

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
 Data File : VN081476.D
 Acq On : 19 Mar 2024 17:21
 Operator : JC\MD
 Sample : P1773-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-6A

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\82N031824W.M
 Title : SW846 8260

Signal : TIC: VN081476.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.512	89	95	104	rBV	403095	654533	4.16%	0.603%
2	3.248	211	220	238	rVB	1680459	3840516	24.43%	3.540%
3	3.648	279	288	303	rVB2	439501	1095604	6.97%	1.010%
4	4.148	364	373	385	rVB2	81851	218977	1.39%	0.202%
5	4.430	407	421	434	rBV	72306	225870	1.44%	0.208%
6	5.283	552	566	569	rVV2	162004	522771	3.32%	0.482%
7	5.377	570	582	607	rVB4	405479	2323354	14.78%	2.141%
8	5.812	642	656	671	rBV2	249504	849455	5.40%	0.783%
9	6.318	729	742	756	rVB4	91906	278498	1.77%	0.257%
10	6.653	794	799	810	rVB3	61539	172571	1.10%	0.159%
11	6.889	831	839	849	rBV4	57163	189130	1.20%	0.174%
12	7.330	903	914	930	rVB2	809246	2295292	14.60%	2.115%
13	8.165	1047	1056	1061	rBV	335124	819603	5.21%	0.755%
14	8.230	1061	1067	1079	rVV2	731433	2598588	16.53%	2.395%
15	8.330	1079	1084	1095	rVB5	97817	271949	1.73%	0.251%
16	8.583	1119	1127	1134	rBV2	349657	914068	5.81%	0.842%
17	8.736	1146	1153	1159	rBV4	135363	355855	2.26%	0.328%
18	8.853	1168	1173	1183	rVB2	99677	226373	1.44%	0.209%
19	9.100	1204	1215	1229	rBV	950270	2008917	12.78%	1.851%
20	9.600	1283	1300	1317	rBV3	237674	762287	4.85%	0.703%
21	10.147	1388	1393	1405	rVB2	82874	183452	1.17%	0.169%
22	10.565	1457	1464	1470	rBV	1322913	2481712	15.78%	2.287%
23	10.629	1470	1475	1487	rVB	647028	1253919	7.98%	1.156%
24	11.865	1677	1685	1694	rBV	1177495	2101304	13.36%	1.937%
25	11.965	1694	1702	1711	rVV	9409710	15596326	99.19%	14.374%
26	12.076	1711	1721	1732	rVB	7923170	15722974	100.00%	14.491%
27	12.400	1764	1776	1788	rBV	2828893	4776584	30.38%	4.402%
28	12.700	1819	1827	1835	rVB	482006	812748	5.17%	0.749%
29	12.847	1845	1852	1863	rVB	898964	1570795	9.99%	1.448%
30	13.035	1875	1884	1890	rBV	1280714	2068920	13.16%	1.907%
31	13.100	1890	1895	1896	rVV	427961	587039	3.73%	0.541%
32	13.129	1896	1900	1904	rVV	1433786	2355104	14.98%	2.171%
33	13.176	1904	1908	1916	rVB	645956	1035727	6.59%	0.955%
34	13.335	1927	1935	1944	rBV	1911332	3150691	20.04%	2.904%
35	13.482	1952	1960	1972	rBV	5771248	9281423	59.03%	8.554%
36	13.612	1972	1982	1988	rVB3	107181	269874	1.72%	0.249%

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Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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37	13.794	2006	2013	2014	rBV	1214005	1694009	10.77%	1.561%
38	13.823	2014	2018	2026	rVB	1922769	3380292	21.50%	3.115%
39	13.953	2033	2040	2042	rBV2	478947	710686	4.52%	0.655%
40	13.994	2042	2047	2063	rVB	2458165	4928758	31.35%	4.542%
41	14.118	2063	2068	2073	rVB2	120994	177720	1.13%	0.164%
42	14.182	2073	2079	2084	rBV2	188894	319651	2.03%	0.295%
43	14.247	2084	2090	2093	rBV	396370	669167	4.26%	0.617%
44	14.329	2099	2104	2111	rVB	1084052	1731956	11.02%	1.596%
45	14.400	2111	2116	2119	rBV	218822	363727	2.31%	0.335%
46	14.447	2119	2124	2132	rVB	983414	1629395	10.36%	1.502%
47	14.576	2140	2146	2152	rVB2	186031	298720	1.90%	0.275%
48	14.653	2152	2159	2163	rBV	706020	1166068	7.42%	1.075%
49	14.694	2163	2166	2171	rVB	447640	620928	3.95%	0.572%
50	14.929	2201	2206	2212	rBV	499460	822459	5.23%	0.758%
51	15.053	2218	2227	2233	rBV3	918248	2044932	13.01%	1.885%
52	15.212	2247	2254	2261	rBV2	144513	271487	1.73%	0.250%
53	15.317	2261	2272	2277	rBV3	177968	437769	2.78%	0.403%
54	15.441	2285	2293	2304	rVB3	224392	590010	3.75%	0.544%
55	15.641	2320	2327	2335	rVB	1377702	2584277	16.44%	2.382%
56	15.747	2340	2345	2350	rVV2	94762	188759	1.20%	0.174%

