

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120125\
 Data File : VN088379.D
 Acq On : 01 Dec 2025 13:52
 Operator : JC\MD
 Sample : Q3716-04 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW7

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\82N112425W.M

Title : SW846 8260

Signal : TIC: VN088379.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.336	58	65	82	rBV	660001	1175847	1.36%	0.292%
2	2.536	86	99	111	rBV	2566151	4716682	5.46%	1.170%
3	3.265	211	223	252	rBV	4385485	10911964	12.62%	2.707%
4	3.665	281	291	314	rVV3	1822420	5924089	6.85%	1.470%
5	3.865	314	325	342	rVV	1061947	2742371	3.17%	0.680%
6	4.048	344	356	364	rVV	590033	1637253	1.89%	0.406%
7	4.148	364	373	392	rVB	1982128	5709210	6.60%	1.416%
8	5.153	526	544	552	rBV4	324616	1201913	1.39%	0.298%
9	5.265	552	563	566	rVV2	528472	1616036	1.87%	0.401%
10	5.330	567	574	611	rVB3	1279013	6573372	7.60%	1.631%
11	5.800	631	654	673	rBV	842372	2933289	3.39%	0.728%
12	6.300	727	739	755	rBV2	491068	1520272	1.76%	0.377%
13	6.642	790	797	810	rVB	384143	1179475	1.36%	0.293%
14	7.065	859	869	883	rVB2	452786	1283312	1.48%	0.318%
15	7.312	901	911	920	rBV	1311489	3816887	4.42%	0.947%
16	7.988	1018	1026	1034	rVB	538493	1273380	1.47%	0.316%
17	8.200	1056	1062	1074	rVV4	947748	3175234	3.67%	0.788%
18	8.312	1074	1081	1091	rVB2	481530	1255761	1.45%	0.312%
19	8.424	1091	1100	1109	rBV	764994	1758855	2.03%	0.436%
20	8.588	1116	1128	1140	rBV	2896045	7305276	8.45%	1.812%
21	8.741	1140	1154	1165	rVV	1673601	5857004	6.78%	1.453%
22	8.947	1179	1189	1202	rVB3	399213	1088072	1.26%	0.270%
23	9.083	1202	1212	1218	rBV2	943856	2208300	2.55%	0.548%
24	9.577	1279	1296	1301	rBV3	1064065	3164567	3.66%	0.785%
25	9.994	1359	1367	1376	rVB	1243783	2549218	2.95%	0.632%
26	10.124	1383	1389	1395	rVB	1615239	3143713	3.64%	0.780%
27	10.318	1413	1422	1434	rBV	525787	1259083	1.46%	0.312%
28	10.541	1454	1460	1464	rBV2	1017736	1862865	2.16%	0.462%
29	10.606	1464	1471	1485	rVV	25100138	46024014	53.24%	11.418%
30	10.724	1485	1491	1498	rVB3	458464	942730	1.09%	0.234%
31	11.841	1672	1681	1689	rBV	766145	1479580	1.71%	0.367%
32	11.941	1689	1698	1707	rBV	10704711	17894854	20.70%	4.440%
33	12.047	1707	1716	1728	rBV2	45939037	86440451	100.00%	21.446%
34	12.376	1761	1772	1782	rBV	19436256	33111106	38.31%	8.215%
35	12.671	1816	1822	1828	rBV	523507	930113	1.08%	0.231%
36	12.829	1843	1849	1859	rVB3	573406	1341857	1.55%	0.333%

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Integrator: RTE

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

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37	13.012	1874	1880	1885	rBV	2119720	3469495	4.01%	0.861%
38	13.071	1885	1890	1894	rVV	10482274	18012491	20.84%	4.469%
39	13.106	1894	1896	1900	rVV	4685352	6706661	7.76%	1.664%
40	13.147	1900	1903	1921	rVB	5654757	8991521	10.40%	2.231%
41	13.312	1922	1931	1939	rBV	3781647	6434534	7.44%	1.596%
42	13.459	1949	1956	1969	rVB	19680499	31635815	36.60%	7.849%
43	13.794	2003	2013	2029	rVB	4457659	9152008	10.59%	2.271%
44	13.929	2029	2036	2037	rBV	682780	1024202	1.18%	0.254%
45	13.965	2037	2042	2058	rVB3	3180014	10832494	12.53%	2.688%
46	14.159	2068	2075	2080	rBV2	559093	939274	1.09%	0.233%
47	14.218	2080	2085	2088	rVV	1185009	2064998	2.39%	0.512%
48	14.247	2088	2090	2095	rVV	1123462	1457487	1.69%	0.362%
49	14.306	2095	2100	2106	rVB	1917721	3018804	3.49%	0.749%
50	14.417	2114	2119	2128	rVB2	1009410	1716165	1.99%	0.426%
51	14.629	2147	2155	2158	rBV	1159190	2042024	2.36%	0.507%
52	14.665	2158	2161	2166	rVB	1462495	2084756	2.41%	0.517%
53	14.900	2196	2201	2206	rBV	1048158	1945881	2.25%	0.483%
54	15.023	2213	2222	2228	rBV2	1626064	3807014	4.40%	0.945%
55	15.288	2256	2267	2273	rBV2	525110	1493932	1.73%	0.371%
56	15.406	2280	2287	2296	rVB3	379139	961192	1.11%	0.238%
57	15.612	2308	2322	2334	rBV	2585674	5242753	6.07%	1.301%
58	16.747	2507	2515	2522	rBV	1311802	3026480	3.50%	0.751%

