

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
 Data File : VN070201.D
 Acq On : 18 Dec 2021 7:57
 Operator : JC/MD
 Sample : M5115-09
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-7

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN070201.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	80	92	109	rBV2	131458	328149	3.36%	0.419%
2	8.021	2226	2249	2260	rBV2	854888	2036436	20.83%	2.601%
3	8.086	2261	2273	2300	rVB	1497073	3400926	34.79%	4.343%
4	8.440	2383	2405	2432	rBV2	1013390	2365330	24.20%	3.021%
5	8.968	2580	2602	2642	rBV	2530948	5332419	54.55%	6.810%
6	10.443	3131	3152	3194	rBV	4142286	7879831	80.61%	10.063%
7	11.744	3618	3637	3664	rBV	4575852	8306043	84.97%	10.608%
8	12.578	3936	3948	3962	rVB2	127241	215561	2.21%	0.275%
9	12.731	3988	4005	4027	rBV	3747594	6629600	67.82%	8.467%
10	13.501	4279	4292	4304	rBV3	125645	221569	2.27%	0.283%
11	13.675	4340	4357	4378	rBV	4288418	7449839	76.21%	9.514%
12	13.772	4382	4393	4403	rVV	159381	270434	2.77%	0.345%
13	13.839	4405	4418	4421	rVV	718316	1004829	10.28%	1.283%
14	13.876	4421	4432	4465	rVV	5513342	9775691	100.00%	12.484%
15	14.002	4466	4479	4492	rVB2	230085	387448	3.96%	0.495%
16	14.214	4548	4558	4568	rBV3	97003	151205	1.55%	0.193%
17	14.278	4569	4582	4590	rBV	593968	1024834	10.48%	1.309%
18	14.327	4590	4600	4615	rVB	1853566	3142559	32.15%	4.013%
19	14.466	4640	4652	4661	rBV	187210	306013	3.13%	0.391%
20	14.539	4671	4679	4698	rVB2	278441	502184	5.14%	0.641%
21	14.622	4700	4710	4715	rBV3	97919	149395	1.53%	0.191%
22	14.657	4716	4723	4731	rVV	124080	165837	1.70%	0.212%
23	14.761	4749	4762	4772	rBV2	209115	346208	3.54%	0.442%
24	14.818	4772	4783	4795	rBV6	234275	438765	4.49%	0.560%
25	14.933	4810	4826	4839	rBV	1621627	2815306	28.80%	3.595%
26	14.997	4840	4850	4861	rVB4	190417	319327	3.27%	0.408%
27	15.080	4873	4881	4892	rVB3	116326	169926	1.74%	0.217%
28	15.193	4911	4923	4931	rBV3	365804	656729	6.72%	0.839%
29	15.236	4932	4939	4949	rVV2	394055	695501	7.11%	0.888%
30	15.314	4952	4968	4986	rVB	1214916	2934148	30.01%	3.747%
31	15.464	5015	5024	5037	rVB3	88510	145083	1.48%	0.185%
32	15.560	5047	5060	5071	rBV	387726	748836	7.66%	0.956%
33	15.641	5073	5090	5134	rVB3	677938	2284653	23.37%	2.918%
34	15.804	5135	5151	5166	rBV2	288634	625708	6.40%	0.799%
35	15.976	5197	5215	5237	rBV4	363100	1049510	10.74%	1.340%
36	16.110	5253	5265	5277	rBV3	294979	595076	6.09%	0.760%

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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

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37	16.185	5279	5293	5308	rVB5	260028	668370	6.84%	0.854%
38	16.341	5332	5351	5378	rBV4	631867	1584621	16.21%	2.024%
39	16.547	5406	5428	5442	rBV4	356386	947800	9.70%	1.210%
40	16.614	5444	5453	5464	rVB4	121723	231785	2.37%	0.296%