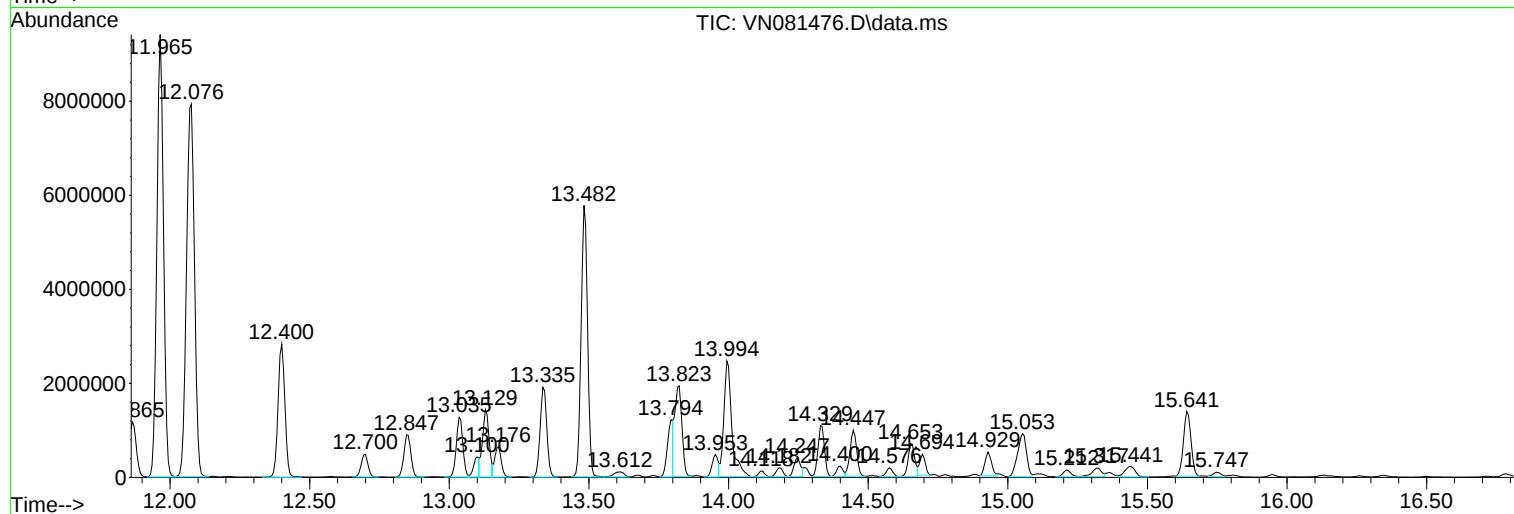
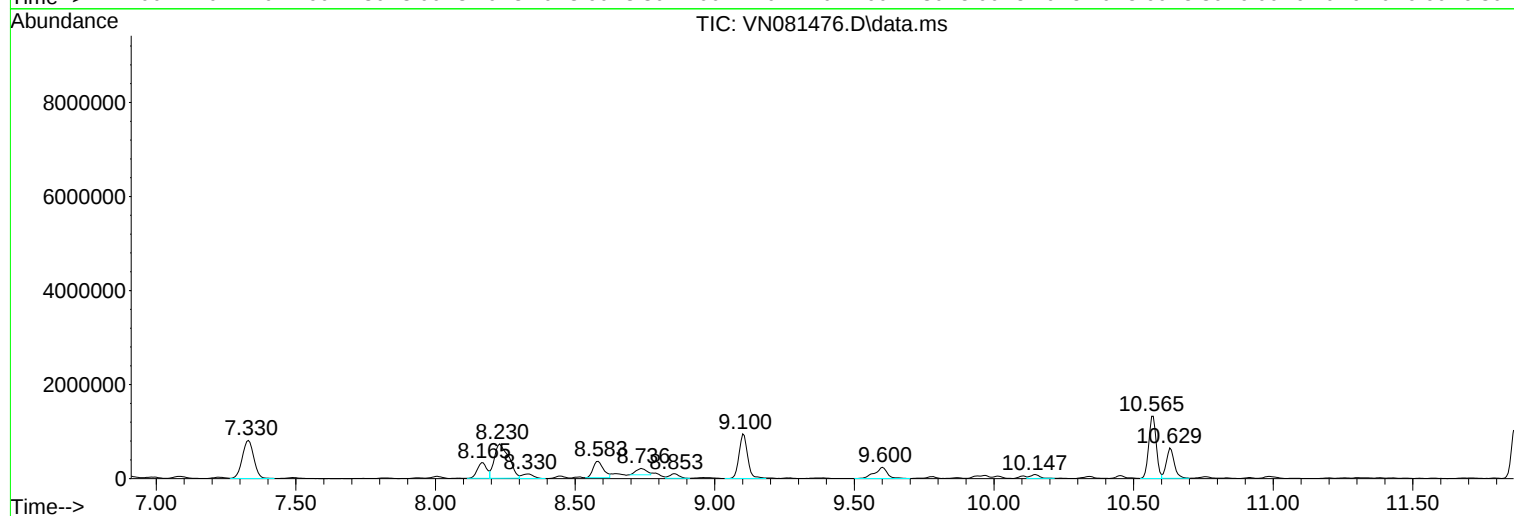
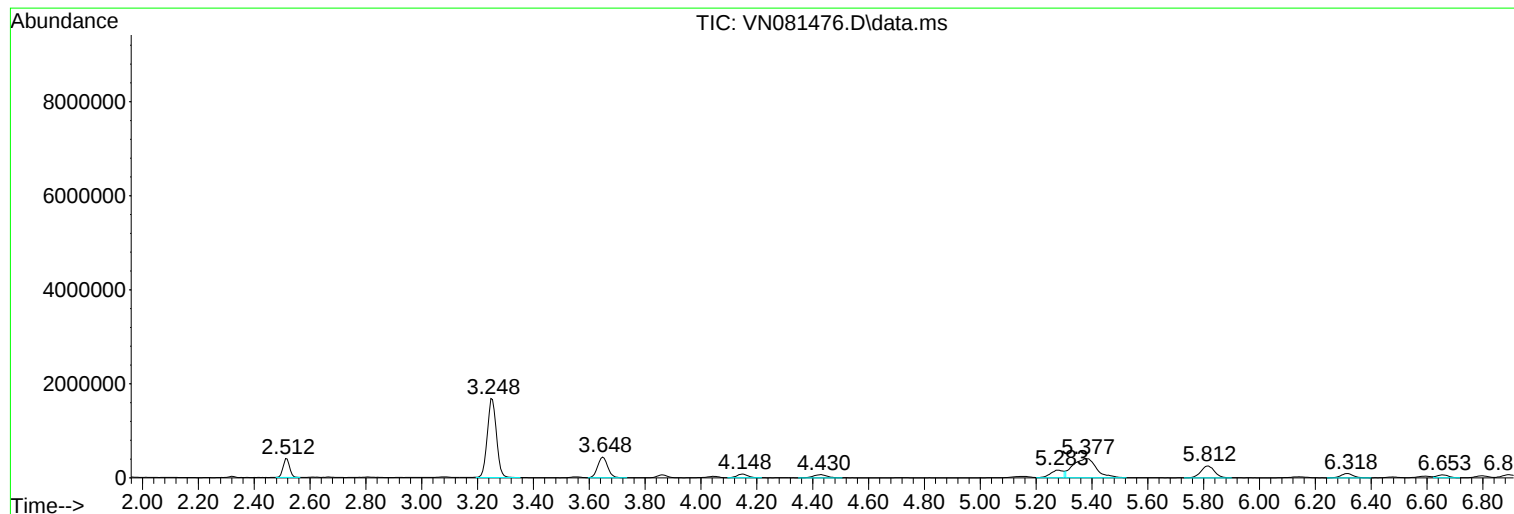
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Quant Title : SW846 8260

