

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
 Data File : VN075855.D
 Acq On : 16 Dec 2022 18:14
 Operator : JC\MD
 Sample : N6096-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 34258

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\82N121422W.M
 Title : SW846 8260

Signal : TIC: VN075855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.442	393	406	428	rBV	458511	1399442	29.60%	6.069%
2	8.177	1030	1041	1045	rBV	247560	595005	12.59%	2.580%
3	8.230	1045	1050	1063	rVB	489420	1095766	23.18%	4.752%
4	8.588	1101	1111	1123	rVV2	252385	631071	13.35%	2.737%
5	9.106	1188	1199	1208	rBV	647150	1324627	28.02%	5.744%
6	10.571	1438	1448	1453	rBV	960677	1782372	37.70%	7.730%
7	10.635	1453	1459	1474	rVB	2591346	4727434	100.00%	20.501%
8	11.871	1660	1669	1680	rBV	865229	1517983	32.11%	6.583%
9	11.965	1680	1685	1693	rVV2	33836	60602	1.28%	0.263%
10	12.077	1697	1704	1713	rVB2	32432	61624	1.30%	0.267%
11	12.400	1749	1759	1767	rBV	350565	601777	12.73%	2.610%
12	12.853	1828	1836	1845	rBV	658449	1110542	23.49%	4.816%
13	13.106	1873	1879	1880	rBV2	29729	48448	1.02%	0.210%
14	13.135	1880	1884	1887	rVV	81104	137686	2.91%	0.597%
15	13.176	1887	1891	1898	rVB	118536	185168	3.92%	0.803%
16	13.265	1898	1906	1913	rBV	367739	570498	12.07%	2.474%
17	13.341	1913	1919	1926	rVB	128160	212355	4.49%	0.921%
18	13.506	1938	1947	1959	rBV2	85399	177851	3.76%	0.771%
19	13.794	1989	1996	2007	rBV2	811007	1712478	36.22%	7.426%
20	13.994	2025	2030	2046	rVB3	153085	453225	9.59%	1.965%
21	14.182	2056	2062	2068	rBV	36385	58988	1.25%	0.256%
22	14.335	2082	2088	2094	rVB	93389	143311	3.03%	0.621%
23	14.447	2102	2107	2112	rVB2	86231	145274	3.07%	0.630%
24	14.576	2124	2129	2135	rVB2	45290	72305	1.53%	0.314%
25	14.659	2135	2143	2146	rBV	76959	131909	2.79%	0.572%
26	14.694	2146	2149	2154	rVV	113215	168576	3.57%	0.731%
27	14.882	2172	2181	2184	rBV4	24809	49274	1.04%	0.214%
28	14.929	2184	2189	2194	rBV2	91016	160778	3.40%	0.697%
29	15.059	2201	2211	2217	rBV2	263681	645080	13.65%	2.797%
30	15.123	2217	2222	2228	rVB5	32496	73691	1.56%	0.320%
31	15.212	2230	2237	2245	rBV	200474	353650	7.48%	1.534%
32	15.323	2245	2256	2260	rBV4	94563	229678	4.86%	0.996%
33	15.447	2269	2277	2285	rVB4	99433	250925	5.31%	1.088%
34	15.641	2305	2310	2315	rVV	50057	97164	2.06%	0.421%
35	15.706	2315	2321	2325	rVV2	68804	134526	2.85%	0.583%
36	15.753	2325	2329	2330	rVV2	45583	61955	1.31%	0.269%

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Peak Location: TOP

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

Peak separation: 5

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37	15.788	2331	2335	2352	rVB5	69814	236809	5.01%	1.027%
38	15.953	2355	2363	2372	rBV	74552	165509	3.50%	0.718%
39	16.135	2382	2394	2395	rBV2	67958	151595	3.21%	0.657%
40	16.170	2395	2400	2410	rVV2	196119	427753	9.05%	1.855%
41	16.264	2410	2416	2421	rVV4	29824	62441	1.32%	0.271%
42	16.347	2421	2430	2443	rVB4	64369	222414	4.70%	0.965%
43	16.512	2446	2458	2470	rBV2	155048	385248	8.15%	1.671%
44	16.717	2482	2493	2499	rBV3	83764	224534	4.75%	0.974%

