

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
 Data File : VN068505.D
 Acq On : 16 Sep 2021 19:35
 Operator : JC/MD
 Sample : M3759-19 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41094

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\82N090721W.M
 Title : SW846 8260

Signal : TIC: VN068505.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.231	79	90	108	rVB2	43916	72354	3.32%	0.313%
2	2.590	215	224	239	rVB3	22456	37489	1.72%	0.162%
3	2.740	267	280	291	rVB4	15553	31474	1.44%	0.136%
4	7.316	1970	1986	2005	rBV3	8147	24384	1.12%	0.105%
5	8.024	2228	2250	2261	rBV3	310124	743803	34.12%	3.213%
6	8.088	2262	2274	2303	rVB	598849	1380686	63.34%	5.964%
7	8.440	2384	2405	2433	rBV	290409	691299	31.71%	2.986%
8	8.971	2582	2603	2640	rBV	760557	1601107	73.45%	6.916%
9	10.443	3134	3152	3186	rBV	1132618	2179927	100.00%	9.417%
10	11.140	3380	3412	3443	rBV	318846	821338	37.68%	3.548%
11	11.746	3617	3638	3665	rBV	1030337	1884648	86.45%	8.141%
12	11.953	3697	3715	3738	rBV	321085	627818	28.80%	2.712%
13	12.283	3816	3838	3857	rBV	307651	538564	24.71%	2.326%
14	12.733	3990	4006	4029	rVB2	811581	1415018	64.91%	6.113%
15	12.985	4086	4100	4108	rBV	295342	511114	23.45%	2.208%
16	13.061	4120	4128	4142	rVB	194624	323897	14.86%	1.399%
17	13.224	4175	4189	4203	rBV	215331	359193	16.48%	1.552%
18	13.369	4229	4243	4265	rBV	680654	1110735	50.95%	4.798%
19	13.503	4280	4293	4303	rVB3	16396	27311	1.25%	0.118%
20	13.562	4303	4315	4325	rBV2	51098	80204	3.68%	0.346%
21	13.616	4325	4335	4343	rBV2	26887	40135	1.84%	0.173%
22	13.677	4343	4358	4367	rBV	987890	1856839	85.18%	8.021%
23	13.876	4407	4432	4441	rBV3	340367	719901	33.02%	3.110%
24	13.999	4467	4478	4490	rBV6	73713	125069	5.74%	0.540%
25	14.072	4494	4505	4516	rVV	84465	134593	6.17%	0.581%
26	14.131	4516	4527	4533	rVV	119421	194045	8.90%	0.838%
27	14.160	4535	4538	4549	rVV	125216	150576	6.91%	0.650%
28	14.219	4549	4560	4571	rVB	158984	242053	11.10%	1.046%
29	14.284	4573	4584	4589	rBV3	40970	62676	2.88%	0.271%
30	14.329	4590	4601	4613	rVB2	194919	323475	14.84%	1.397%
31	14.461	4638	4650	4661	rBV3	77680	134545	6.17%	0.581%
32	14.544	4672	4681	4686	rVV2	88905	132769	6.09%	0.574%
33	14.581	4687	4695	4704	rVB	164060	236134	10.83%	1.020%
34	14.621	4705	4710	4719	rVB3	39724	50424	2.31%	0.218%
35	14.662	4720	4725	4744	rVB4	32495	54889	2.52%	0.237%
36	14.764	4745	4763	4770	rBV5	41945	80546	3.69%	0.348%

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37	14.812	4771	4781	4790	rBV	177725	294730	13.52%	1.273%
38	14.933	4807	4826	4839	rBV4	449029	1015472	46.58%	4.387%
39	15.085	4869	4883	4899	rBV	382383	661529	30.35%	2.858%
40	15.198	4915	4925	4933	rBV6	68479	124280	5.70%	0.537%
41	15.313	4955	4968	4985	rVB4	122405	289353	13.27%	1.250%
42	15.509	5034	5041	5050	rVB	45082	67670	3.10%	0.292%
43	15.566	5051	5062	5072	rBV2	87558	151474	6.95%	0.654%
44	15.646	5073	5092	5108	rBV5	66178	214698	9.85%	0.927%
45	15.807	5136	5152	5170	rBV2	86920	190976	8.76%	0.825%
46	16.019	5208	5231	5253	rVB3	229606	598095	27.44%	2.584%
47	16.349	5337	5354	5375	rBV3	148667	343911	15.78%	1.486%
48	16.553	5417	5430	5444	rVB5	62659	132262	6.07%	0.571%
49	16.620	5445	5455	5471	rBV5	31693	63738	2.92%	0.275%