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



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

Instrument :
MSVOA_N
ClientSampleId :
MW-6A

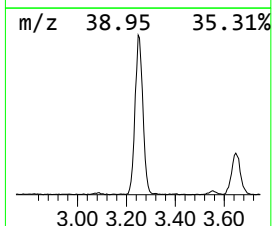
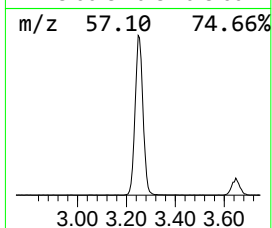
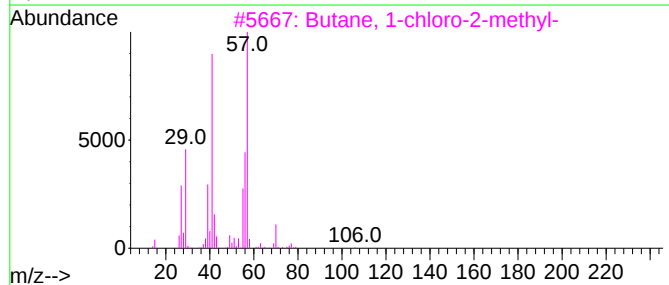
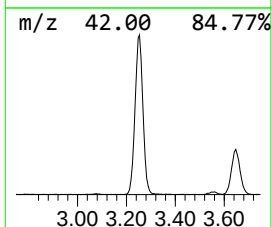
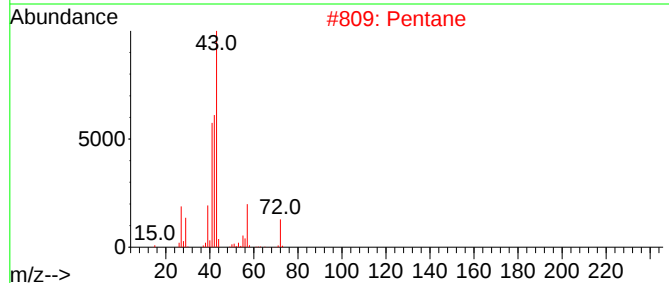
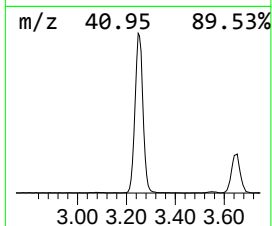
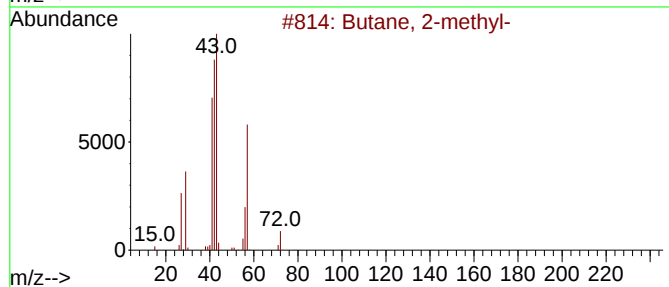
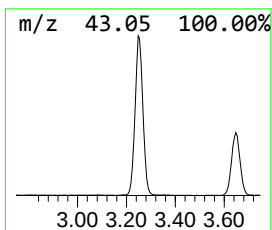
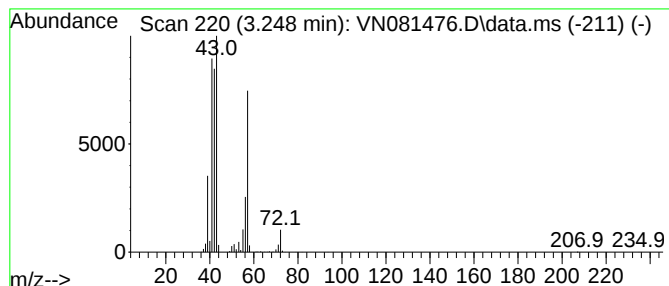
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.248	73.90 ug/l	3840520	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	28
3			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	27
4			3-Buten-1-ol	72	C4H8O	000627-27-0	25
5			1-Butene	56	C4H8	000106-98-9	10



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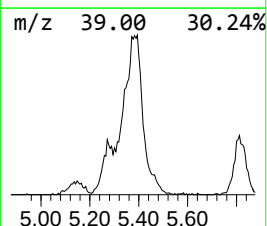
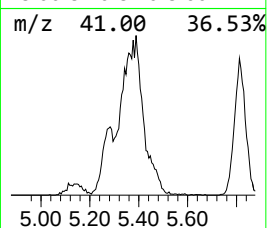
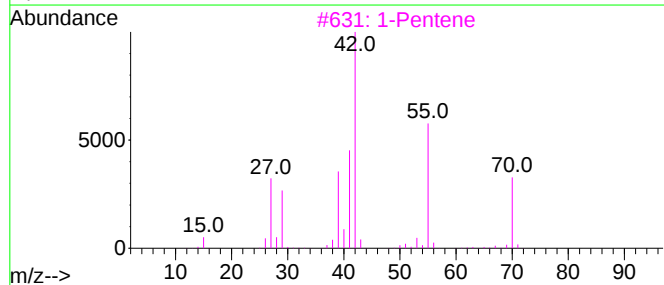
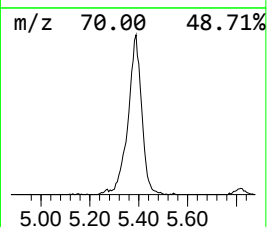
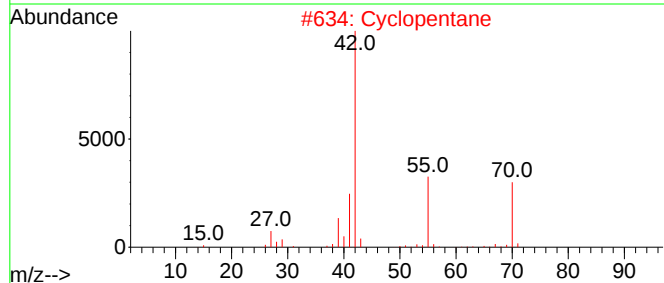
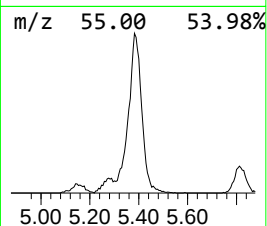
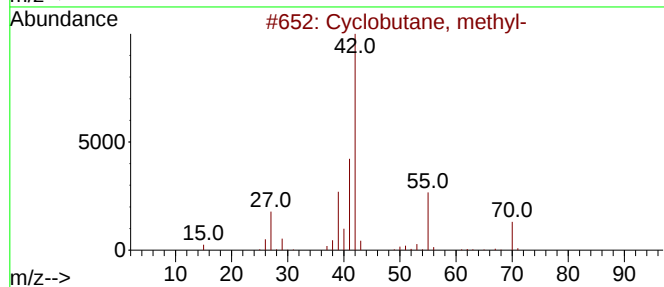
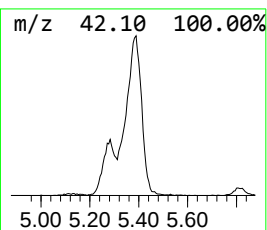
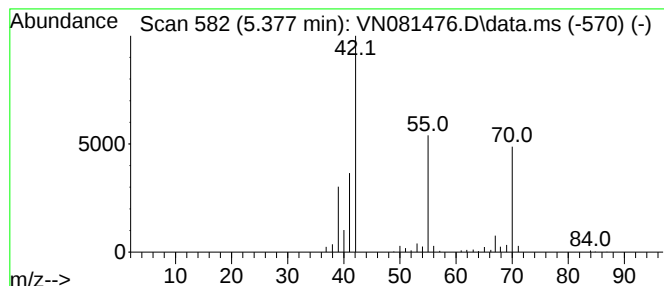
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclobutane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.377	44.70 ug/l	2323350	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2			Cyclopentane	70	C5H10	000287-92-3	78
3			1-Pentene	70	C5H10	000109-67-1	64
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	43