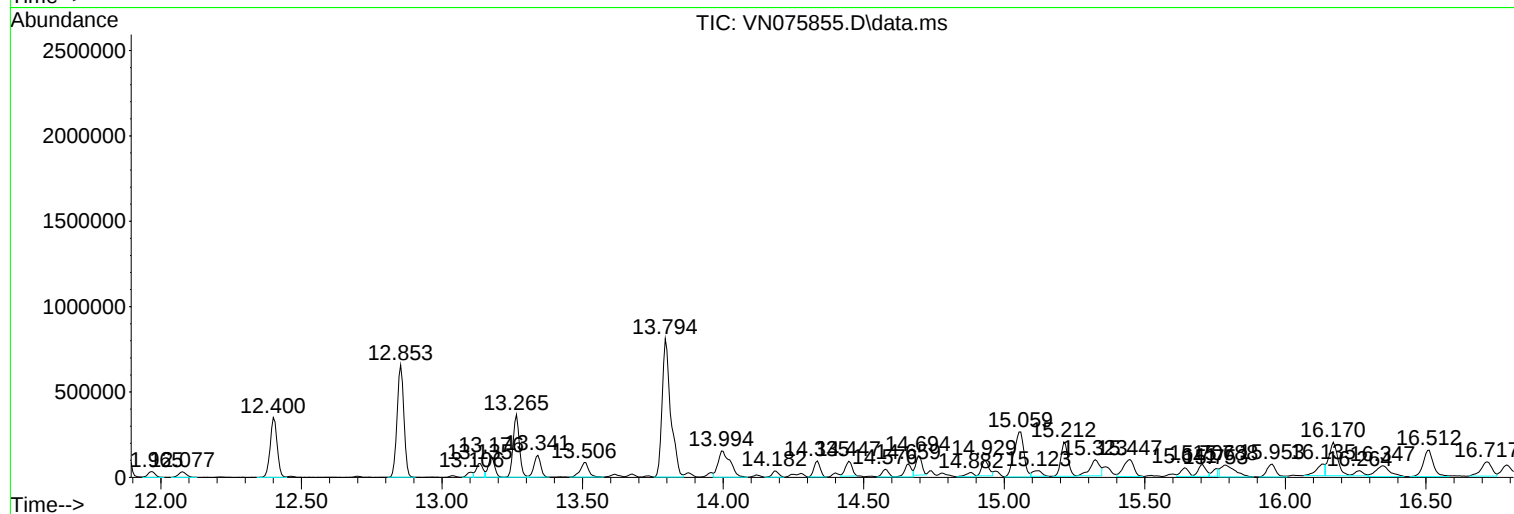
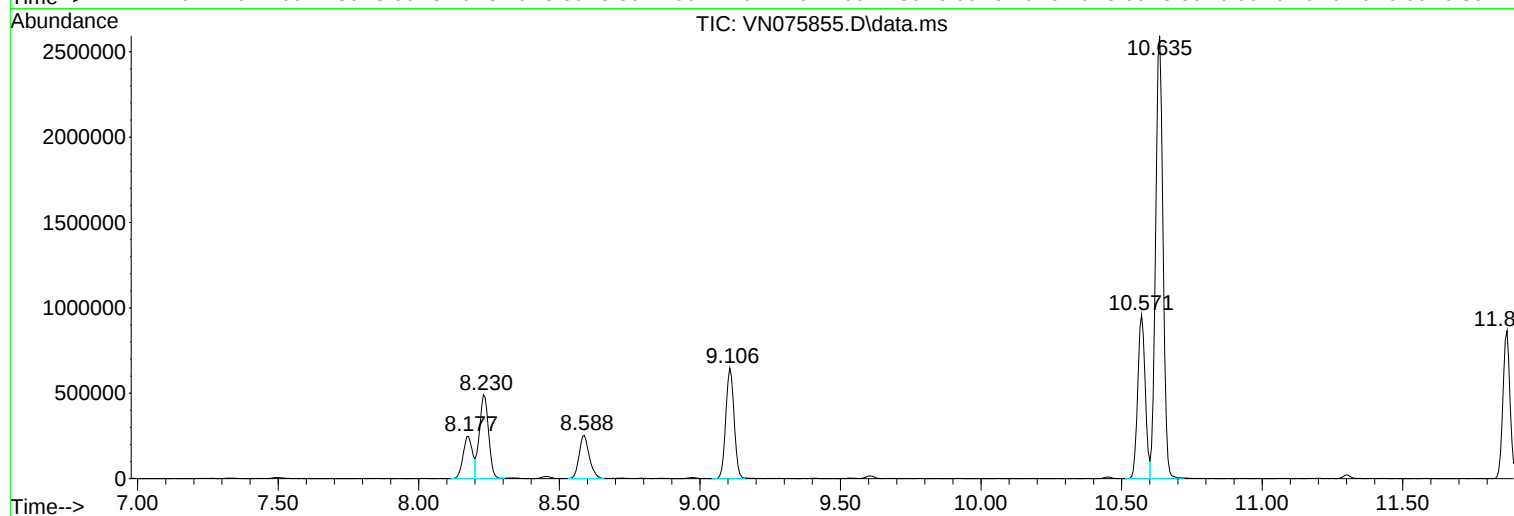
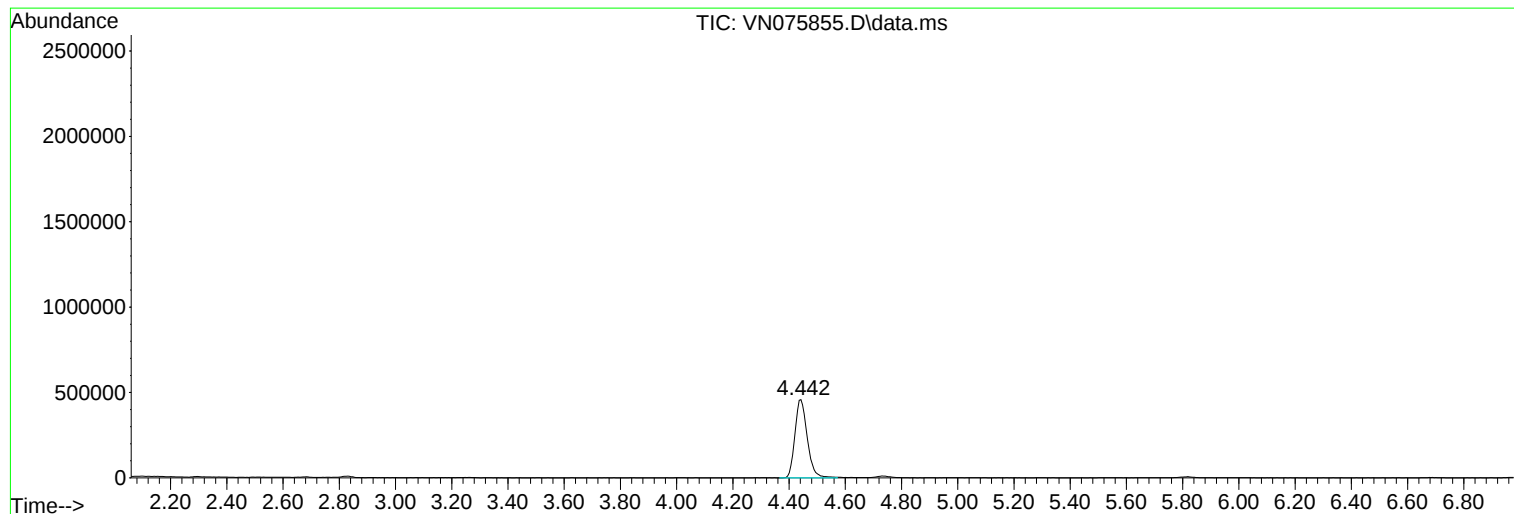
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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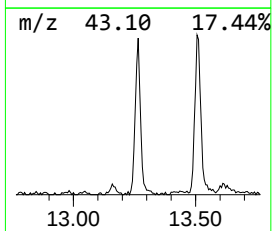
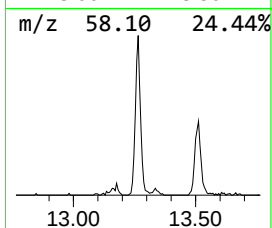
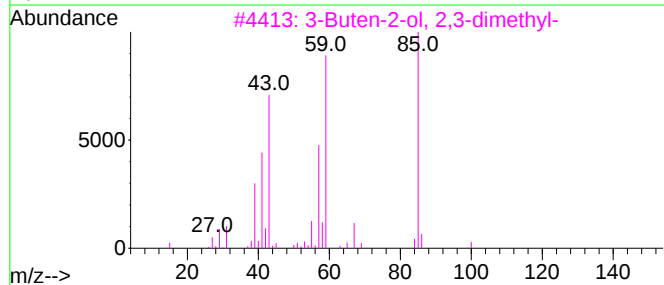
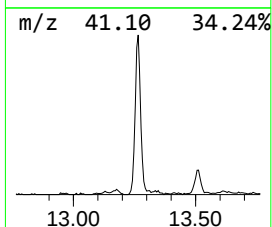
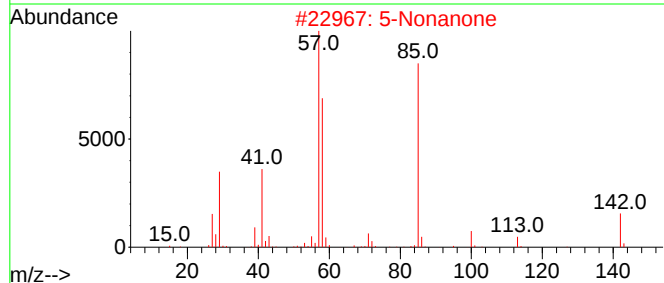
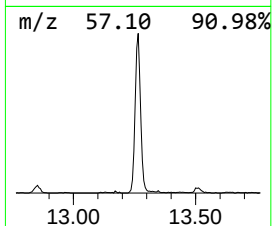
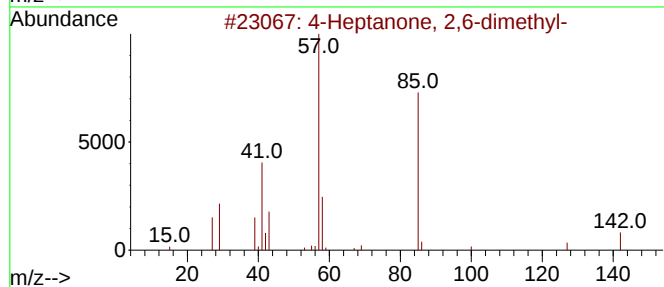
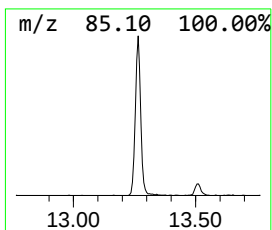
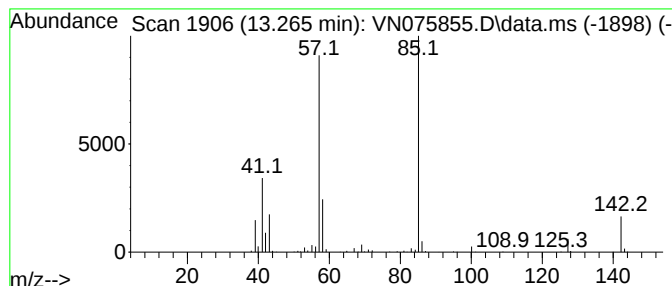
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 1 4-Heptanone, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.265	16.66 ug/l	570498	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			5-Nonanone	142	C9H18O	000502-56-7	59
3			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	53
4			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	50
5			4-Methoxy-3-buten-2-one	100	C5H8O2	004652-27-1	47



