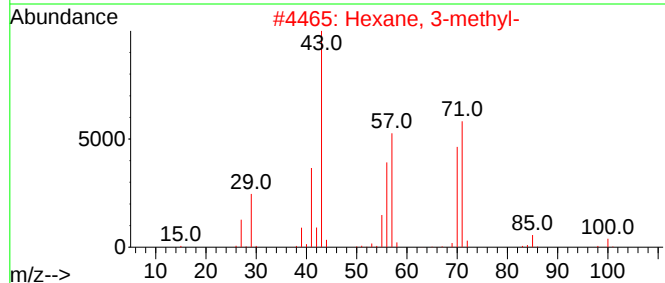
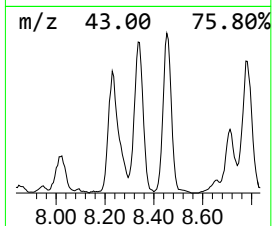
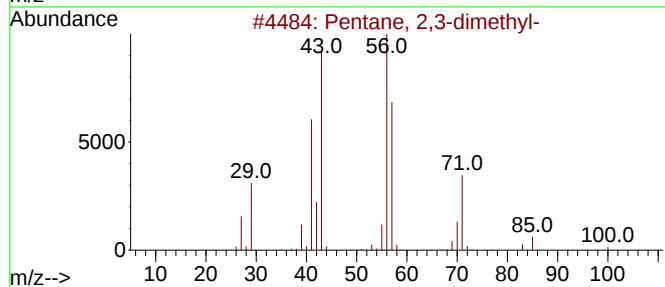
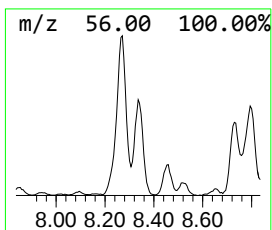
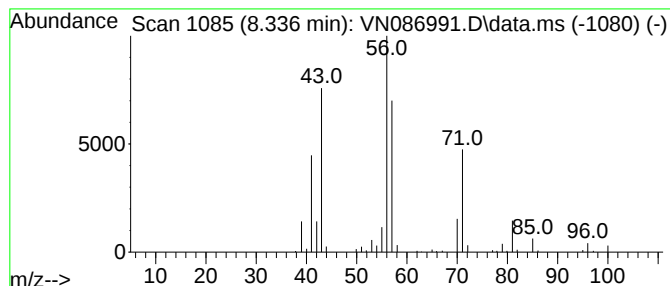
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.336	39.29 ug/l	589909	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	46
3			Heptane	100	C7H16	000142-82-5	43
4			Ethane, isocyanato-	71	C3H5NO	000109-90-0	42
5			Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086991.D
Acq On : 12 Jun 2025 20:26
Operator : JC\MD
Sample : Q2268-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