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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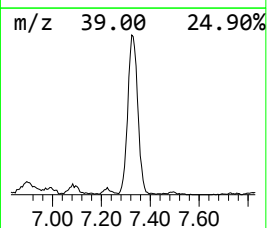
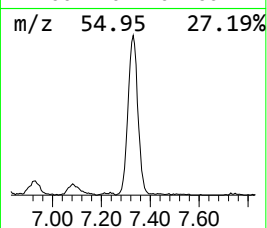
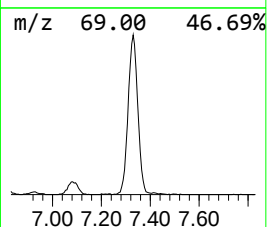
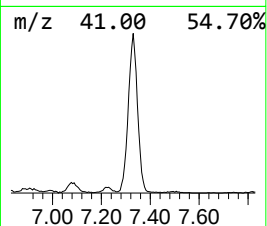
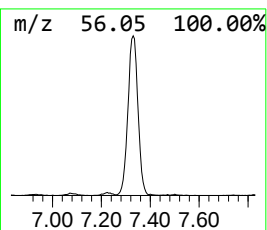
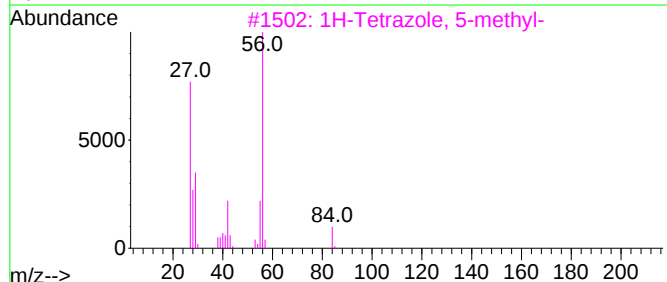
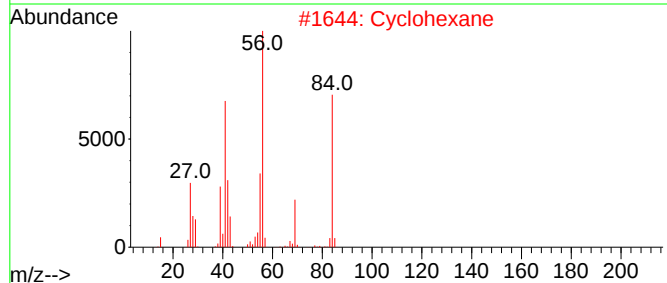
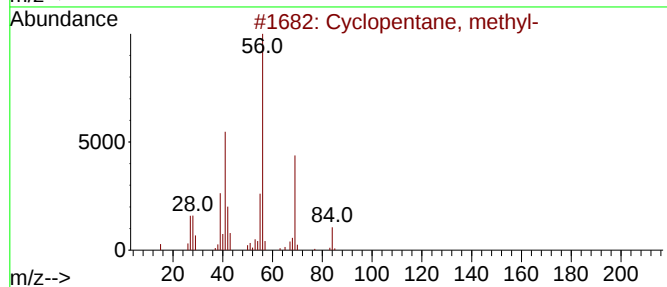
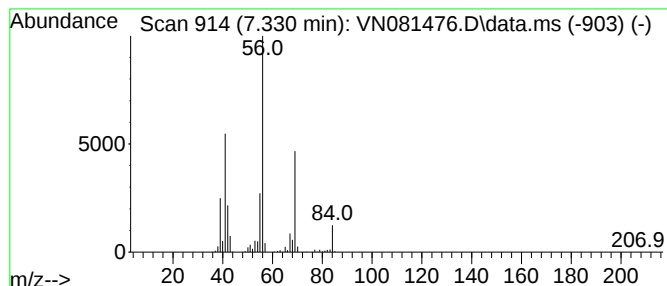
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Quant Title : SW846 8260

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

Peak Number 3 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.330	44.16 ug/l	2295290	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclohexane	84	C6H12	000110-82-7	90
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64