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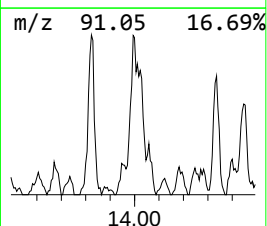
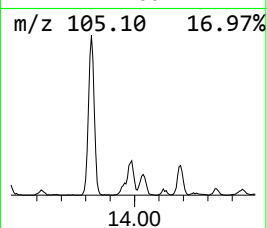
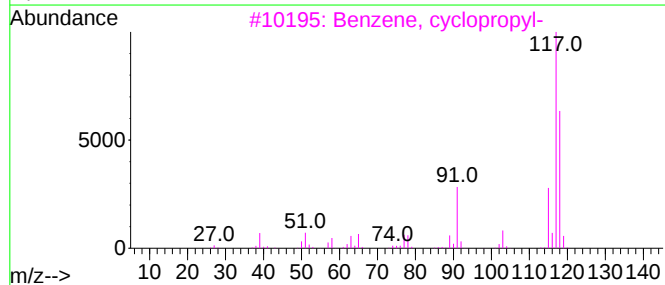
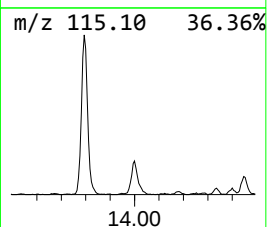
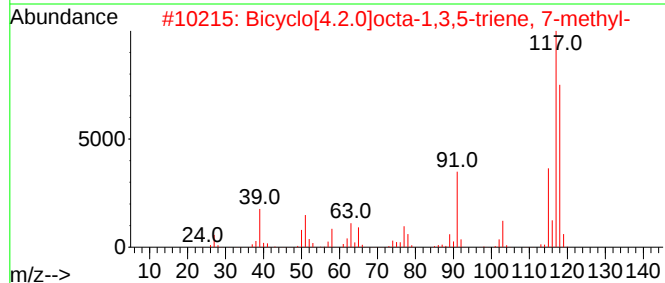
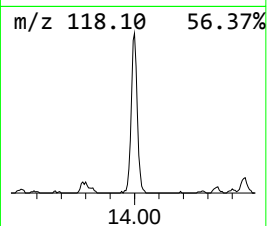
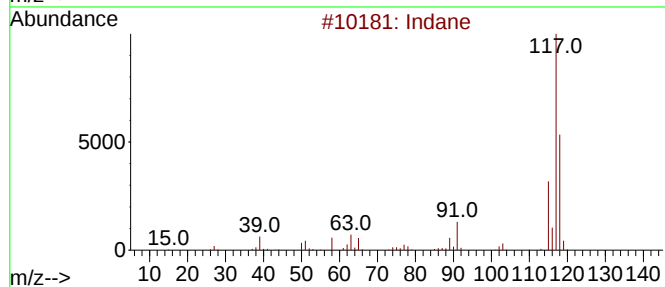
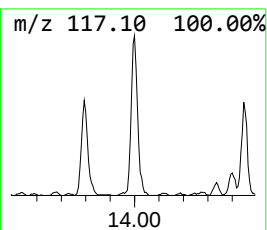
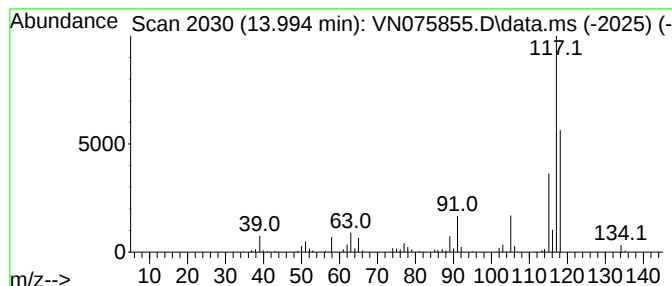
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 2 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	13.23 ug/l	453225	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	68
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	68
4			Delatacyclene	118	C9H10	007785-10-6	64
5			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64