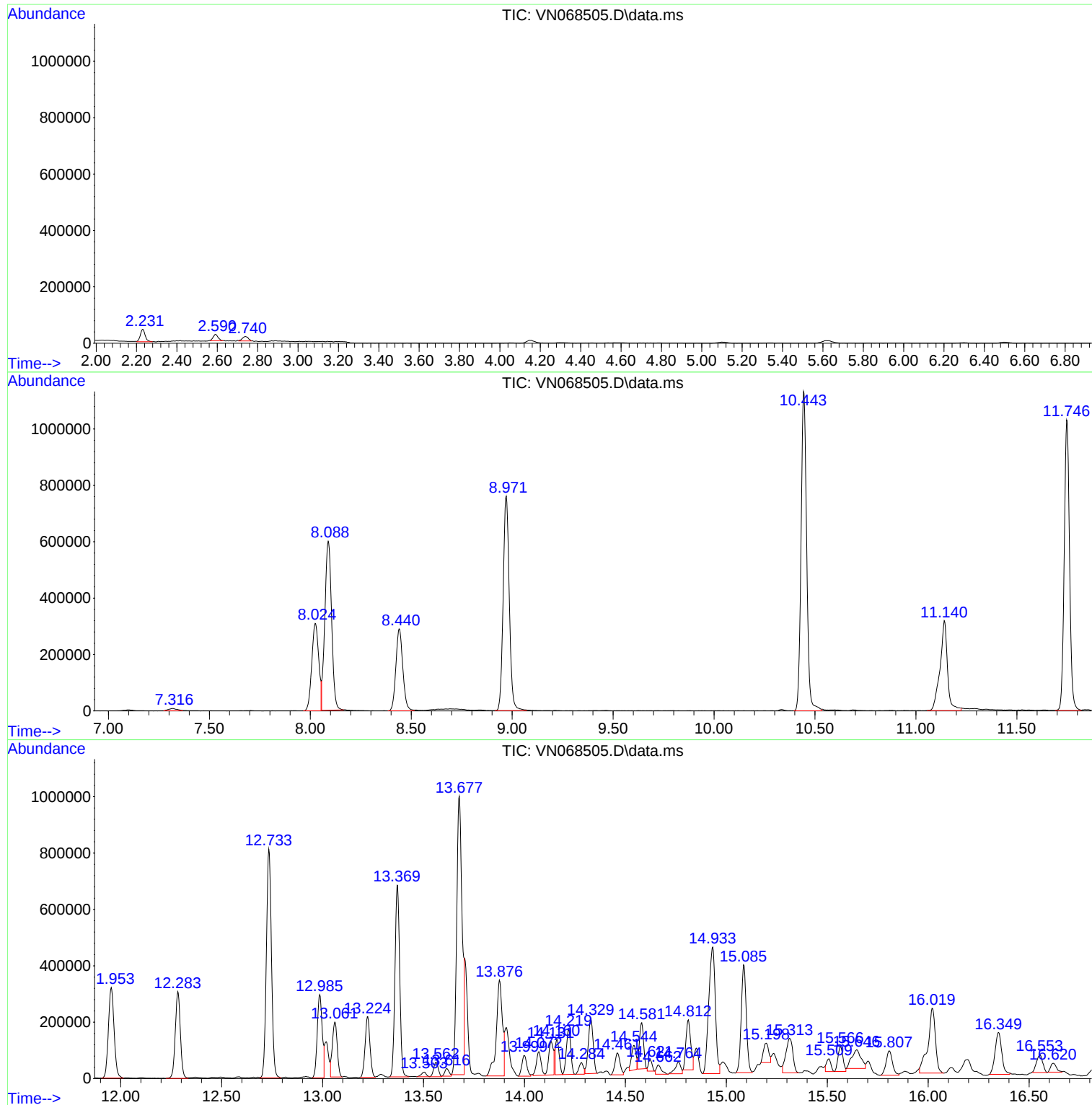
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Quant Title : SW846 8260

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



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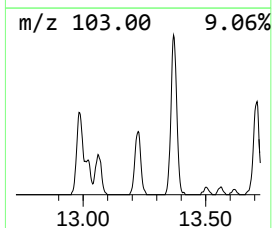
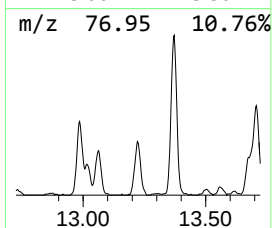
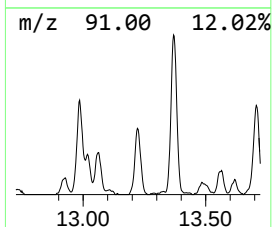
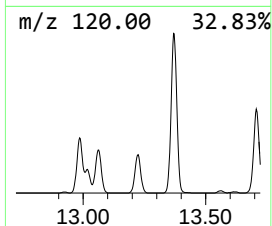
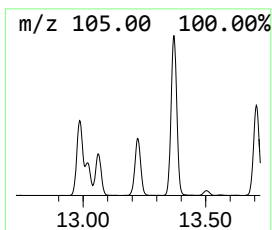
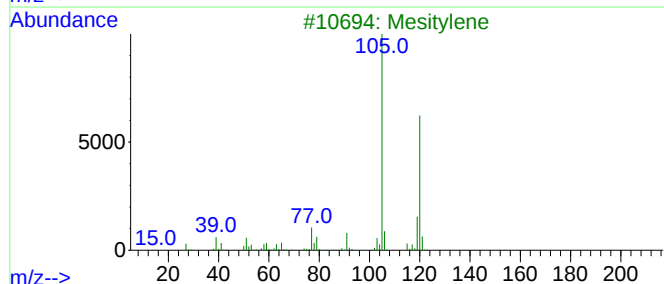
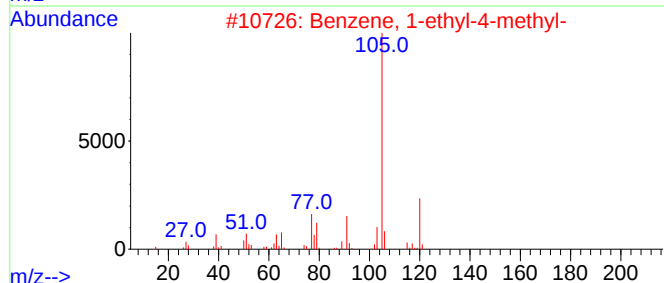
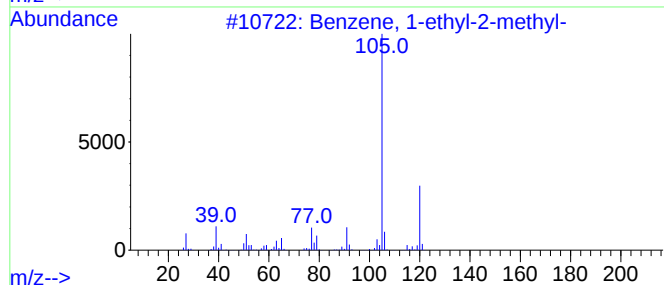
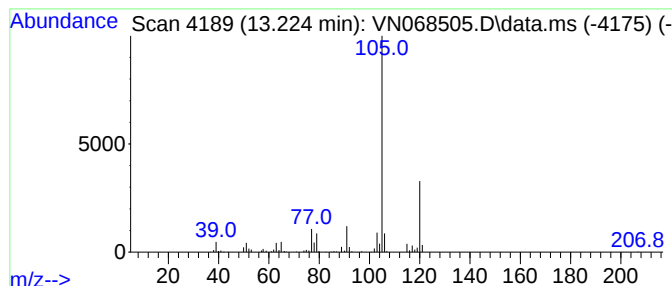
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.224	9.67 ug/l	359193	1,4-Dichlorobenzene-d4	13.677