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Instrument :
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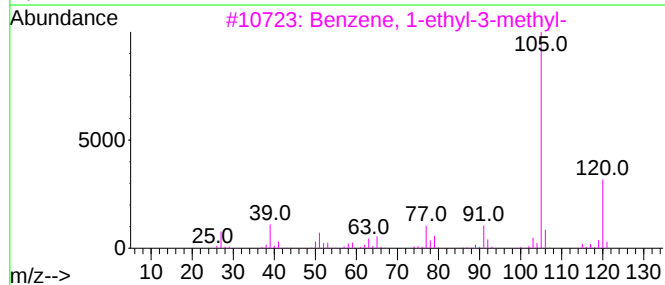
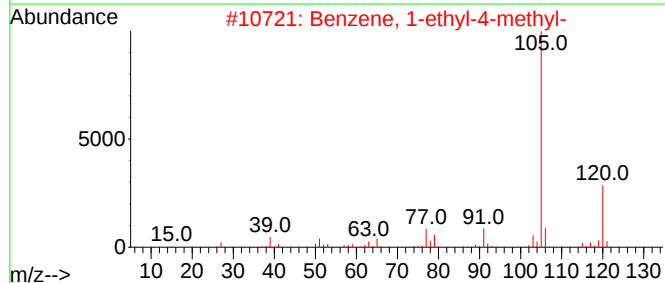
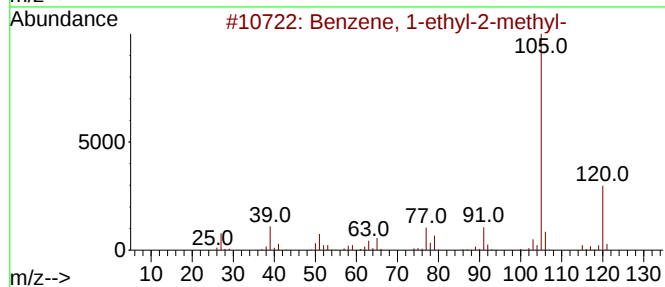
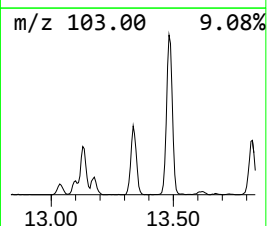
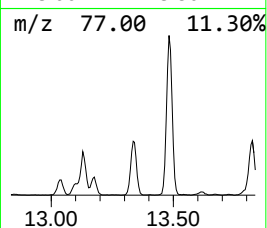
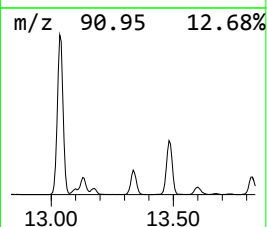
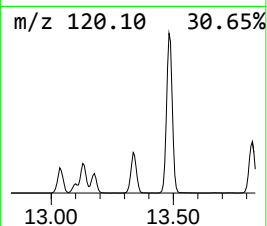
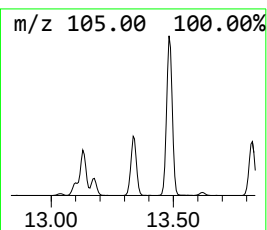
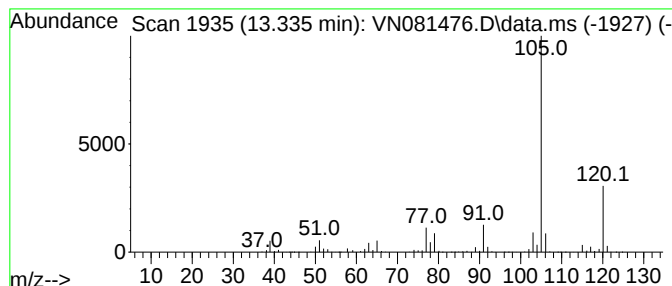
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	93.00 ug/l	3150690	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	91
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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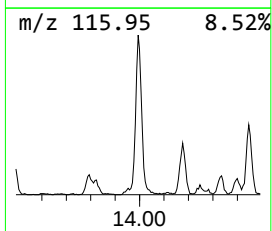
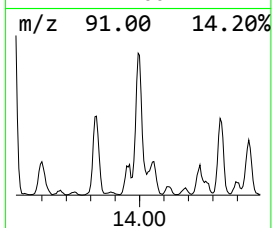
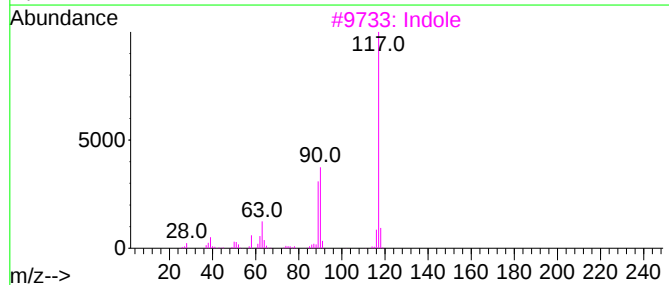
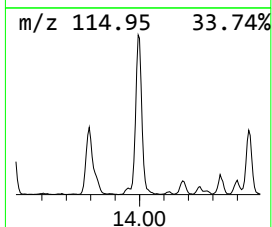
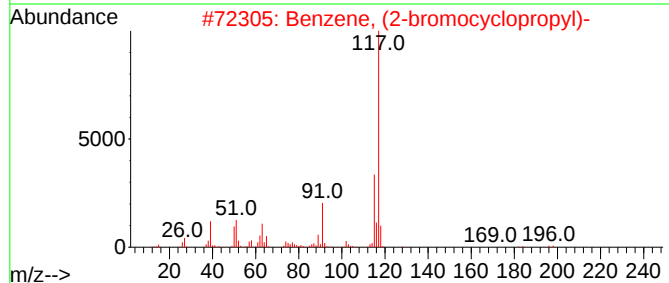
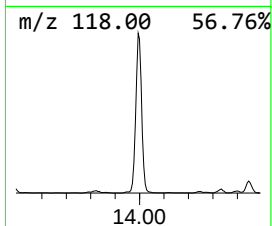
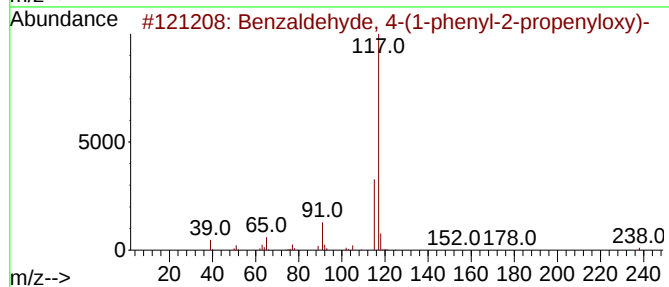
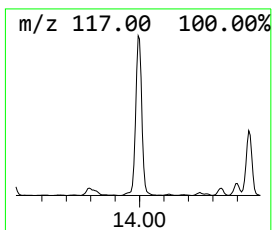
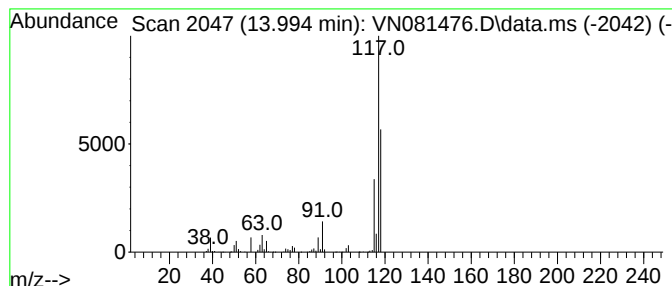
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Quant Title : SW846 8260

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

Peak Number 5 Benzaldehyde, 4-(1-phenyl-2... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	145.48 ug/l	4928760	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	53
2			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
3			Indole	117	C8H7N	000120-72-9	43
4			4-Ethynylaniline	117	C8H7N	014235-81-5	43
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081476.D
Acq On : 19 Mar 2024 17:21
Operator : JC\MD
Sample : P1773-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6A