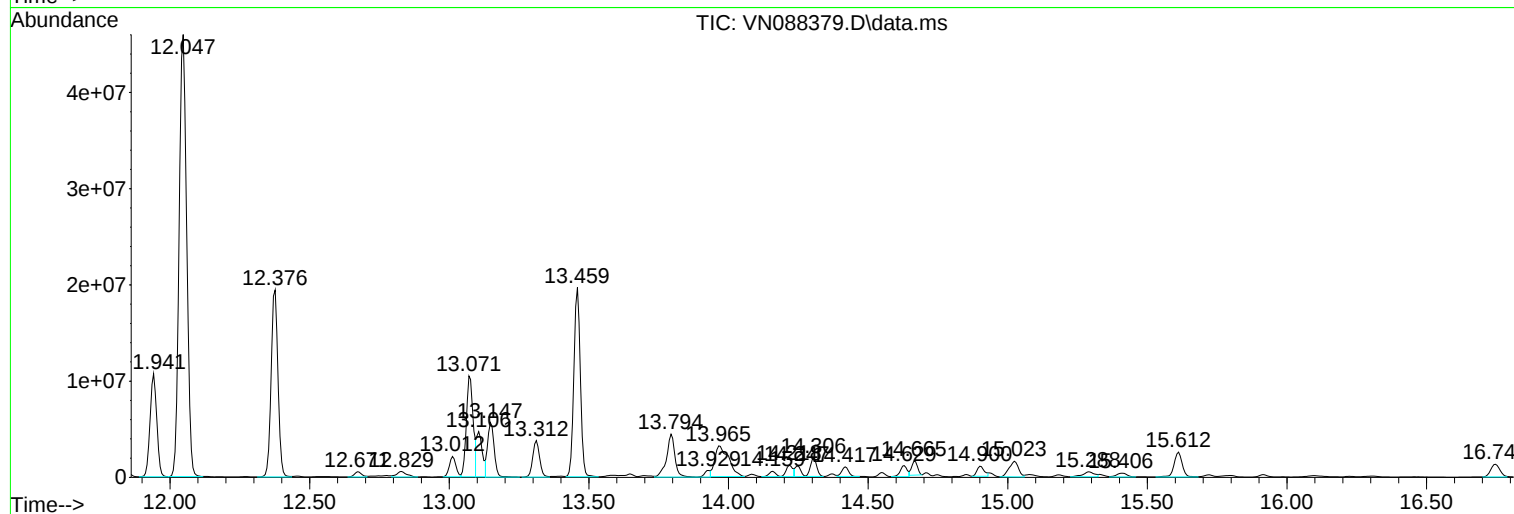
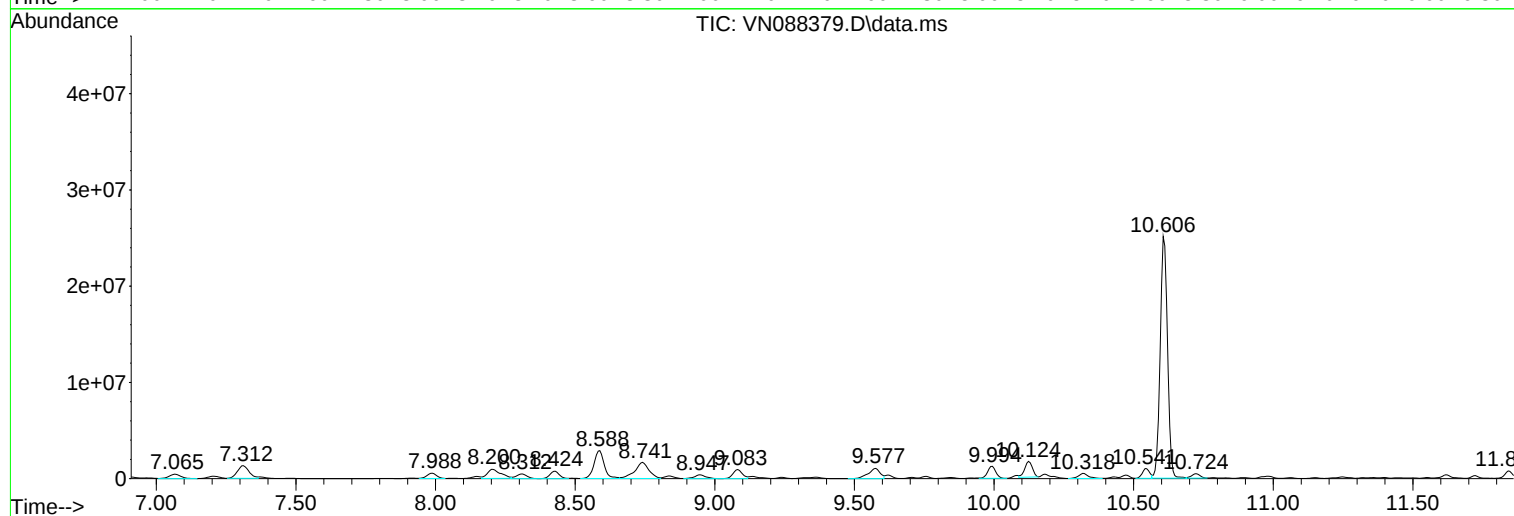
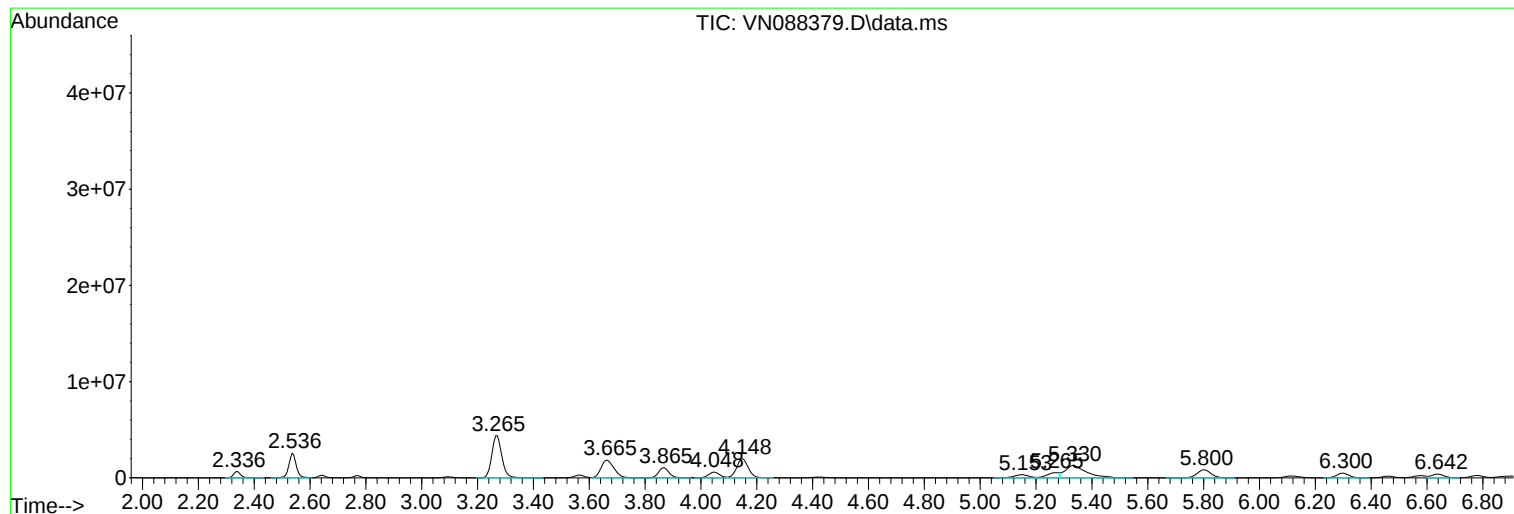
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Quant Title : SW846 8260