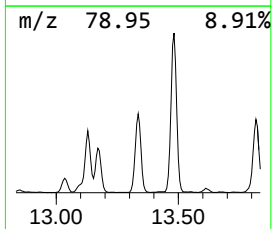
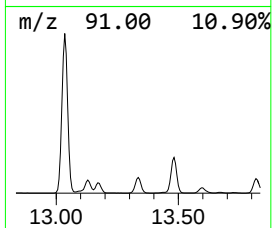
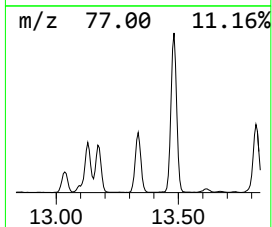
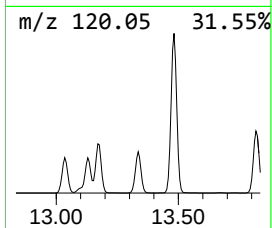
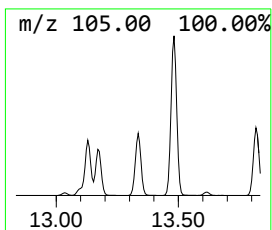
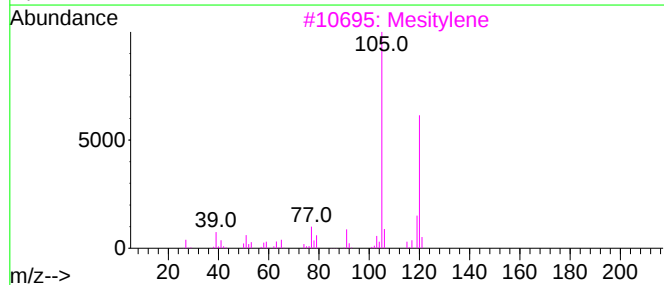
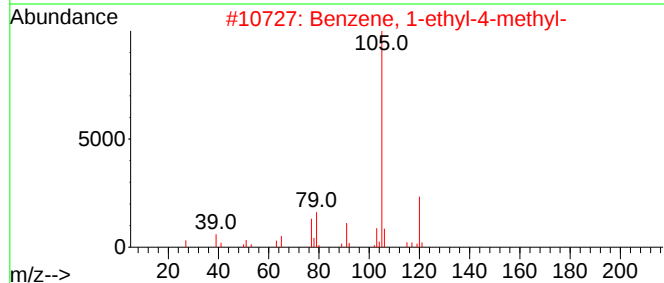
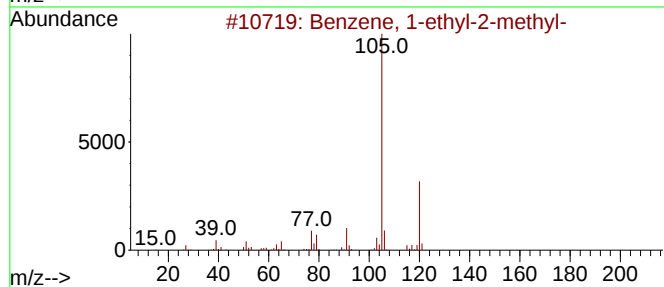
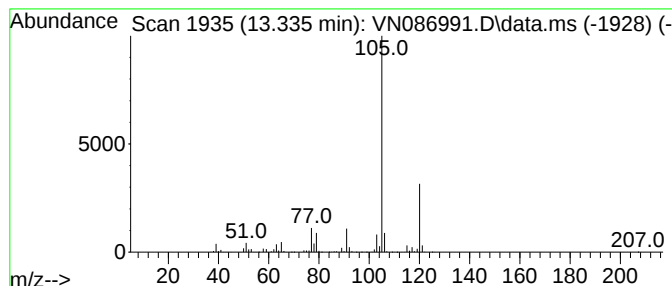
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	30.11 ug/l	3006190	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	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086991.D
Acq On : 12 Jun 2025 20:26
Operator : JC\MD
Sample : Q2268-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