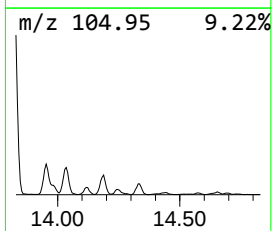
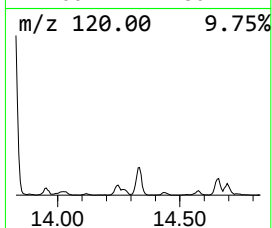
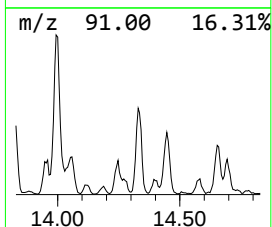
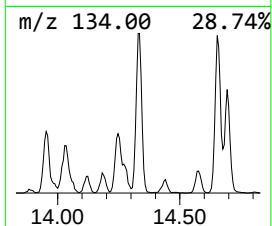
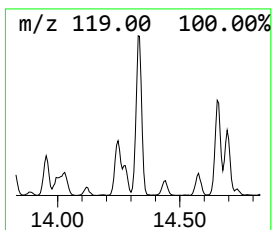
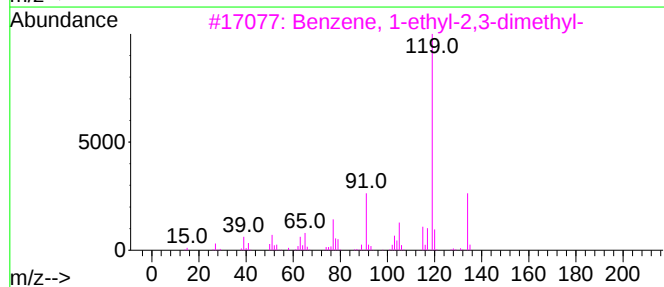
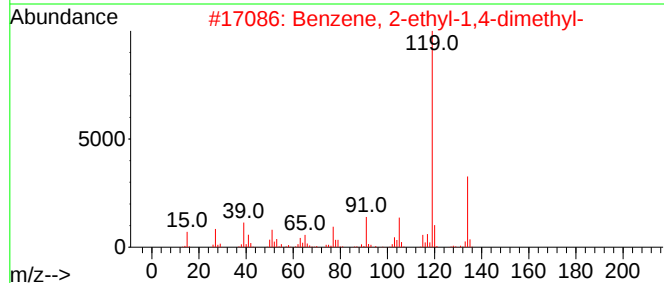
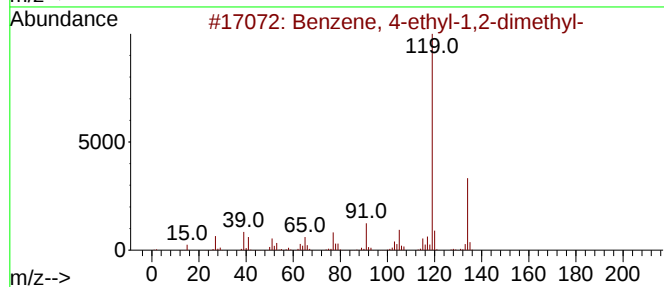
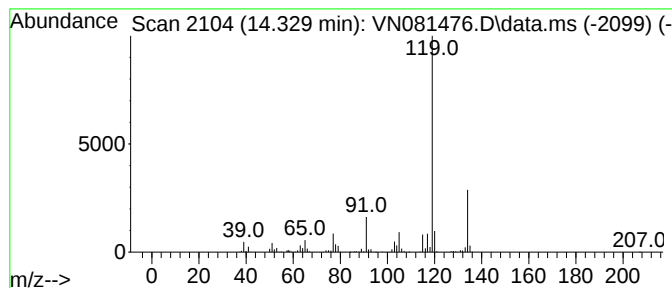
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Quant Title : SW846 8260

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.
14.329	51.12 ug/l	1731960	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	95
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081476.D
Acq On : 19 Mar 2024 17:21
Operator : JC\MD
Sample : P1773-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6A

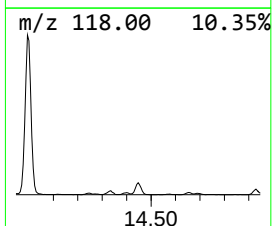
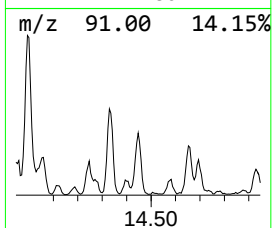
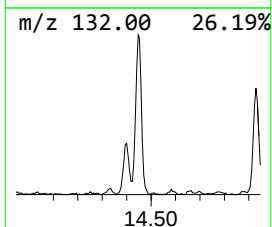
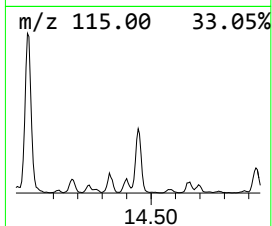
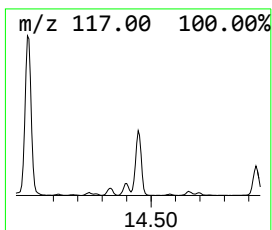
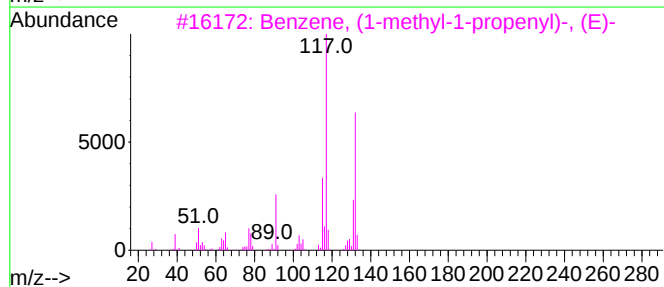
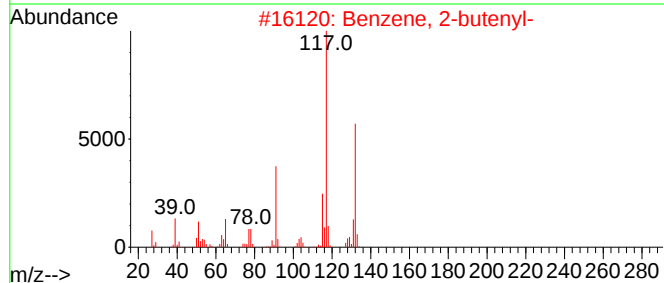
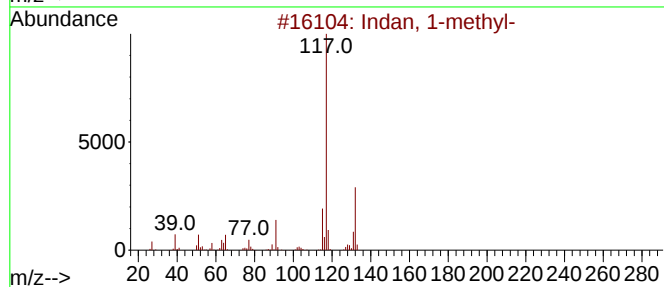
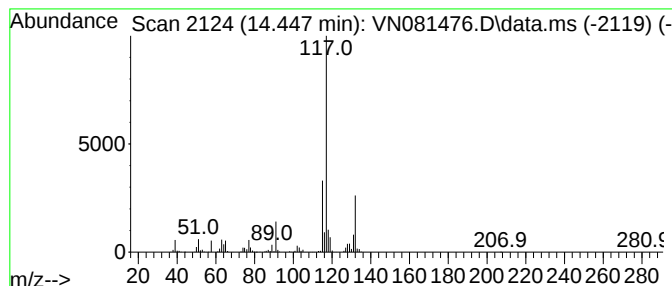
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Quant Title : SW846 8260