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



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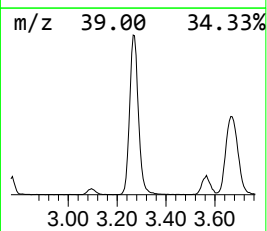
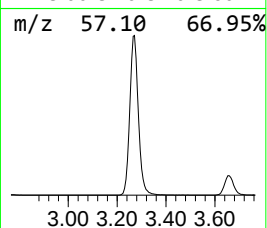
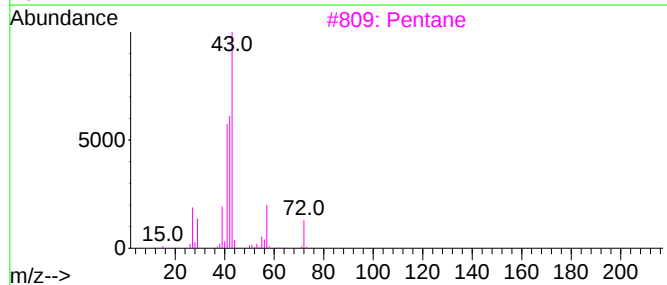
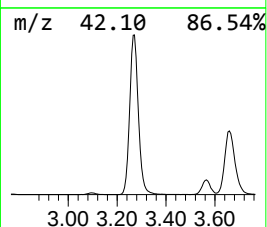
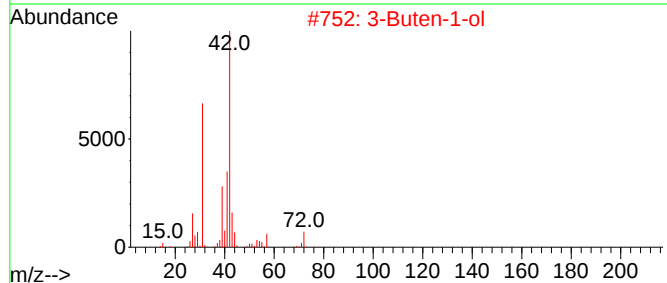
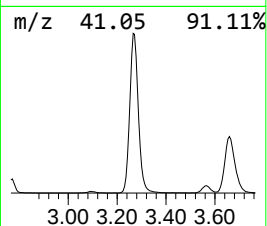
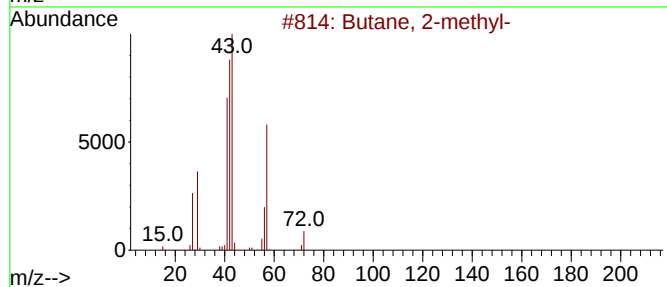
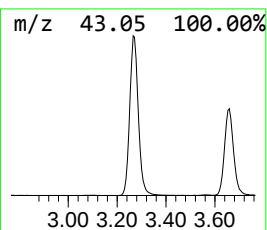
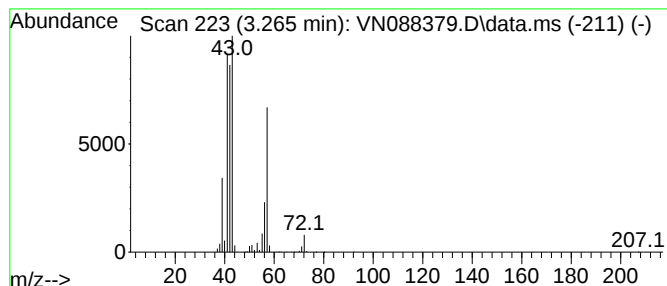
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112425W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.265	171.83 ug/l	10912000	Pentafluorobenzene	8.206