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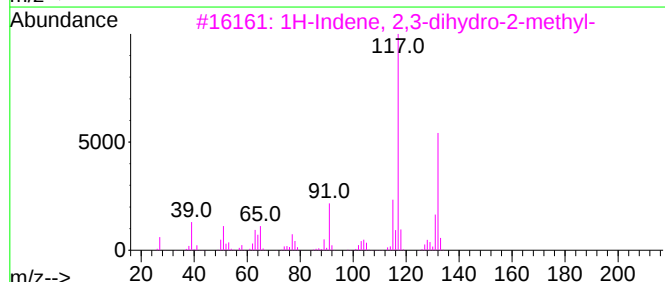
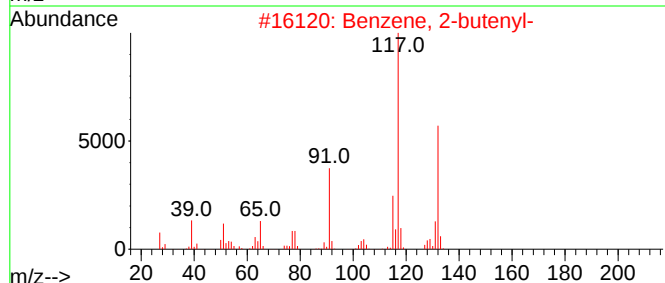
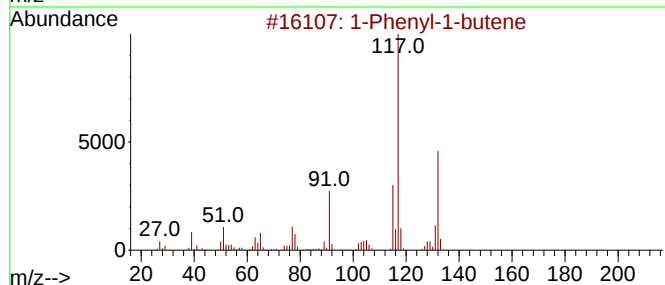
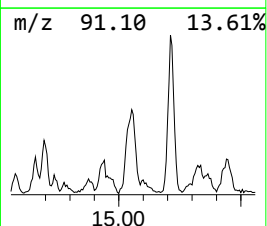
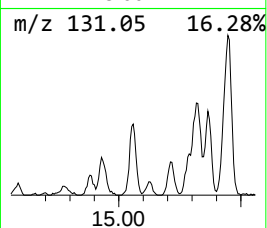
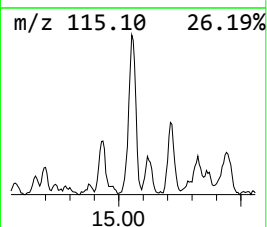
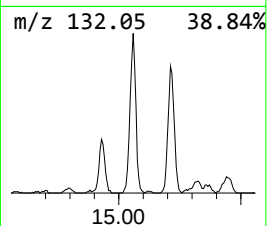
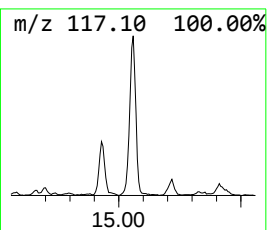
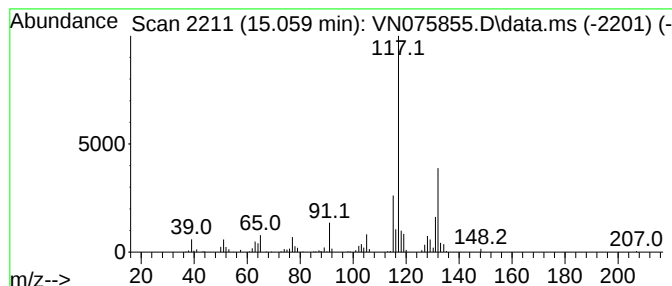
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Phenyl-1-butene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.059	18.83 ug/l	645080	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenyl-1-butene	132	C10H12	000824-90-8	91
2		Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
3		1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	91
4		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	91
5		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	91



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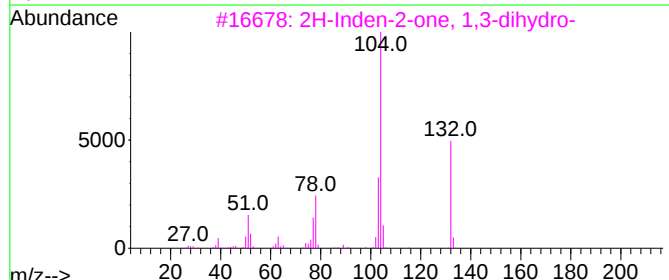
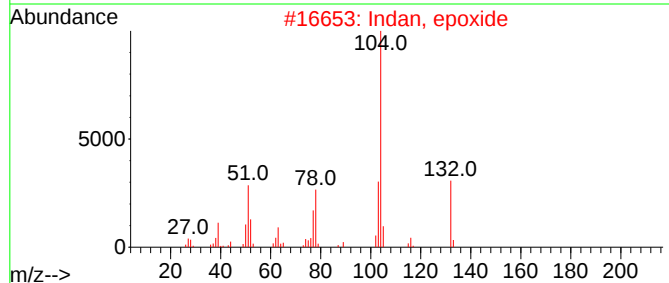
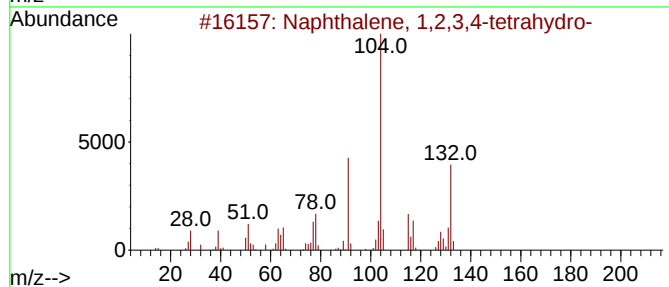
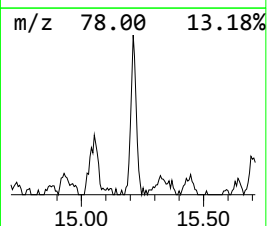
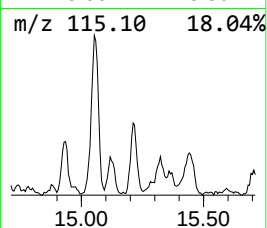
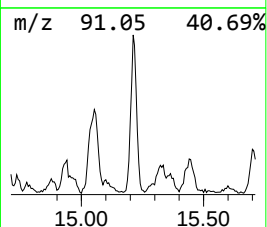
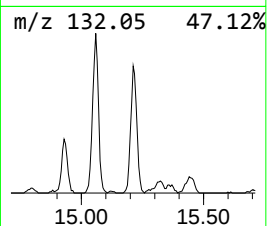
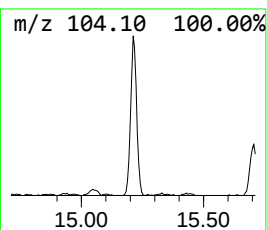
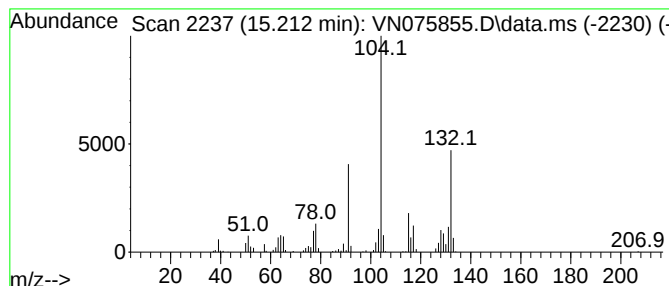
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.212	10.33 ug/l	353650	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			Indan, epoxide	132	C9H8O	000768-22-9	64
3			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	58
4			Benzene, 3-cyclohexen-1-yl-	158	C12H14	004994-16-5	47
5			Phensuximide	189	C11H11NO2	000086-34-0	38