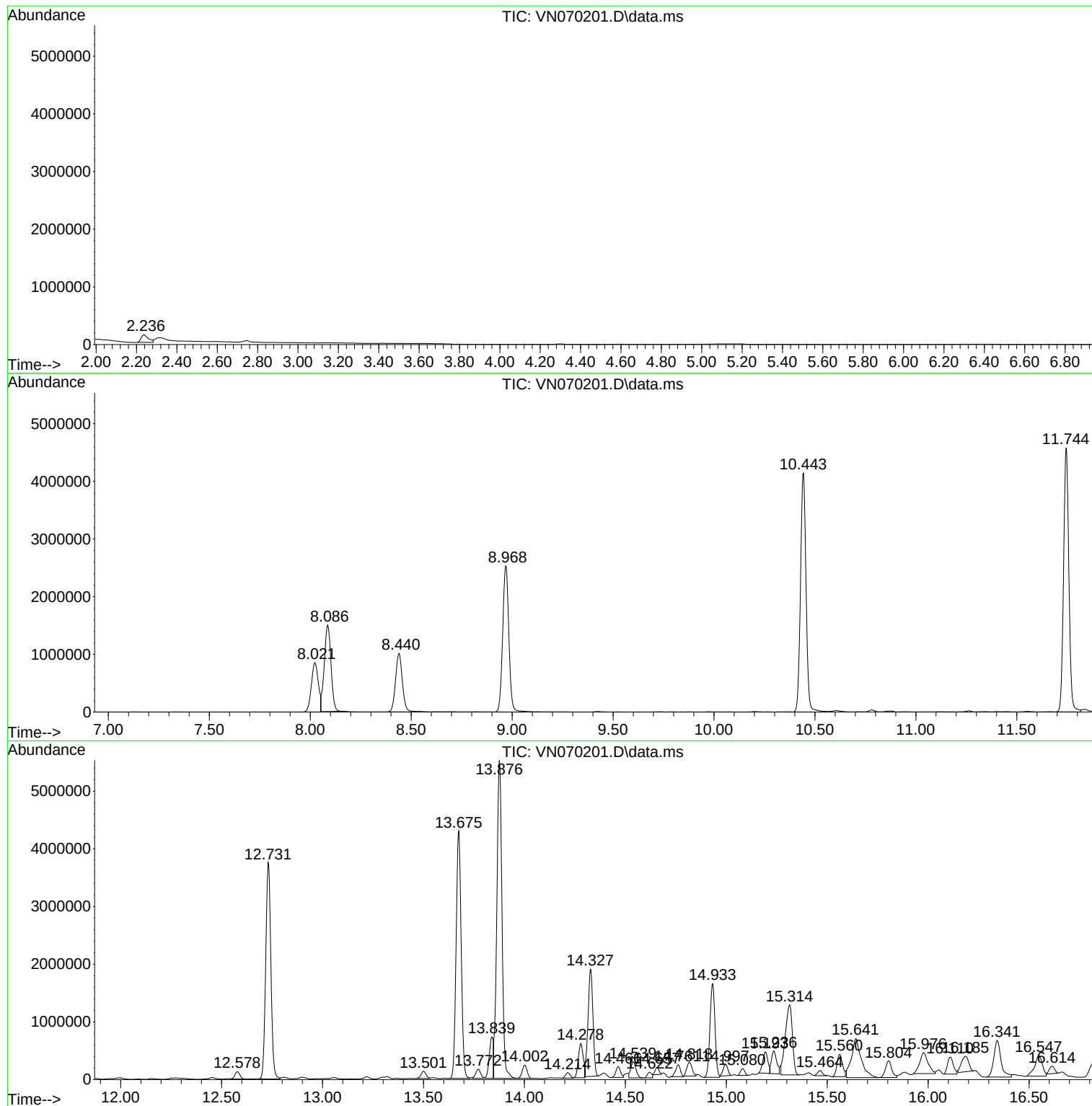
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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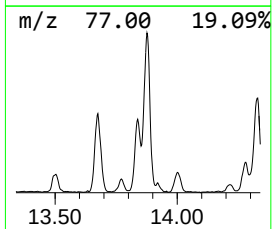
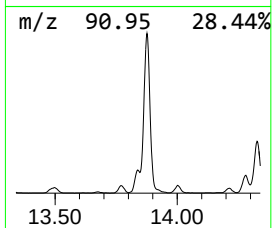
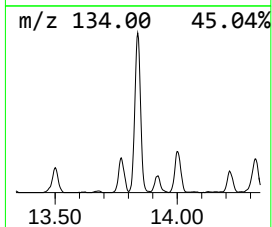
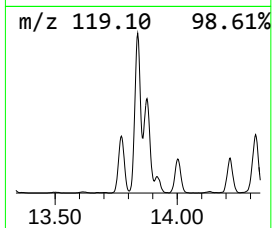
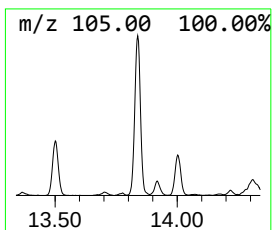
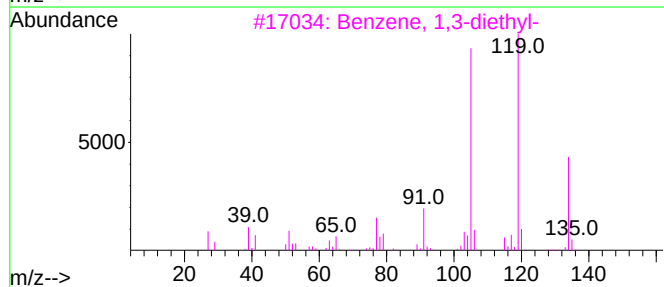
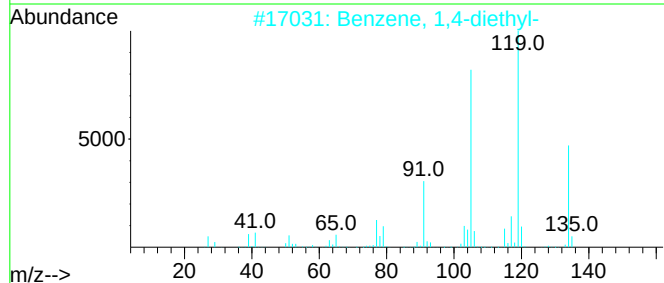
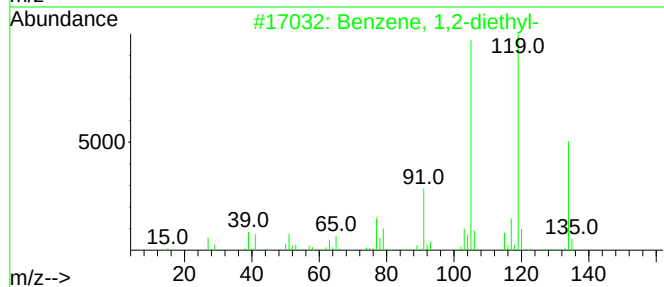
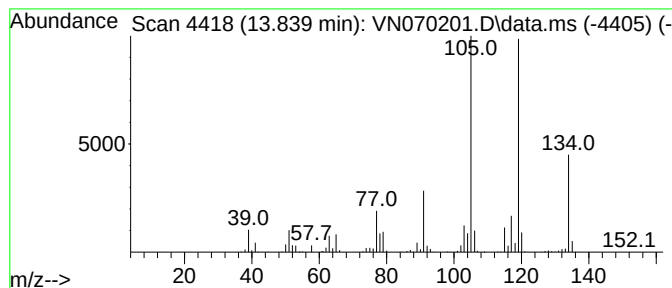
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1,2-diethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	6.74 ug/l	1004830	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	81
5			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	76