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-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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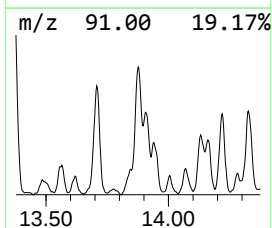
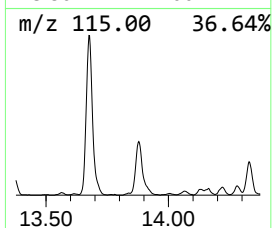
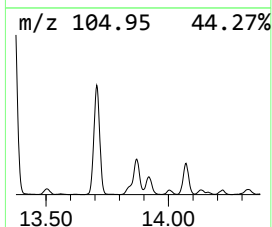
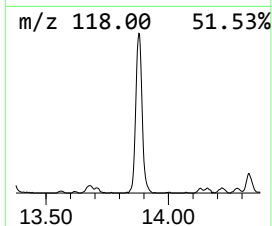
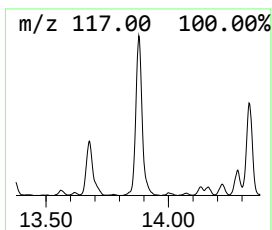
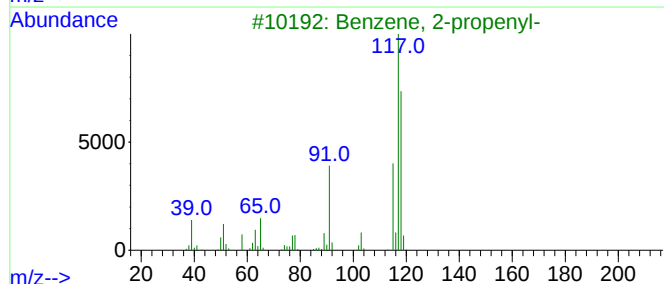
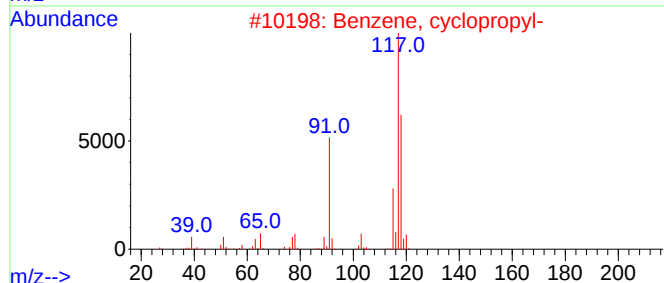
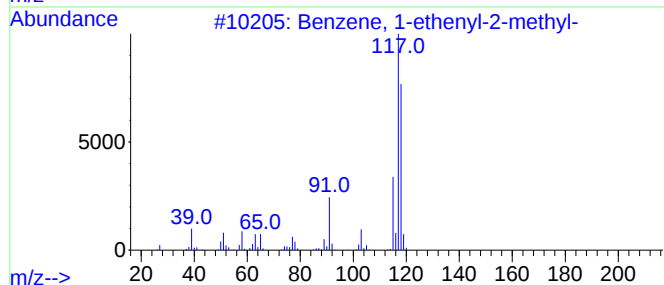
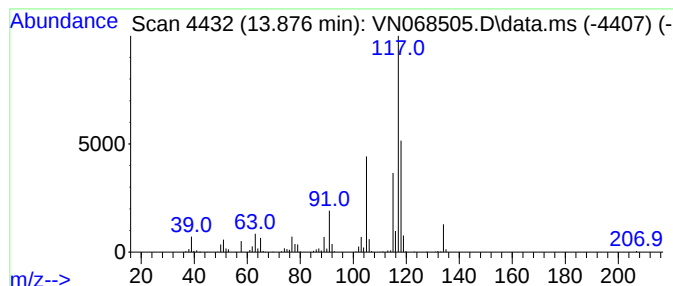
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethenyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	19.39 ug/l	719901	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	76
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	70



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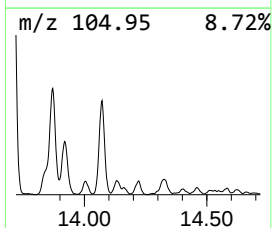
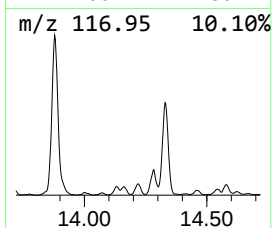
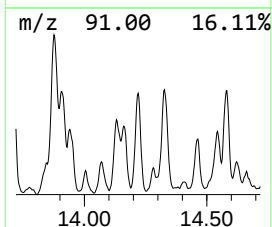
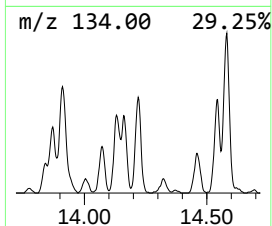
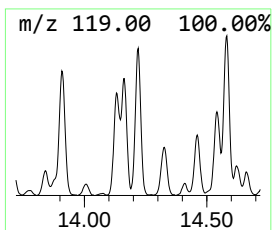
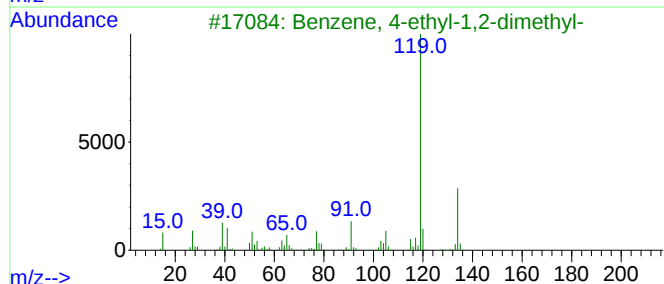
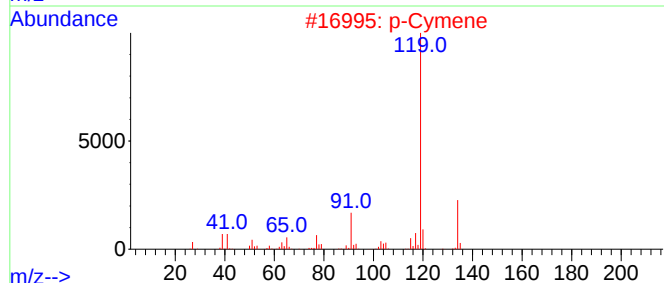
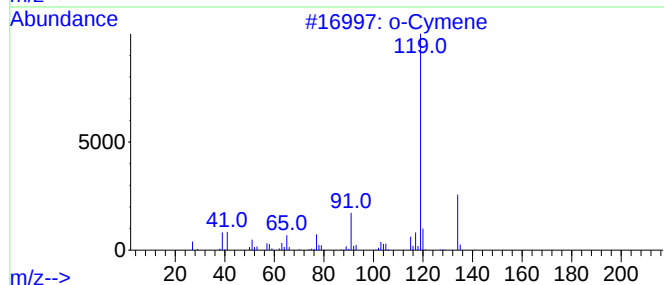
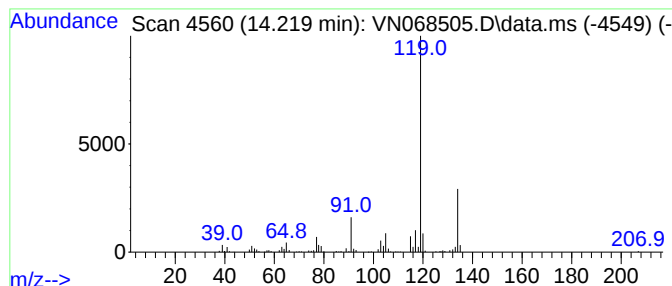
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 3 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	6.52 ug/l	242053	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	97
2			p-Cymene	134	C10H14	000099-87-6	95
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