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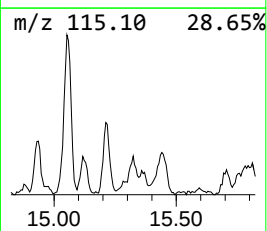
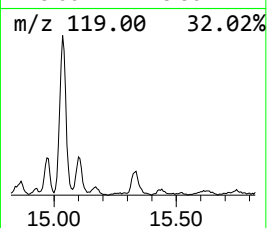
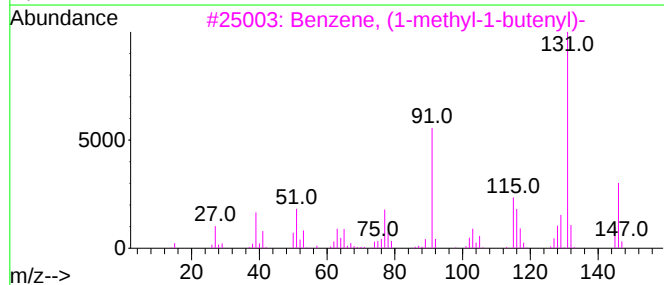
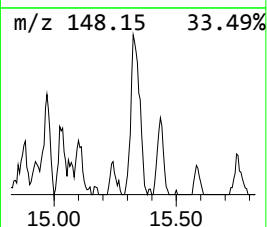
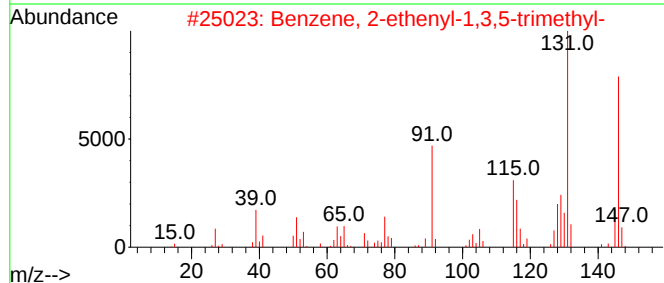
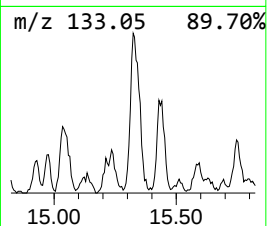
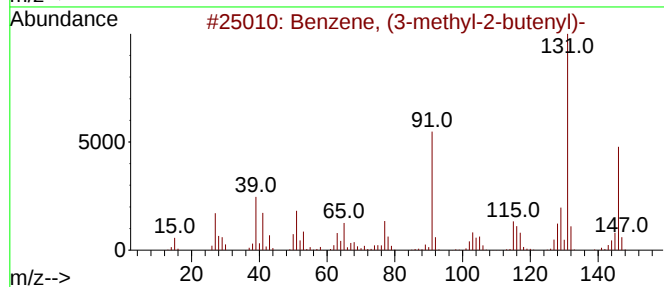
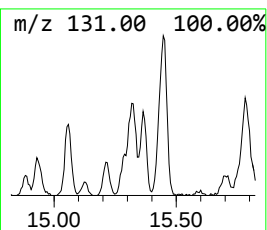
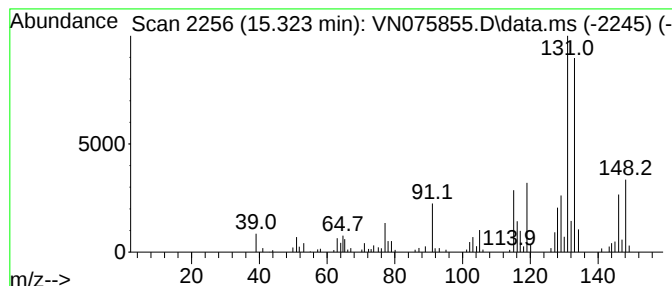
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, (3-methyl-2-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	6.71 ug/l	229678	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	50
2			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	50
3			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	46
4			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	46
5			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075855.D
Acq On : 16 Dec 2022 18:14
Operator : JC\MD
Sample : N6096-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
34258