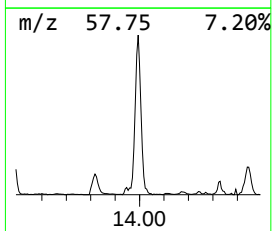
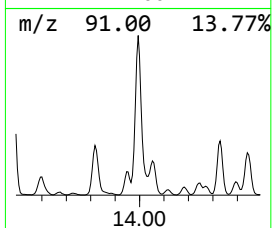
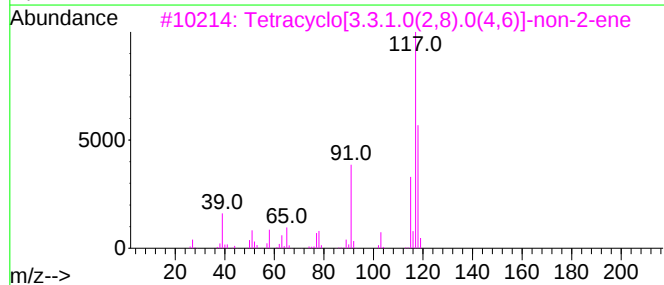
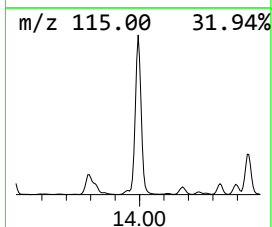
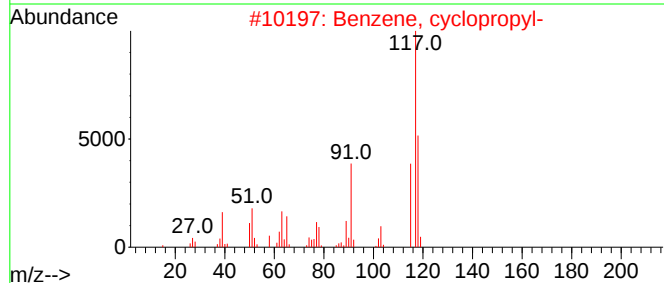
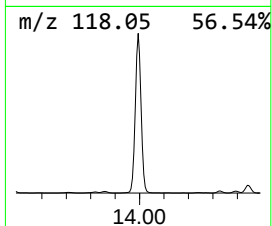
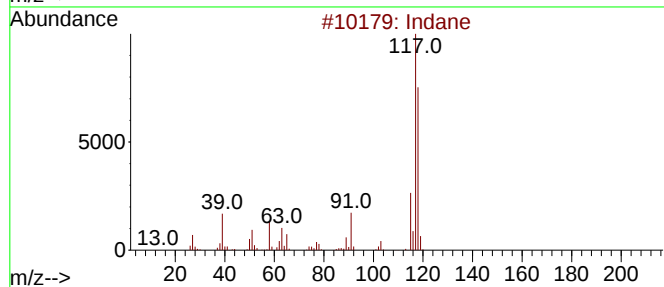
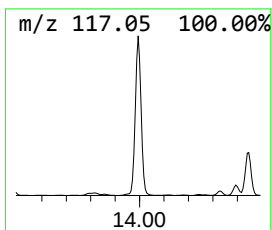
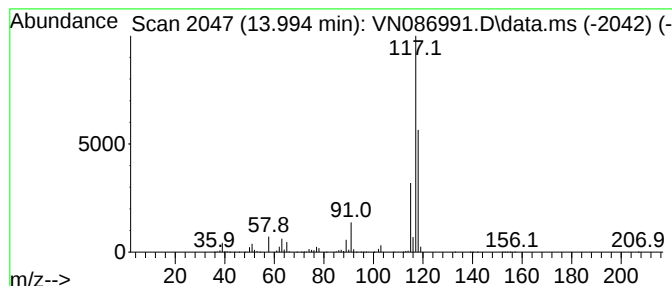
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Quant Title : SW846 8260

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

Peak Number 8 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	92.54 ug/l	9239170	1,4-Dichlorobenzene-d4	13.794

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	74
3			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5			7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086991.D
Acq On : 12 Jun 2025 20:26
Operator : JC\MD
Sample : Q2268-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