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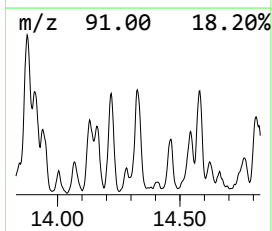
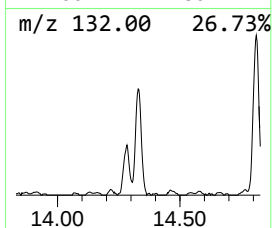
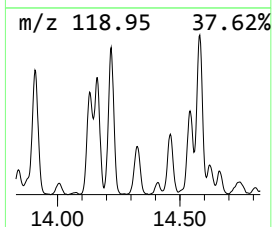
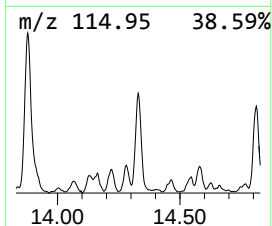
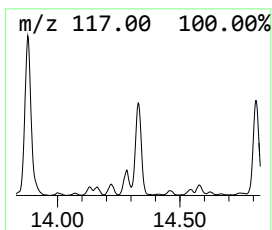
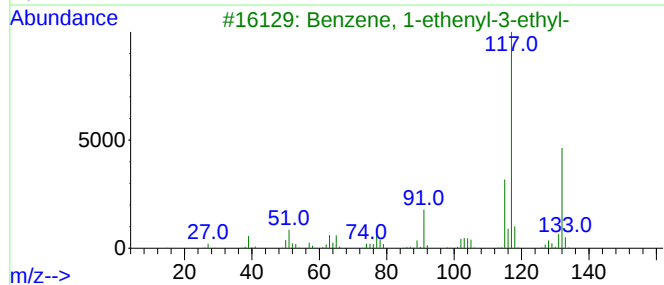
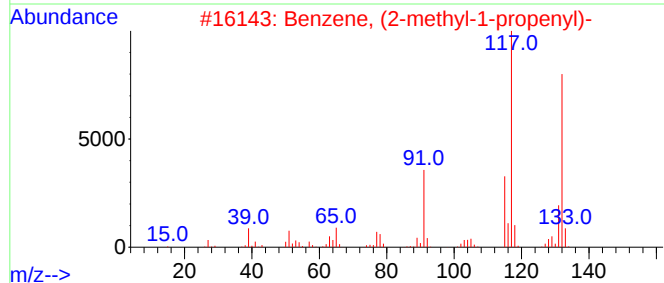
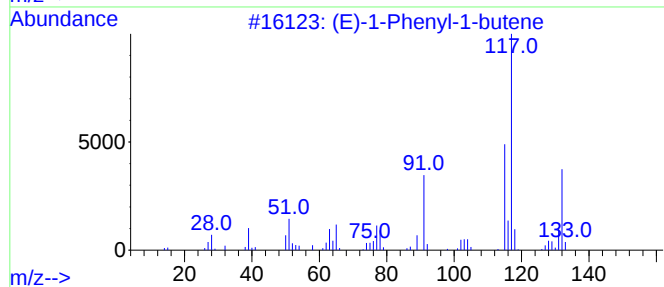
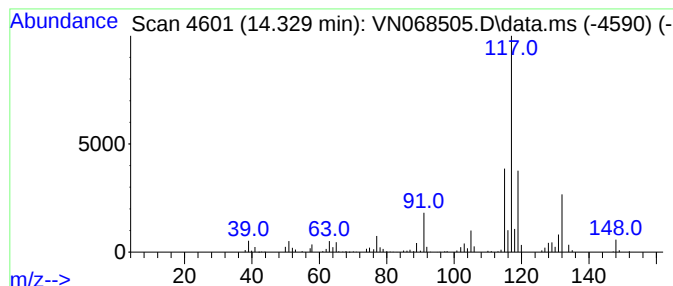
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 4 (E)-1-Phenyl-1-butene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	8.71 ug/l	323475	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	83
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	74
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	74
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	72
5			Indan, 1-methyl-	132	C10H12	000767-58-8	70