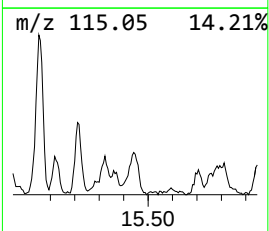
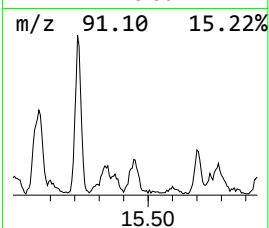
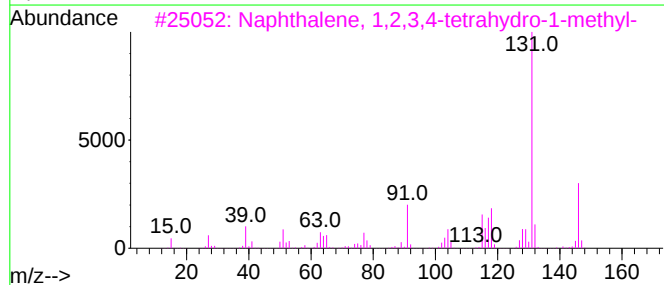
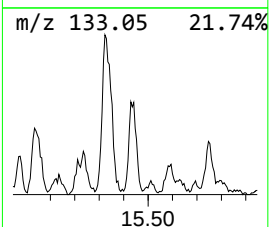
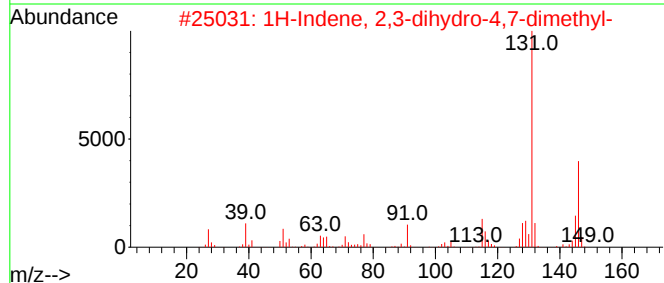
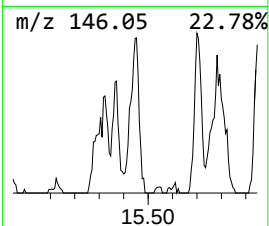
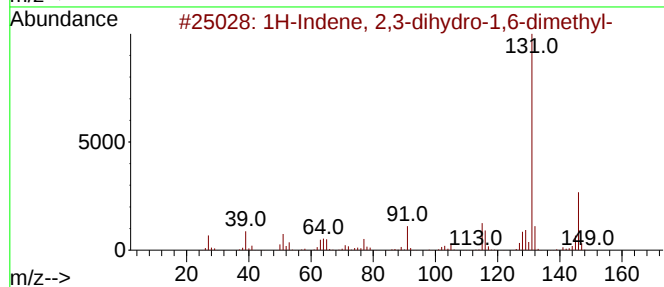
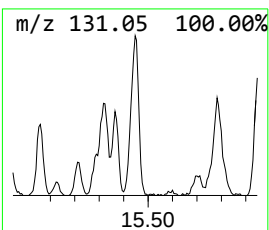
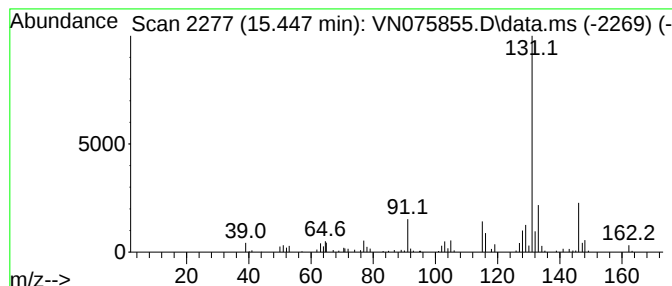
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Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.447	7.33 ug/l	250925	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	93
2			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	81
4			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	81
5			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075855.D
Acq On : 16 Dec 2022 18:14
Operator : JC\MD
Sample : N6096-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
34258

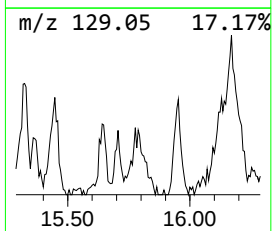
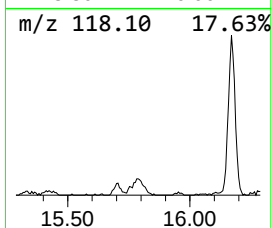
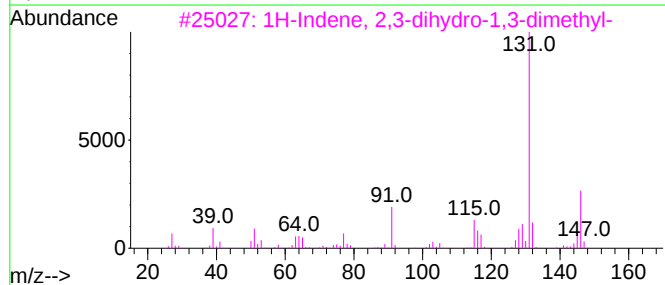
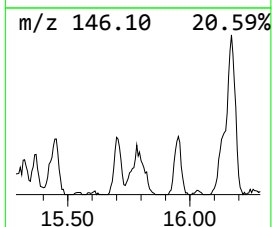
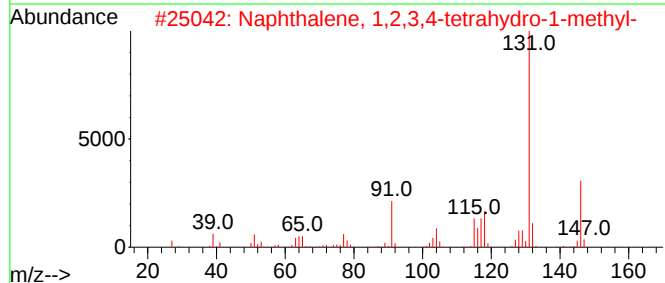
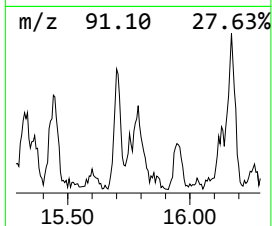
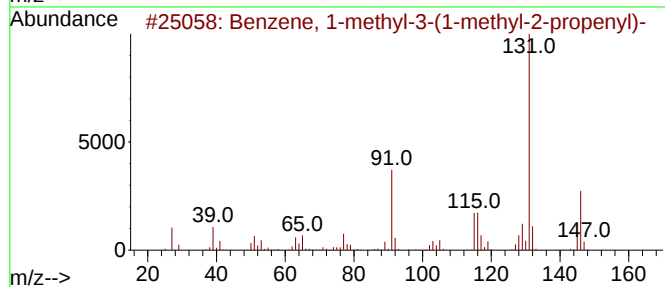
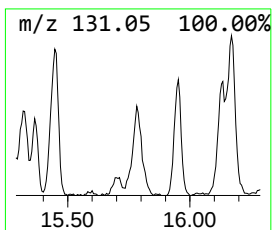
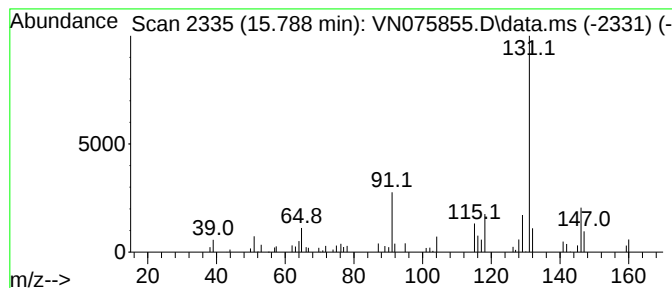
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methyl-3-(1-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.788	6.91 ug/l	236809	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	74
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	74
3			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	68
4			1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	64
5			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075855.D
Acq On : 16 Dec 2022 18:14
Operator : JC\MD
Sample : N6096-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
34258