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

Peak Number 7 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	48.09 ug/l	1629400	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	83
2			Benzene, 2-butenyl-	132	C10H12	001560-06-1	80
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	80
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	80
5			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081476.D
Acq On : 19 Mar 2024 17:21
Operator : JC\MD
Sample : P1773-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6A

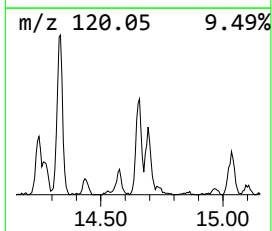
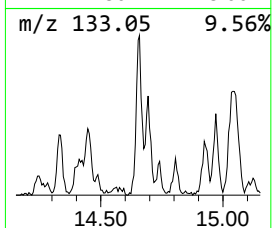
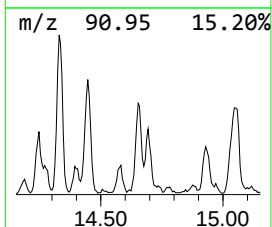
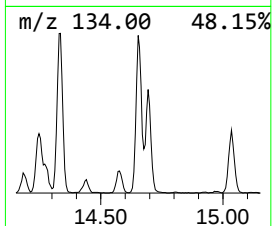
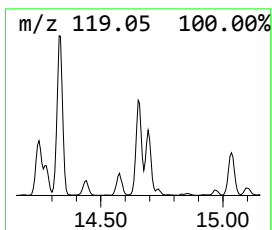
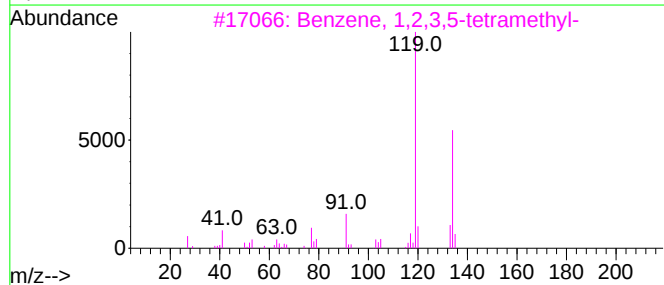
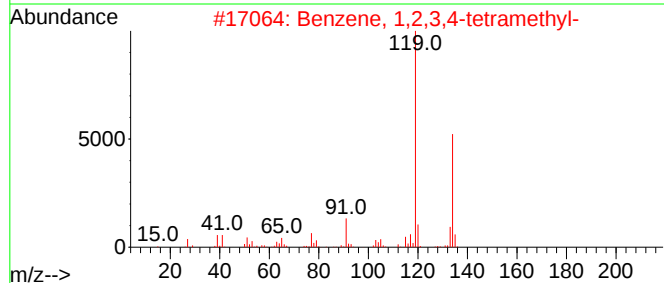
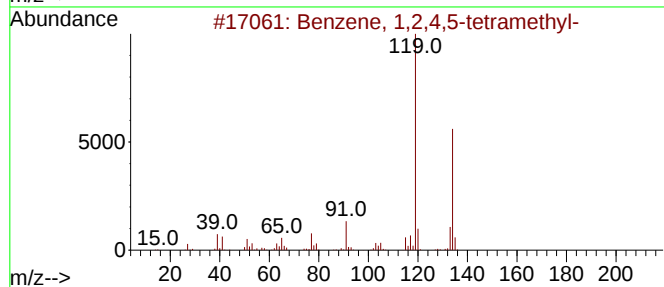
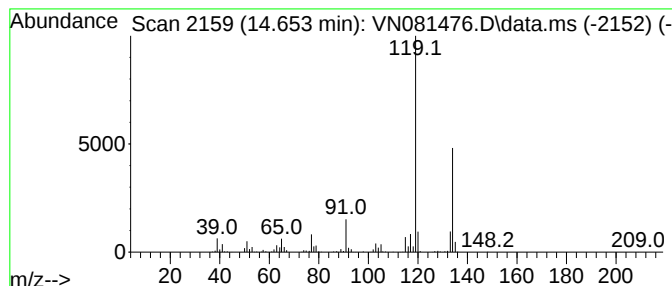
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.653	34.42 ug/l	1166070	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081476.D
Acq On : 19 Mar 2024 17:21
Operator : JC\MD
Sample : P1773-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6A

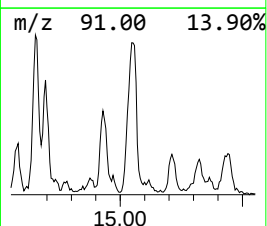
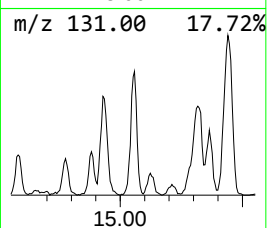
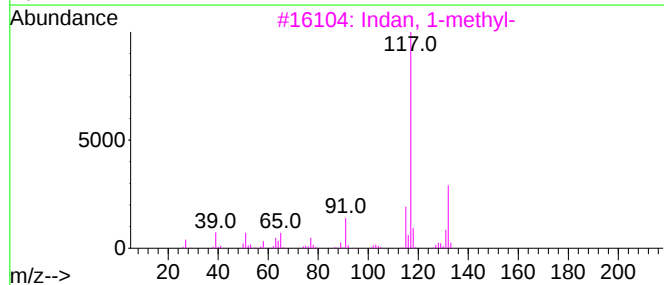
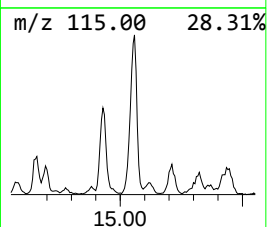
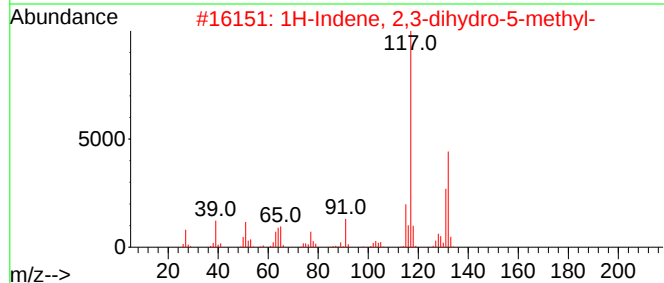
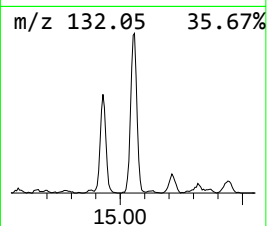
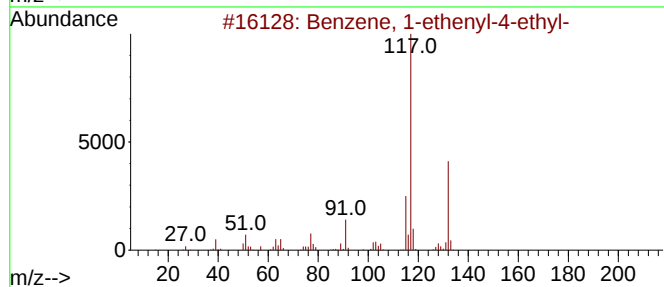
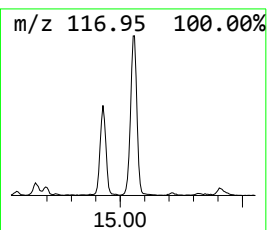
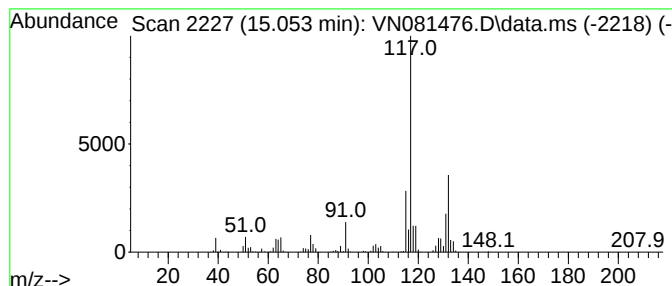
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Quant Title : SW846 8260