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	90
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		Pentane	72	C5H12	000109-66-0	36
4		2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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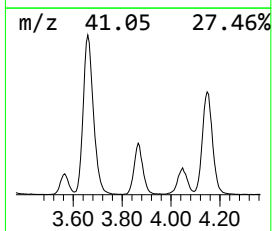
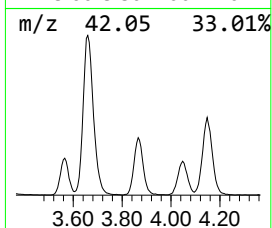
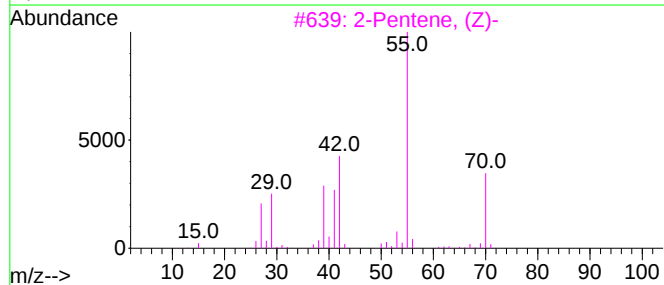
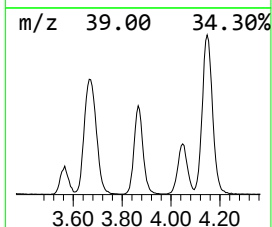
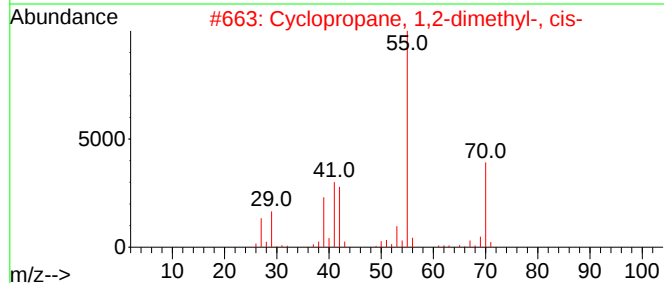
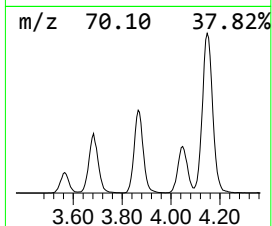
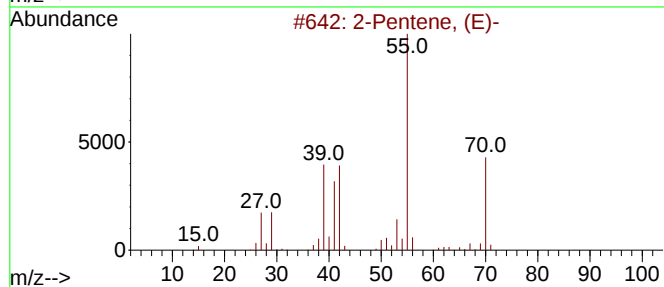
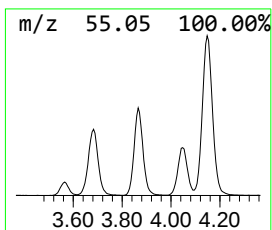
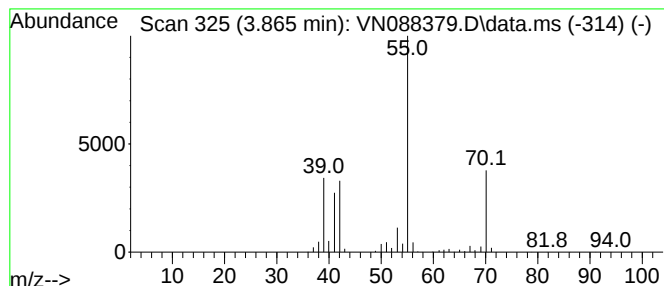
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112425W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentene, (E)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.865	43.18 ug/l	2742370	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, (E)-	70	C5H10	000646-04-8	93
2			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
3			2-Pentene, (Z)-	70	C5H10	000627-20-3	90
4			2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
5			2-Methyl-1-butene	70	C5H10	000563-46-2	87