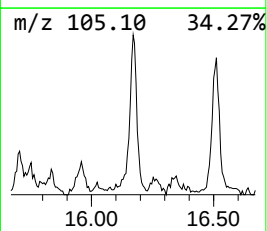
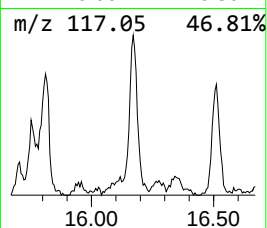
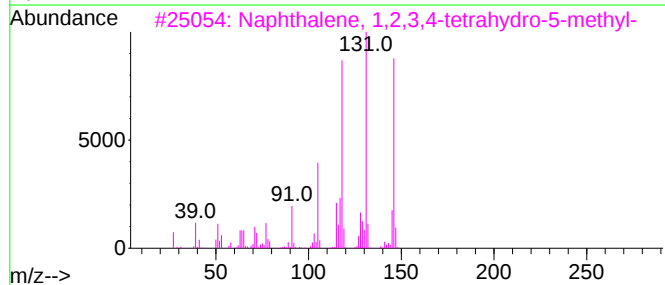
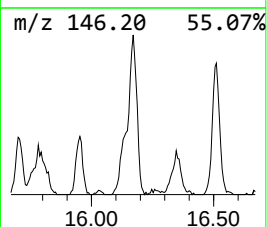
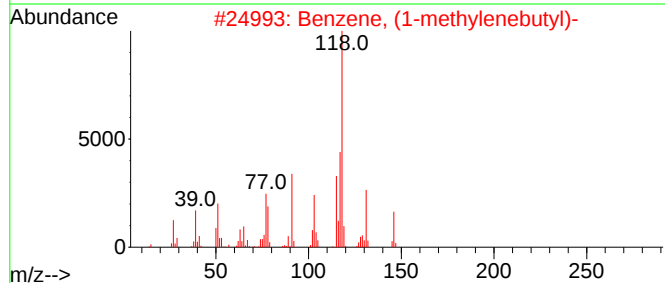
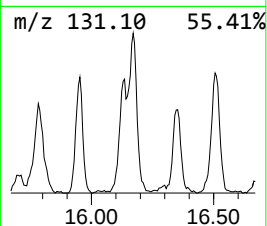
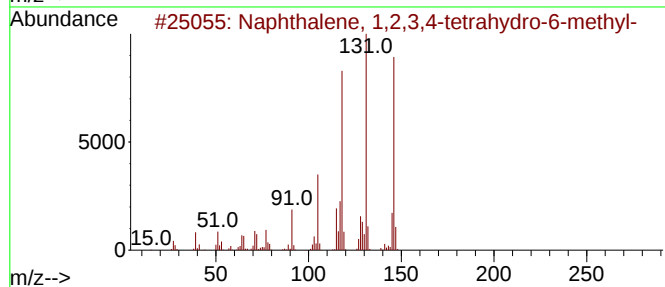
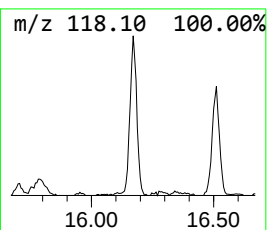
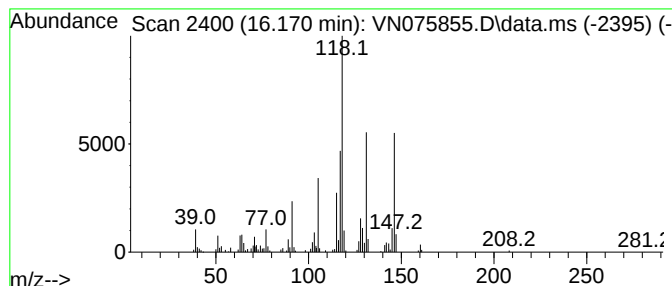
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	12.49 ug/l	427753	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	92
2			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	90
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
4			Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	74
5			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075855.D
Acq On : 16 Dec 2022 18:14
Operator : JC\MD
Sample : N6096-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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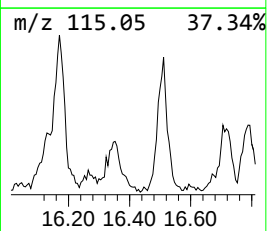
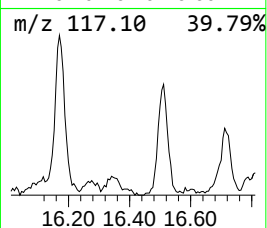
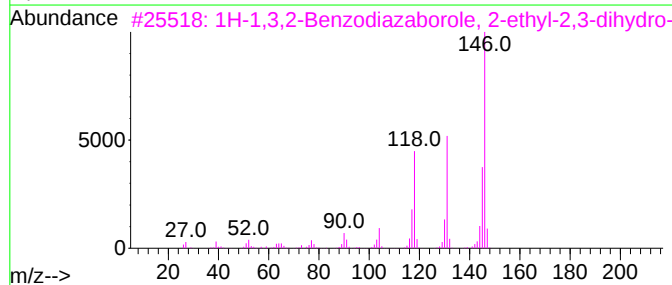
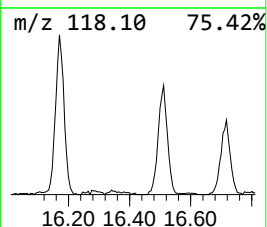
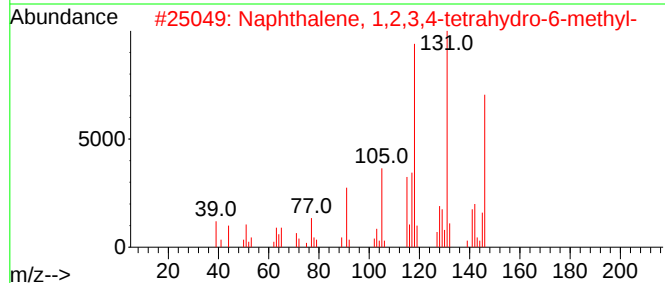
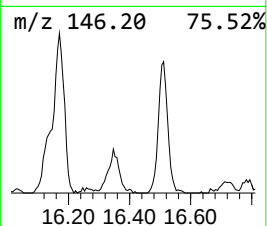
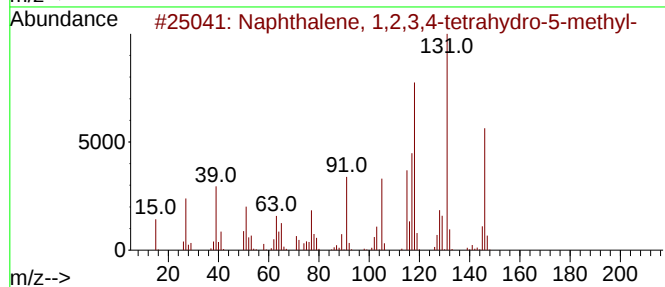
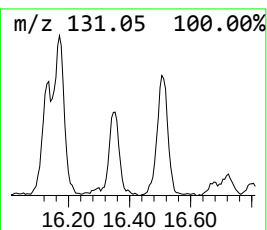
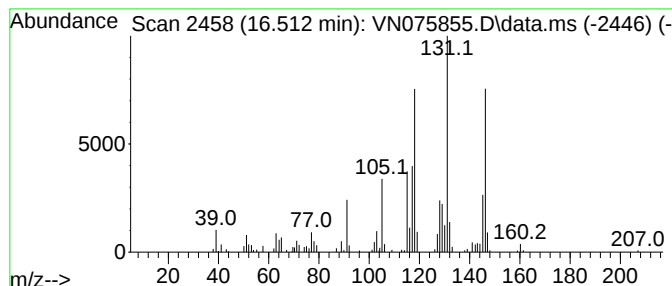
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.512	11.25 ug/l	385248	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	97
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	87
4			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	64
5			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075855.D
Acq On : 16 Dec 2022 18:14
Operator : JC\MD
Sample : N6096-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
34258