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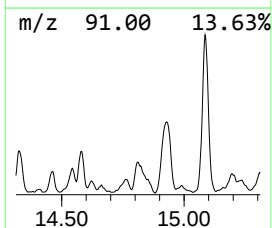
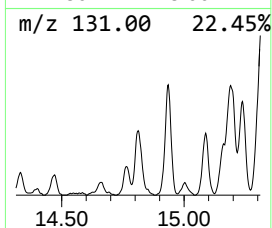
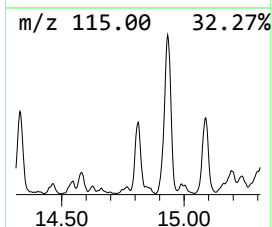
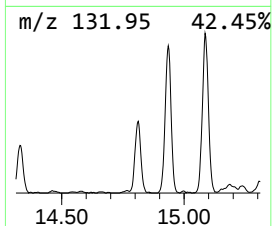
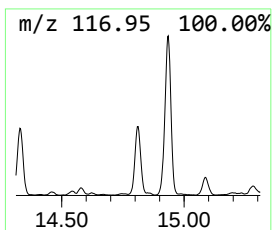
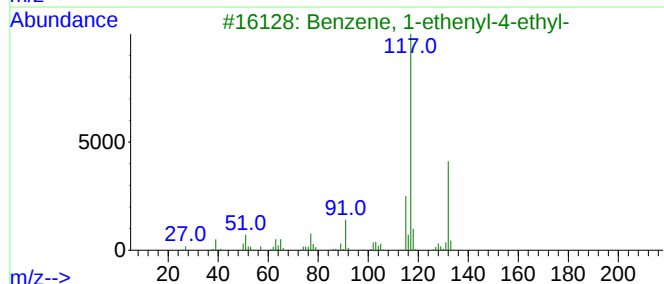
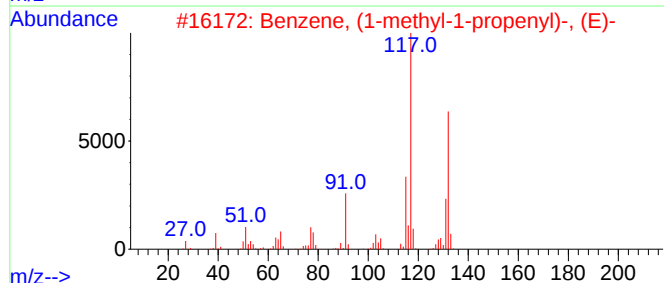
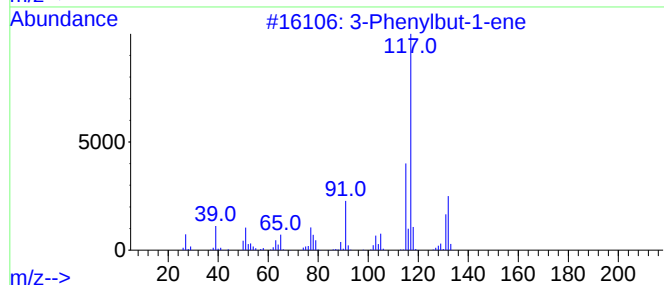
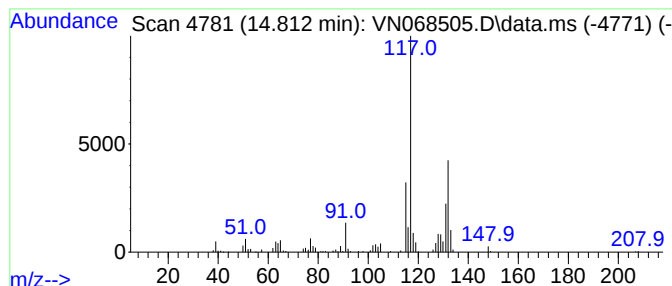
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Quant Title : SW846 8260

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

Peak Number 5 3-Phenylbut-1-ene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.812	7.94 ug/l	294730	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Phenylbut-1-ene	132	C10H12	000934-10-1	86
2			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	81
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	80
5			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068505.D
Acq On : 16 Sep 2021 19:35
Operator : JC/MD
Sample : M3759-19 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41094

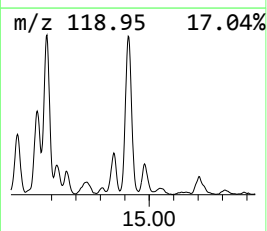
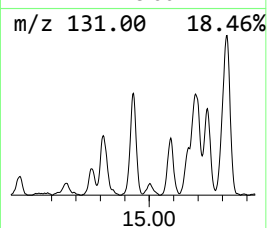
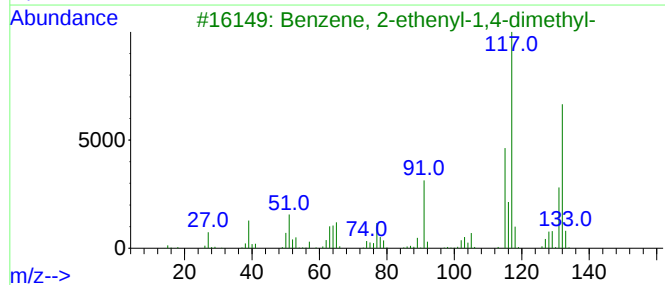
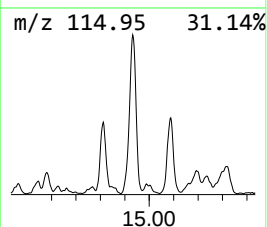
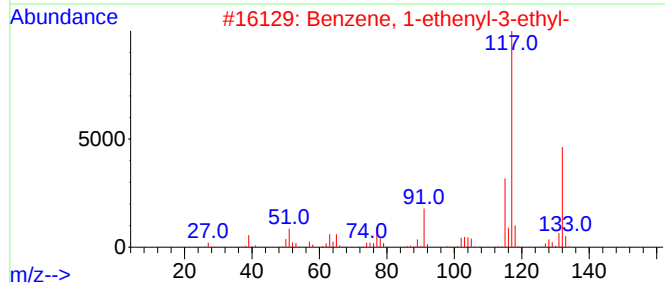
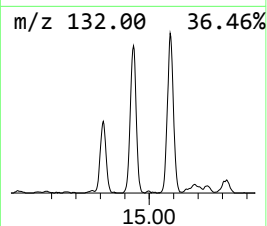
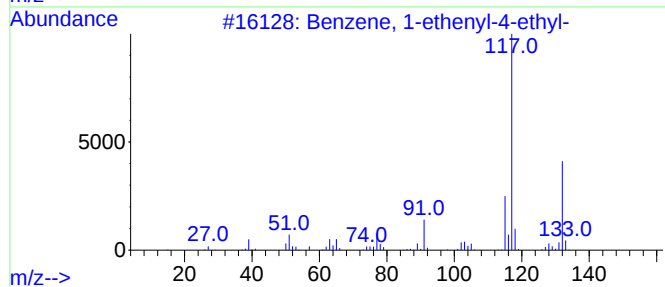
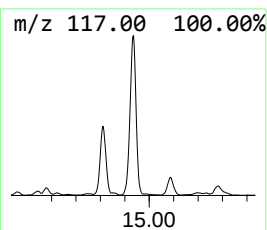
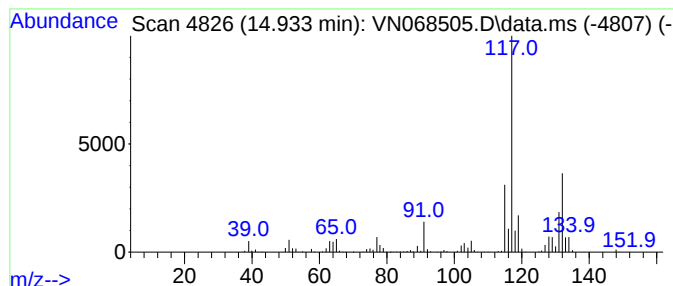
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	27.34 ug/l	1015470	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068505.D
Acq On : 16 Sep 2021 19:35
Operator : JC/MD
Sample : M3759-19 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41094