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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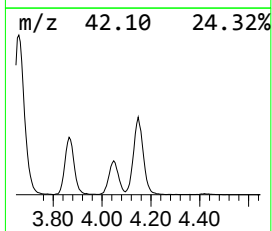
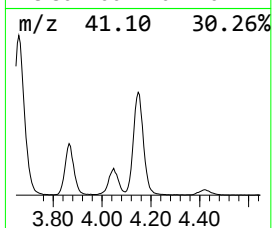
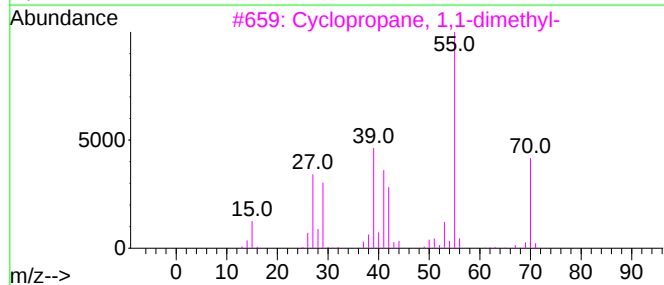
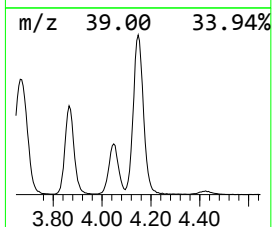
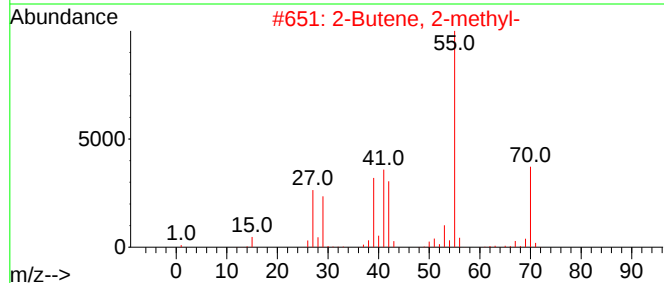
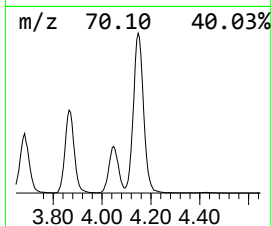
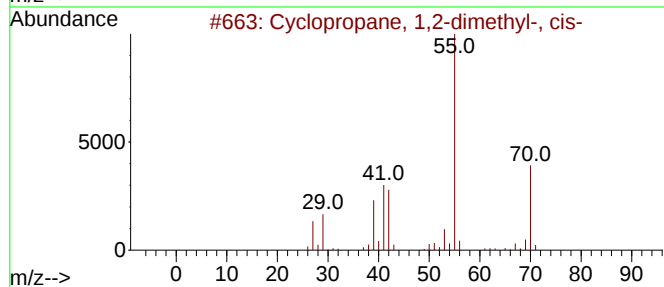
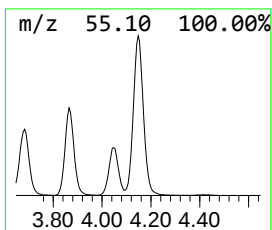
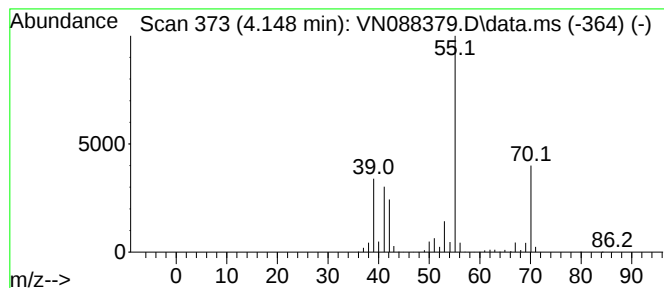
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112425W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.148	89.90 ug/l	5709210	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
4			1-Butene, 3-methyl-	70	C5H10	000563-45-1	87
5			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83



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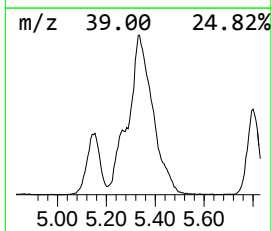
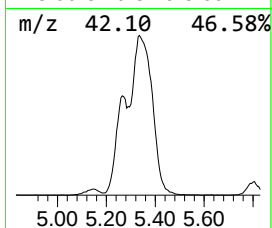
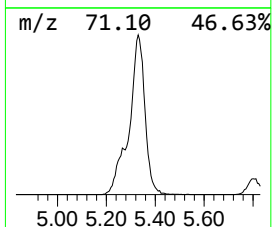
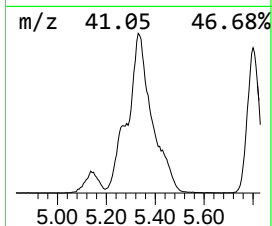
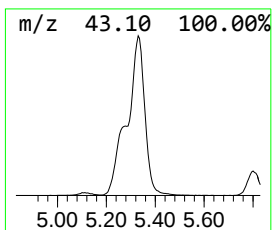
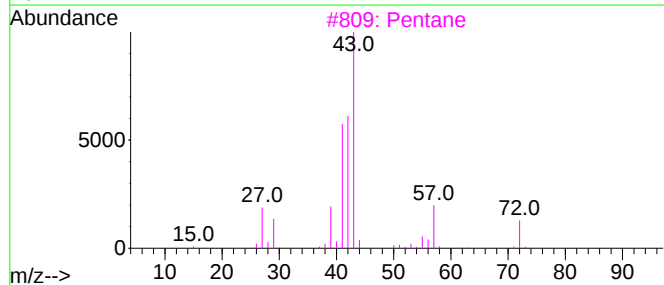
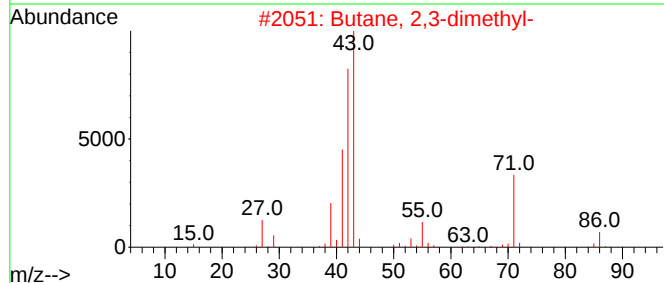
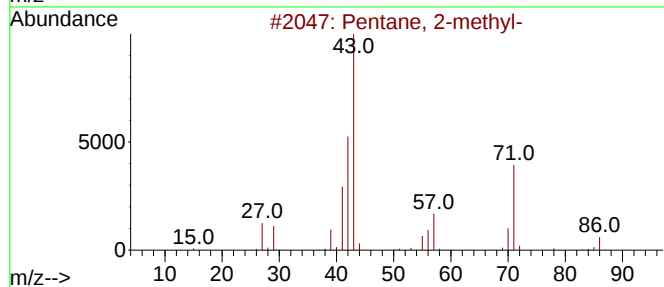
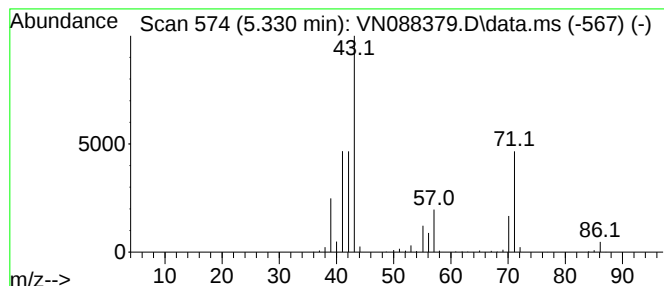
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.330	103.51 ug/l	6573370	Pentafluorobenzene	8.206