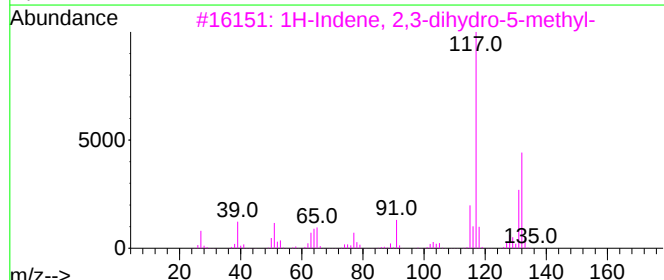
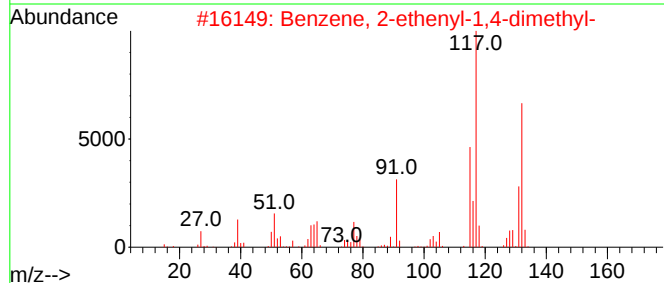
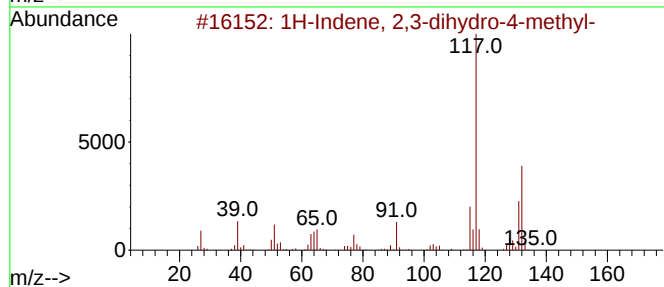
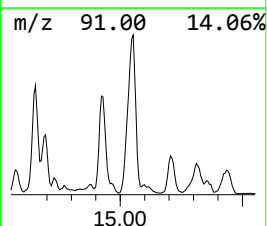
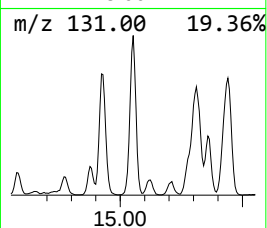
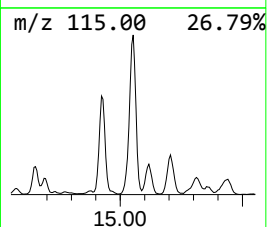
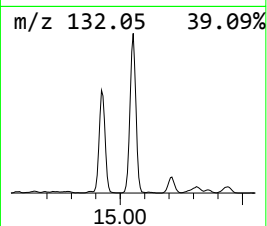
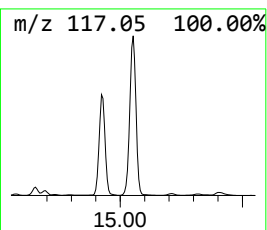
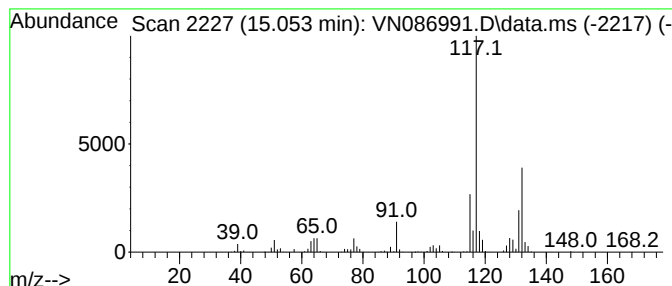
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	35.90 ug/l	3583930	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
2		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	93
3		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
4		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5		1-Phenyl-1-butene	132	C10H12	000824-90-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086991.D
Acq On : 12 Jun 2025 20:26
Operator : JC\MD
Sample : Q2268-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