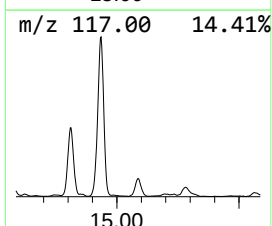
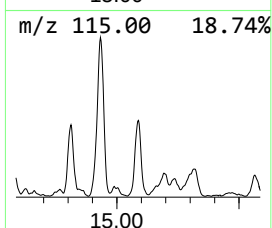
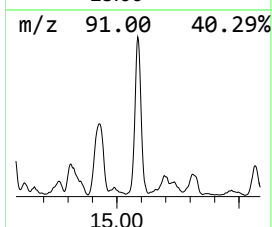
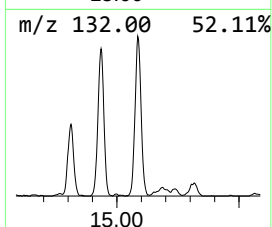
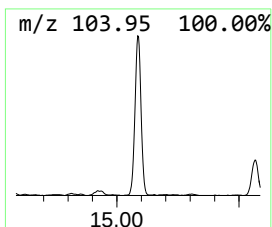
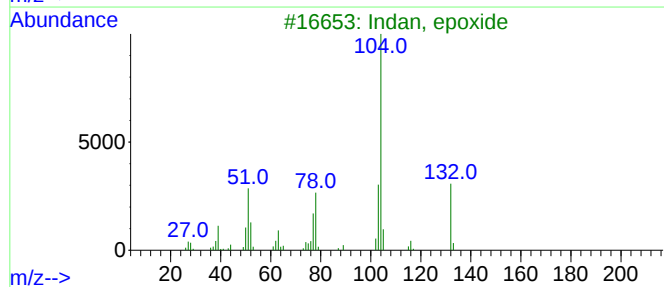
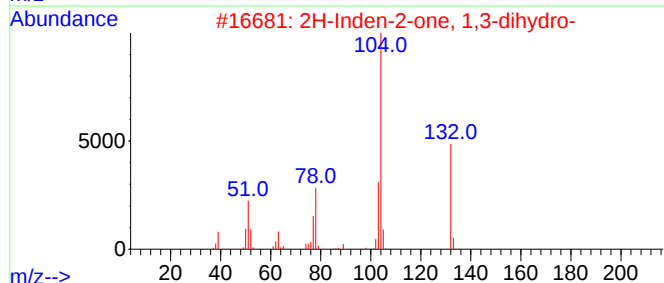
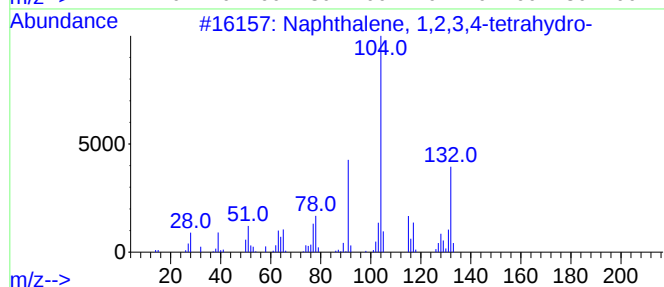
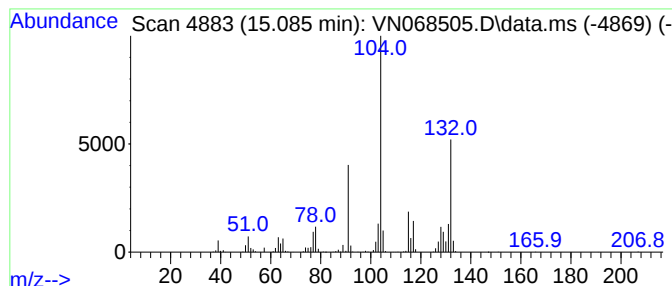
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	17.81 ug/l	661529	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	50
3			Indan, epoxide	132	C9H8O	000768-22-9	50
4			4-Cyanobenzoic acid, 2-phenyleth...	251	C16H13NO2	131786-46-4	35
5			Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068505.D
Acq On : 16 Sep 2021 19:35
Operator : JC/MD
Sample : M3759-19 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41094