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	46
3			Pentane	72	C5H12	000109-66-0	38
4			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	28



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MW7

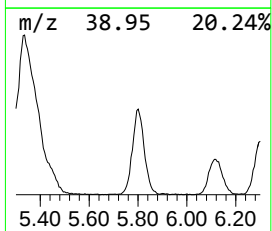
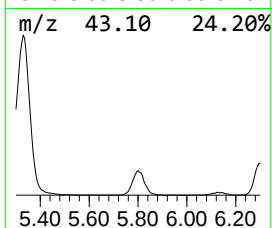
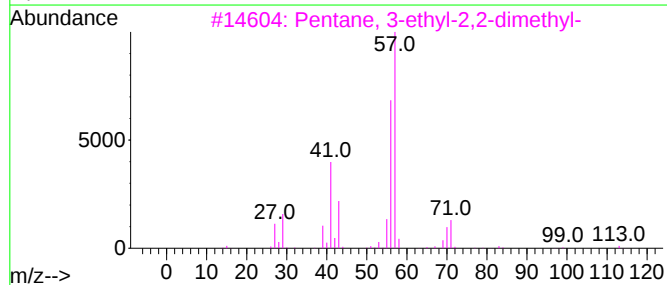
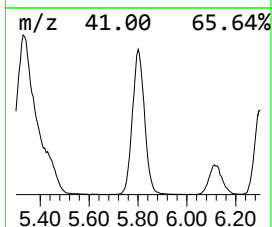
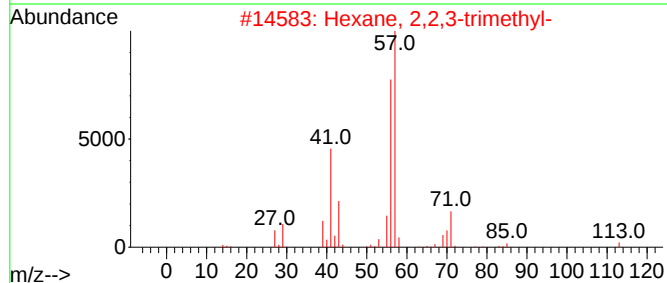
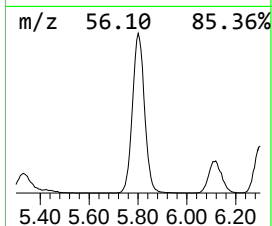
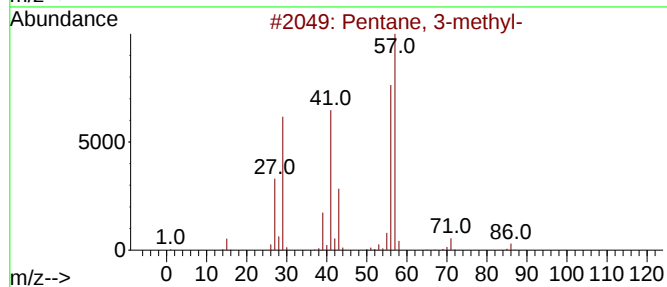
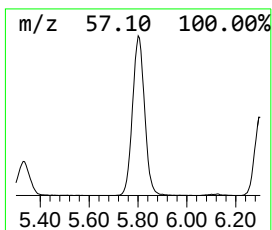
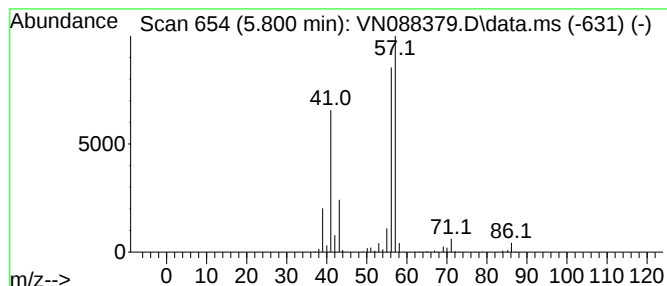
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.800	46.19 ug/l	2933290	Pentafluorobenzene	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	42
5			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120125\
Data File : VN088379.D
Acq On : 01 Dec 2025 13:52
Operator : JC\MD
Sample : Q3716-04 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW7