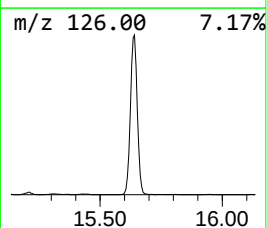
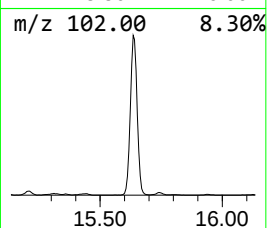
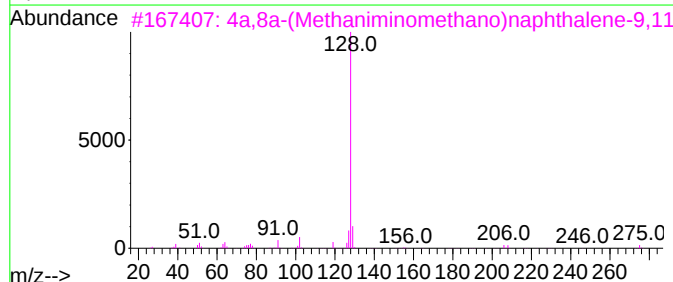
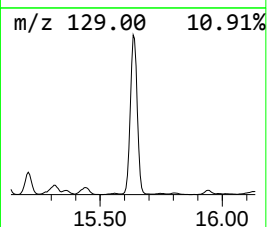
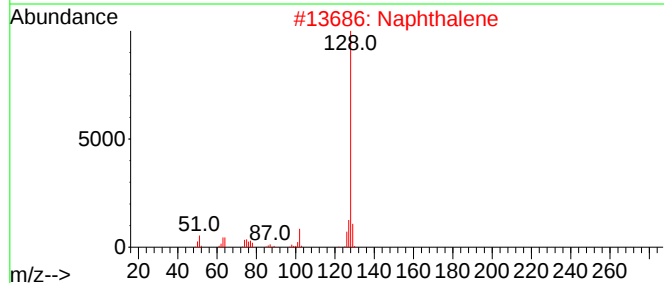
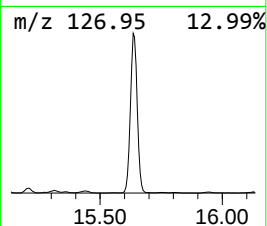
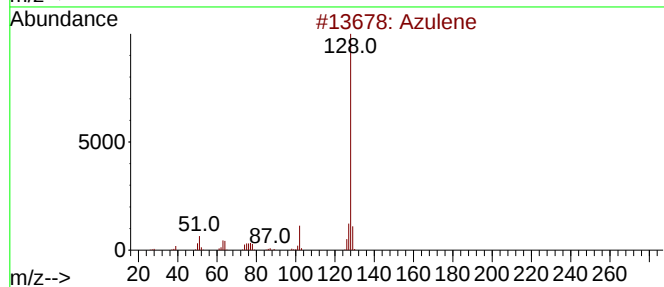
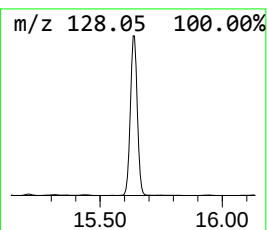
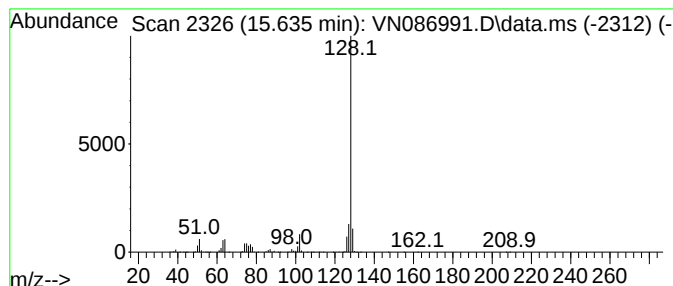
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Quant Title : SW846 8260

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

Peak Number 10 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.635	69.53 ug/l	6941830	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
4			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59
5			4-Phenylbut-3-ene-1-yne	128	C10H8	100022-12-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061225\
Data File : VN086991.D
Acq On : 12 Jun 2025 20:26
Operator : JC\MD
Sample : Q2268-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2-20250605

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N060625W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.283	60.8	ug/l	913370	1	8.230	750752	50.0
Butane, 2,3-dim...	5.300	30.5	ug/l	457292	1	8.230	750752	50.0
Pentane, 2-methyl-	5.371	111.3	ug/l	1671270	1	8.230	750752	50.0
Pentane, 3-methyl-	5.836	113.9	ug/l	1709720	1	8.230	750752	50.0
Cyclopentane, m...	7.341	146.8	ug/l	2204690	1	8.230	750752	50.0
Pentane, 2,3-di...	8.336	39.3	ug/l	589909	1	8.230	750752	50.0
Benzene, 1-ethy...	13.335	30.1	ug/l	3006190	4	13.794	4991990	50.0
Indane	13.994	92.5	ug/l	9239170	4	13.794	4991990	50.0
1H-Indene, 2,3-...	15.053	35.9	ug/l	3583930	4	13.794	4991990	50.0
Azulene	15.635	69.5	ug/l	6941830	4	13.794	4991990	50.0