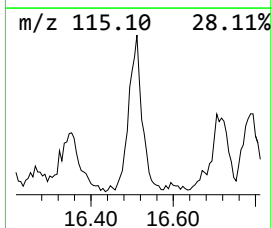
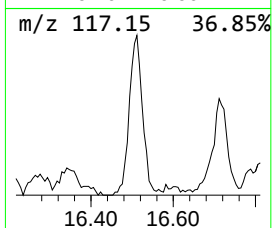
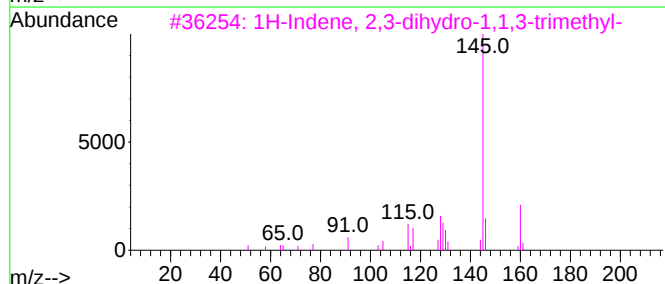
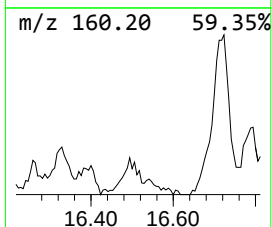
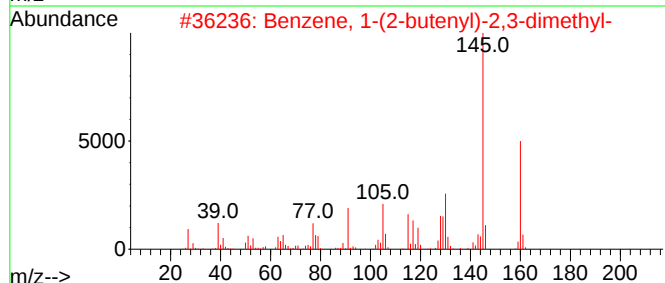
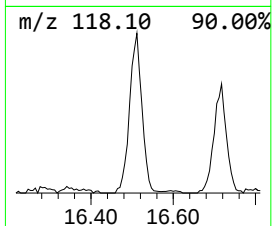
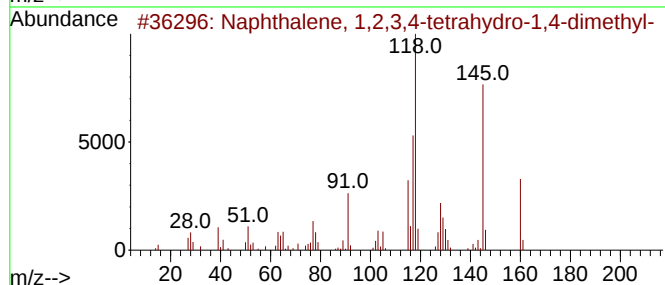
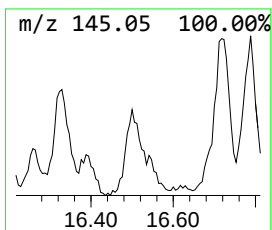
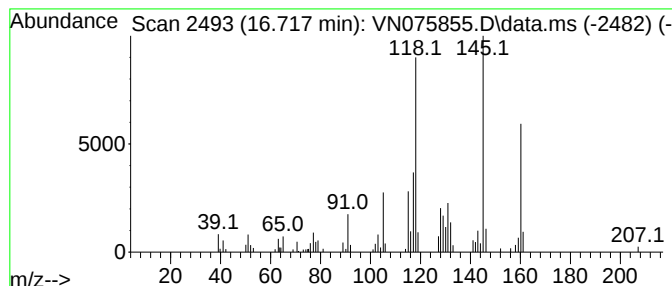
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.717	6.56 ug/l	224534	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	97
2			Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	78
3			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	70
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	70
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121622\
Data File : VN075855.D
Acq On : 16 Dec 2022 18:14
Operator : JC\MD
Sample : N6096-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
34258

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.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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Indane	13.994	13.2	ug/l	453225	4	13.794	1712480	50.0
1-Phenyl-1-butene	15.059	18.8	ug/l	645080	4	13.794	1712480	50.0
Naphthalene, 1,...	15.212	10.3	ug/l	353650	4	13.794	1712480	50.0
Benzene, (3-met...	15.323	6.7	ug/l	229678	4	13.794	1712480	50.0
1H-Indene, 2,3-...	15.447	7.3	ug/l	250925	4	13.794	1712480	50.0
Benzene, 1-meth...	15.788	6.9	ug/l	236809	4	13.794	1712480	50.0
Naphthalene, 1,...	16.170	12.5	ug/l	427753	4	13.794	1712480	50.0
Naphthalene, 1,...	16.512	11.3	ug/l	385248	4	13.794	1712480	50.0
Naphthalene, 1,...	16.717	6.6	ug/l	224534	4	13.794	1712480	50.0