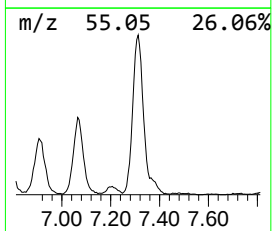
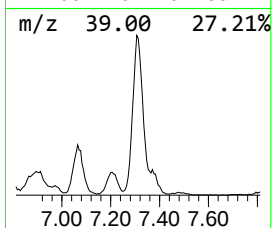
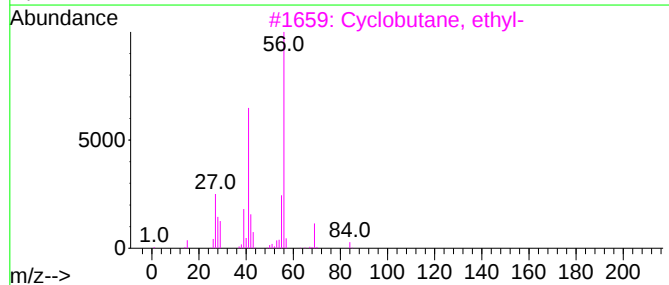
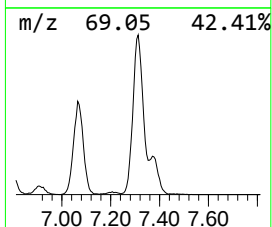
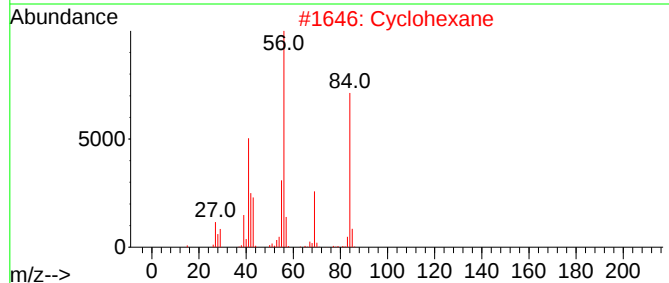
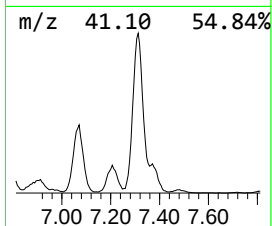
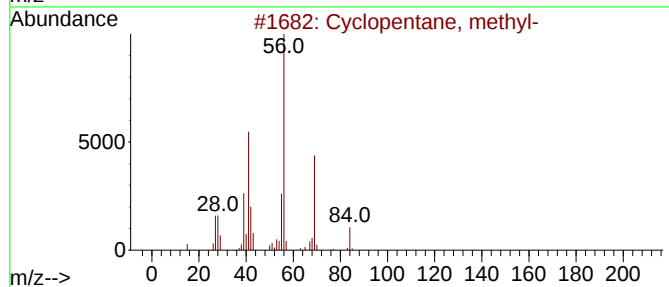
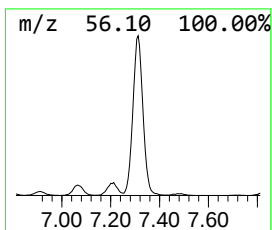
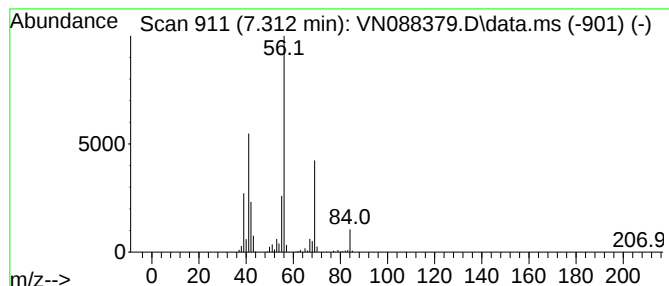
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Quant Title : SW846 8260

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

Peak Number 8 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.312	60.10 ug/l	3816890	Pentafluorobenzene	8.206

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			Cyclobutane	56	C4H8	000287-23-0	50
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120125\
Data File : VN088379.D
Acq On : 01 Dec 2025 13:52
Operator : JC\MD
Sample : Q3716-04 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW7

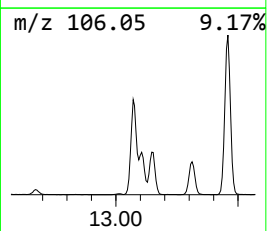
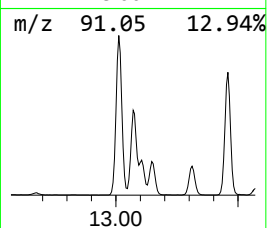
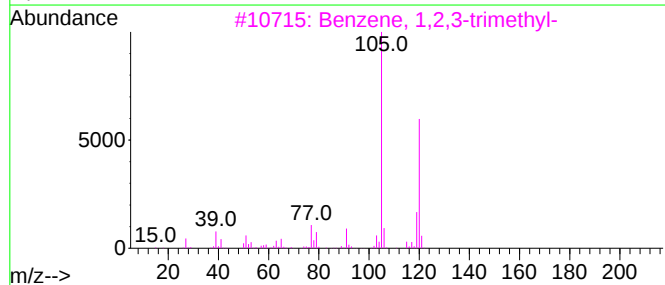
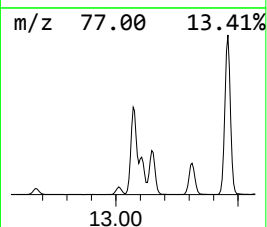
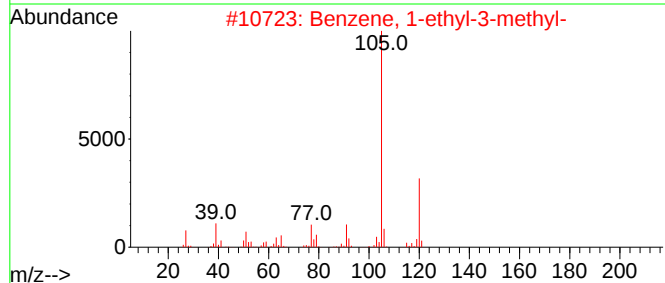
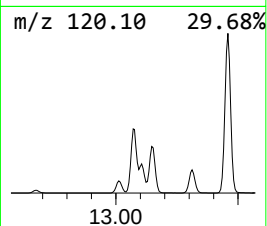
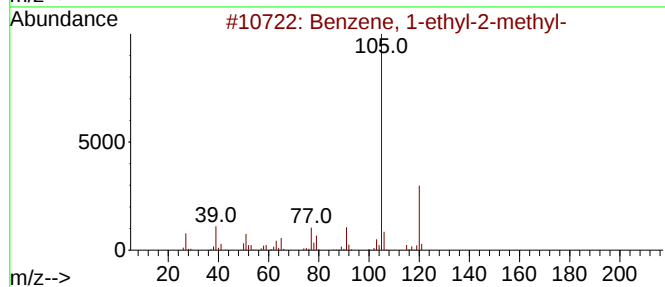
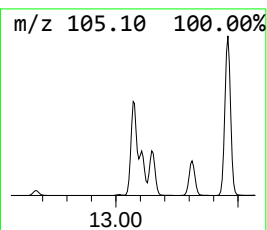
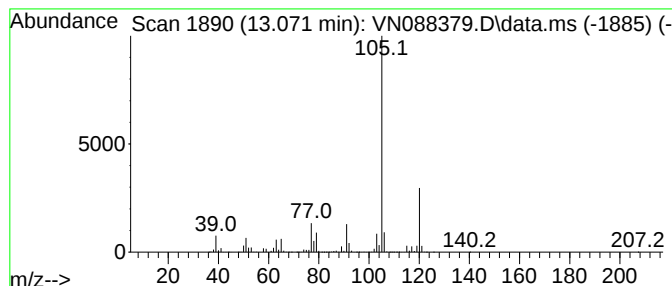
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Quant Title : SW846 8260