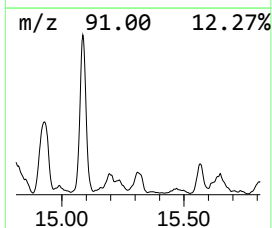
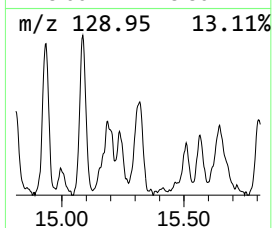
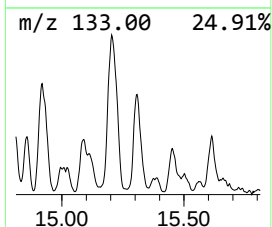
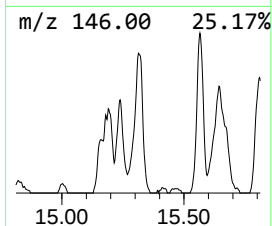
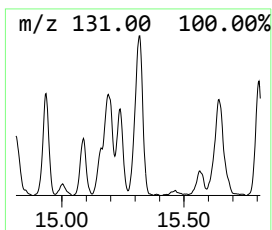
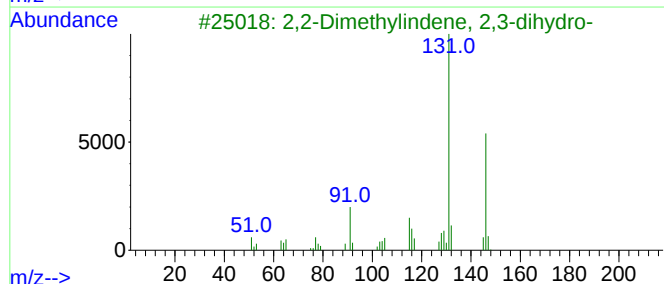
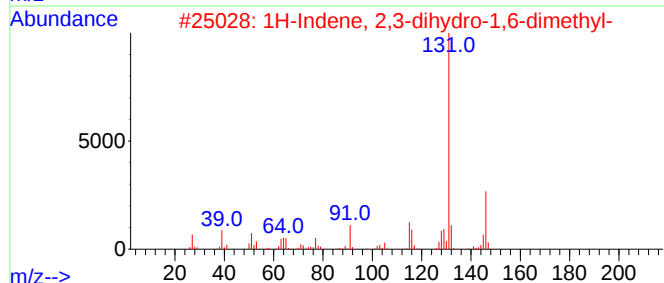
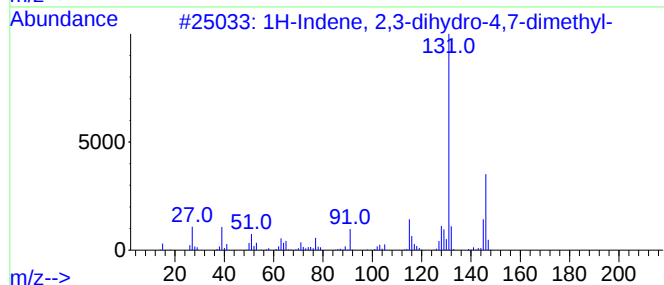
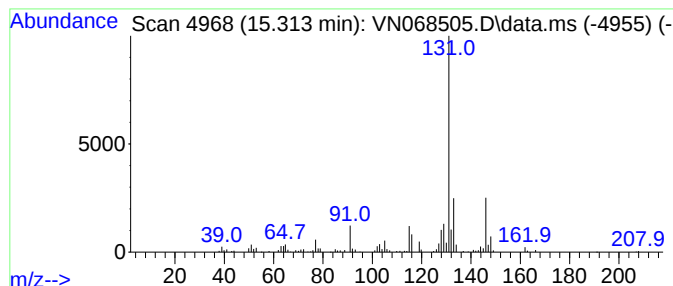
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.313	7.79 ug/l	289353	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90
2			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	90
3			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	81
4			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	81
5			1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068505.D
Acq On : 16 Sep 2021 19:35
Operator : JC/MD
Sample : M3759-19 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41094

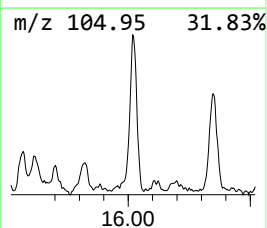
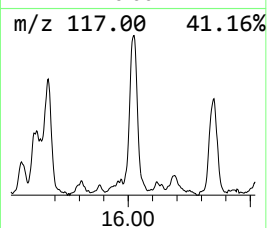
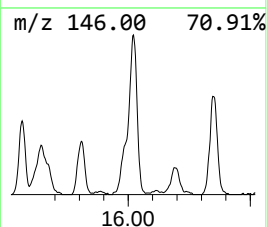
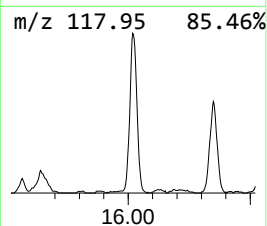
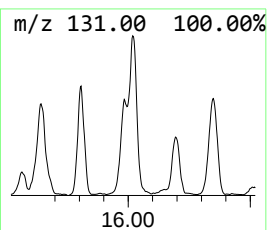
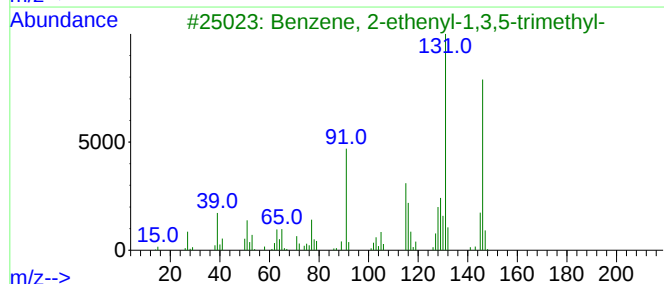
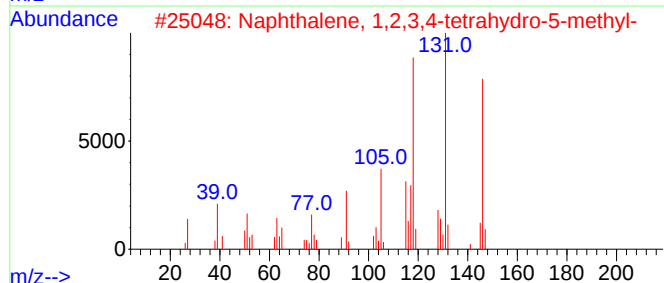
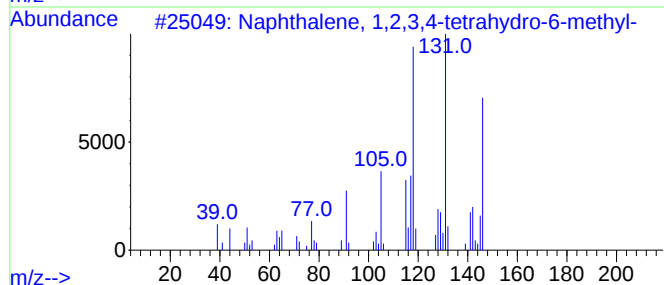
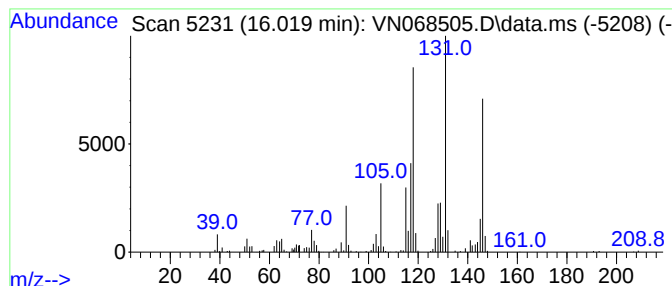
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.019	16.11 ug/l	598095	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
3			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	78
4			Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	55
5			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068505.D
Acq On : 16 Sep 2021 19:35
Operator : JC/MD
Sample : M3759-19 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41094