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	60.36 ug/l	2044930	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
3			Indan, 1-methyl-	132	C10H12	000767-58-8	90
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081476.D
Acq On : 19 Mar 2024 17:21
Operator : JC\MD
Sample : P1773-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6A

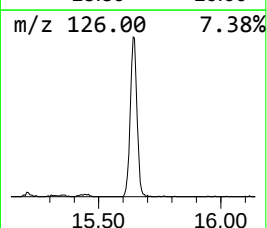
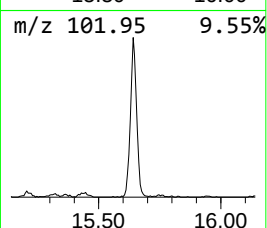
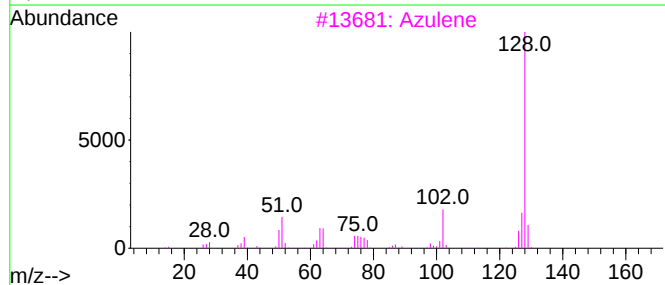
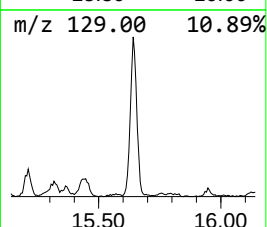
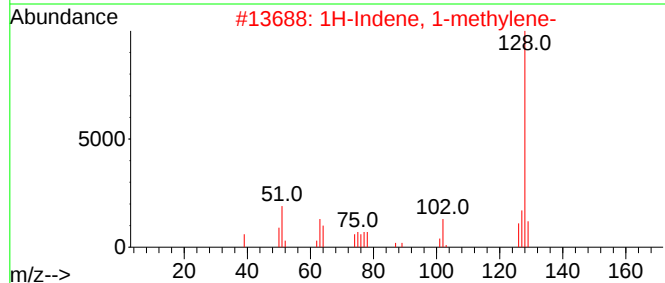
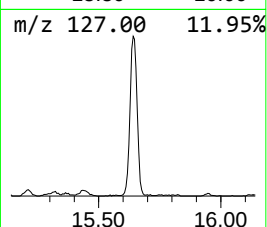
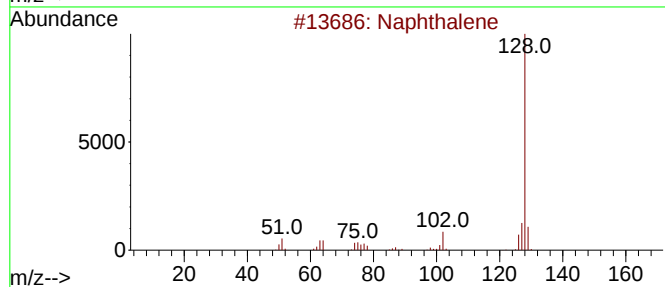
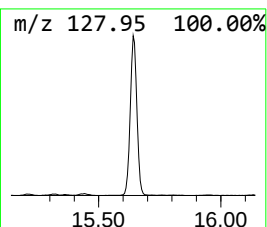
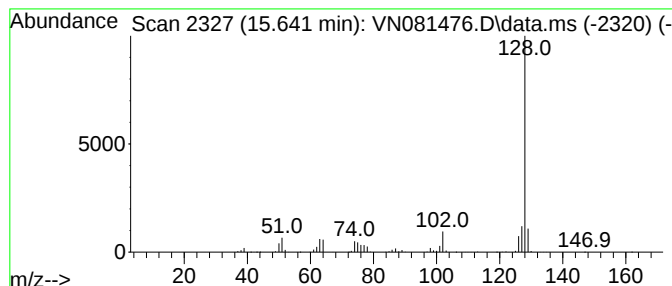
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 1-methylene- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.641	76.28 ug/l	2584280	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3			Azulene	128	C10H8	000275-51-4	91
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	56
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031924\
Data File : VN081476.D
Acq On : 19 Mar 2024 17:21
Operator : JC\MD
Sample : P1773-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.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
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Cyclobutane, me...	5.377	44.7	ug/l	2323350	1	8.230	2598590	50.0
Cyclopentane, m...	7.330	44.2	ug/l	2295290	1	8.230	2598590	50.0
Benzene, 1-ethy...	13.335	93.0	ug/l	3150690	4	13.794	1694010	50.0
Benzaldehyde, 4...	13.994	145.5	ug/l	4928760	4	13.794	1694010	50.0
Benzene, 4-ethy...	14.329	51.1	ug/l	1731960	4	13.794	1694010	50.0
Indan, 1-methyl-	14.447	48.1	ug/l	1629400	4	13.794	1694010	50.0
Benzene, 1,2,4,...	14.653	34.4	ug/l	1166070	4	13.794	1694010	50.0
Benzene, 1-ethe...	15.053	60.4	ug/l	2044930	4	13.794	1694010	50.0
1H-Indene, 1-me...	15.641	76.3	ug/l	2584280	4	13.794	1694010	50.0