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

Peak Number 13 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.070	98.41 ug/l	18012500	1,4-Dichlorobenzene-d4	13.771

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, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120125\
Data File : VN088379.D
Acq On : 01 Dec 2025 13:52
Operator : JC\MD
Sample : Q3716-04 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW7

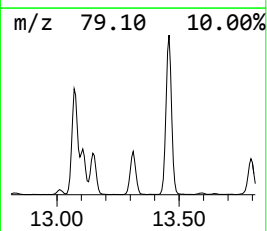
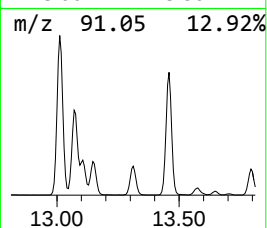
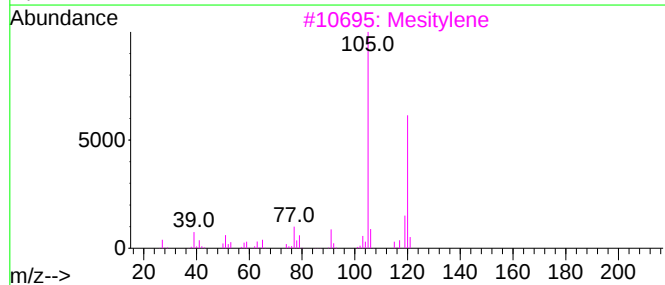
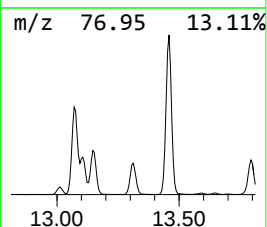
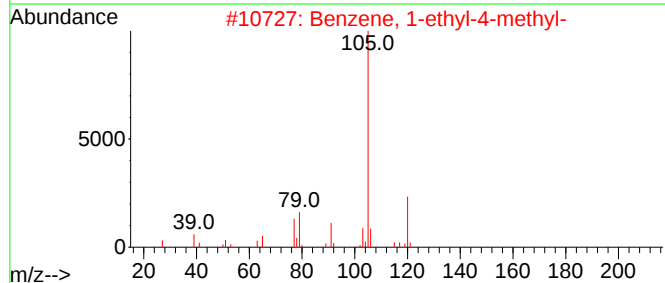
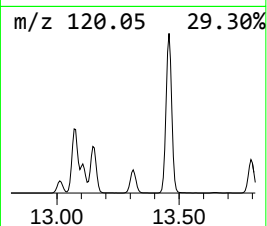
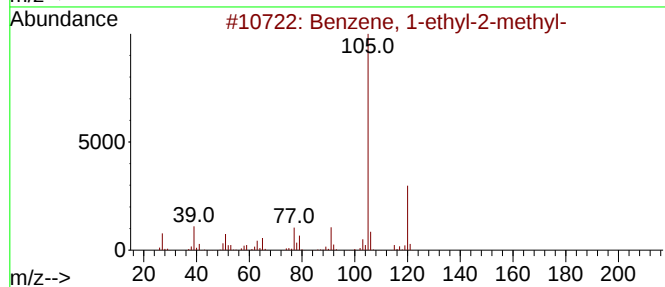
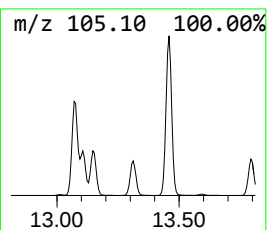
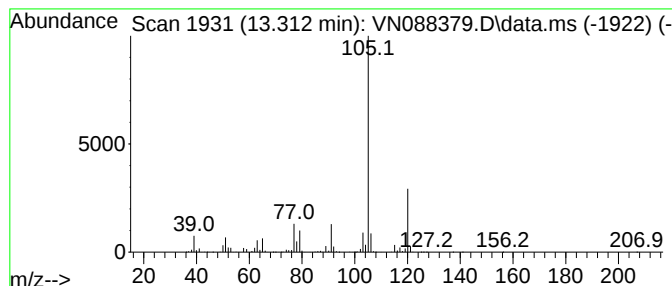
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Quant Title : SW846 8260

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

Peak Number 14 Benzene, 1-ethyl-4-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.312	35.15 ug/l	6434530	1,4-Dichlorobenzene-d4	13.771

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			Mesitylene	120	C9H12	000108-67-8	91
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\VN120125\
Data File : VN088379.D
Acq On : 01 Dec 2025 13:52
Operator : JC\MD
Sample : Q3716-04 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112425W.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-	3.265	171.8	ug/l	10912000	1	8.206	3175230	50.0
2-Pentene, (E)-	3.865	43.2	ug/l	2742370	1	8.206	3175230	50.0
Cyclopropane, 1...	4.148	89.9	ug/l	5709210	1	8.206	3175230	50.0
Pentane, 2-methyl-	5.330	103.5	ug/l	6573370	1	8.206	3175230	50.0
Pentane, 3-methyl-	5.800	46.2	ug/l	2933290	1	8.206	3175230	50.0
Cyclopentane, m...	7.312	60.1	ug/l	3816890	1	8.206	3175230	50.0
Benzene, 1-ethy...	13.070	98.4	ug/l	18012500	4	13.771	9152010	50.0
Benzene, 1-ethy...	13.312	35.1	ug/l	6434530	4	13.771	9152010	50.0