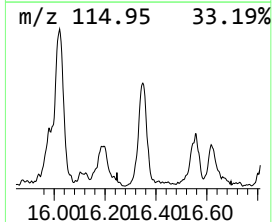
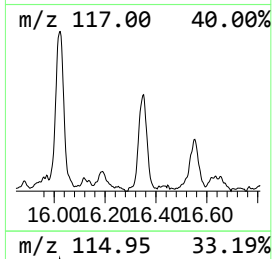
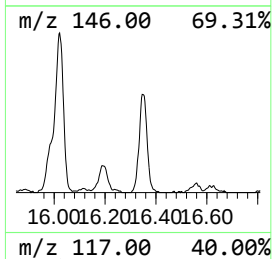
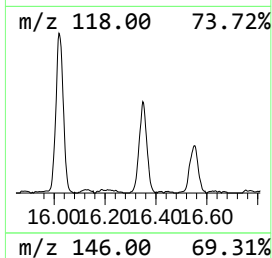
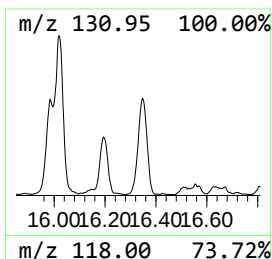
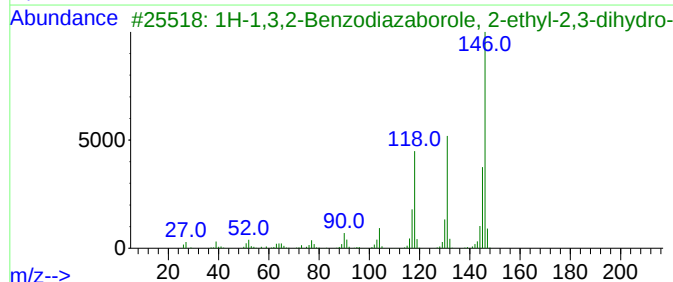
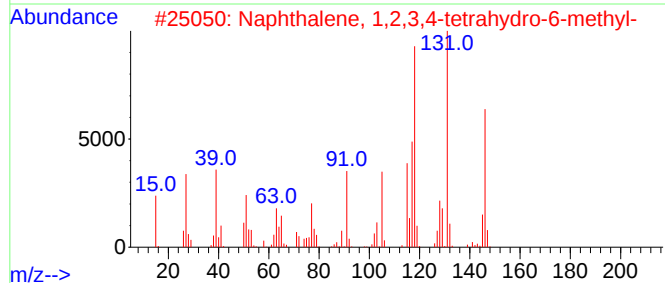
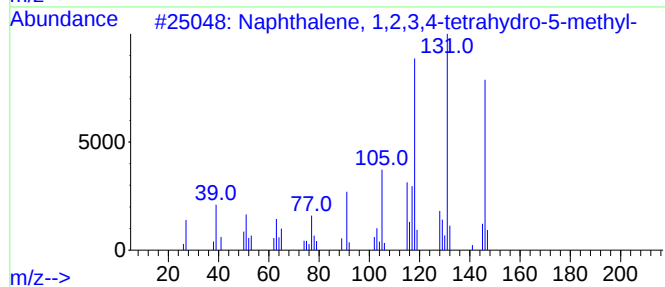
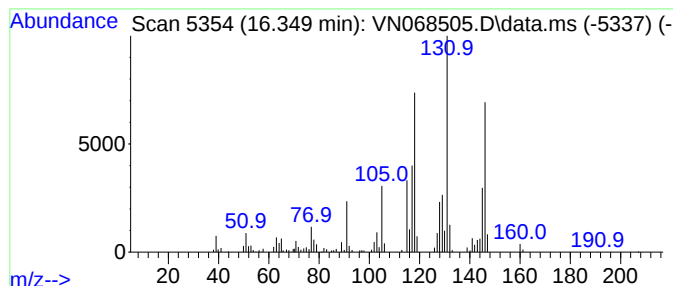
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.349	9.26 ug/l	343911	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	91
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	70
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091621\
Data File : VN068505.D
Acq On : 16 Sep 2021 19:35
Operator : JC/MD
Sample : M3759-19 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41094

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.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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Benzene, 1-ethe...	13.876	19.4	ug/l	719901	4	13.677	1856840	50.0
o-Cymene	14.219	6.5	ug/l	242053	4	13.677	1856840	50.0
(E)-1-Phenyl-1-...	14.329	8.7	ug/l	323475	4	13.677	1856840	50.0
3-Phenylbut-1-ene	14.812	7.9	ug/l	294730	4	13.677	1856840	50.0
Benzene, 1-ethe...	14.933	27.3	ug/l	1015470	4	13.677	1856840	50.0
Naphthalene, 1,...	15.086	17.8	ug/l	661529	4	13.677	1856840	50.0
1H-Indene, 2,3-...	15.313	7.8	ug/l	289353	4	13.677	1856840	50.0
Naphthalene, 1,...	16.019	16.1	ug/l	598095	4	13.677	1856840	50.0
Naphthalene, 1,...	16.349	9.3	ug/l	343911	4	13.677	1856840	50.0