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Instrument :
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ClientSampleId :
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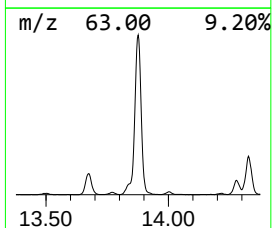
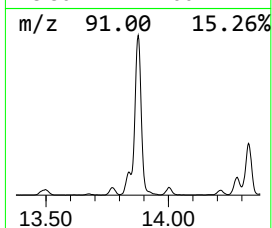
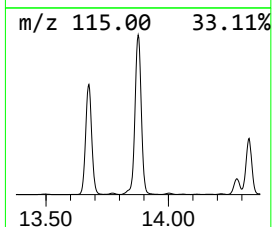
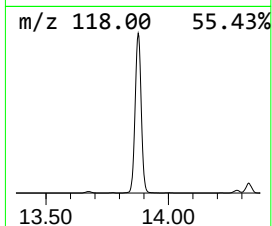
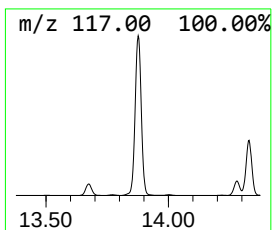
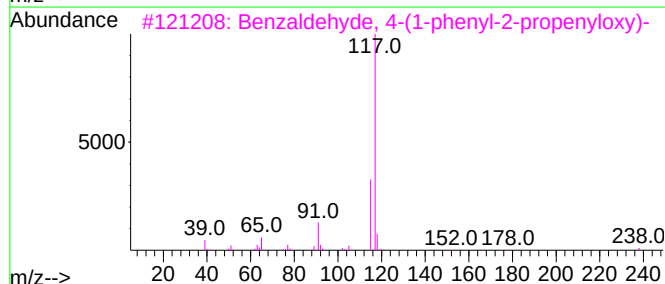
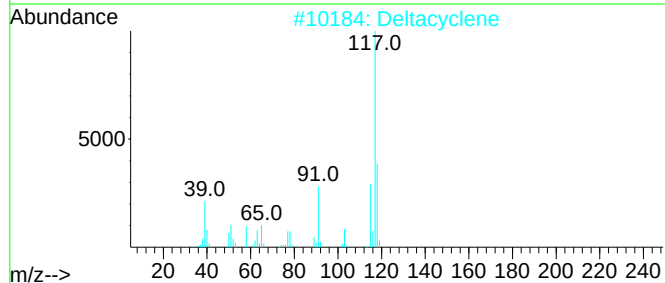
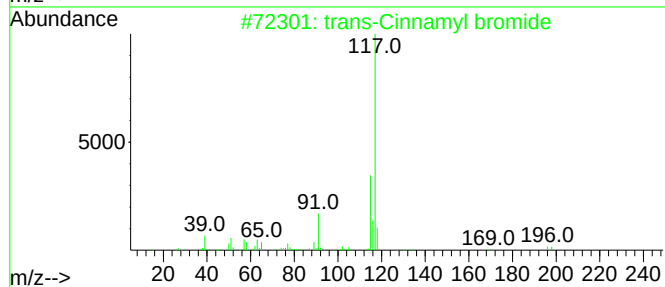
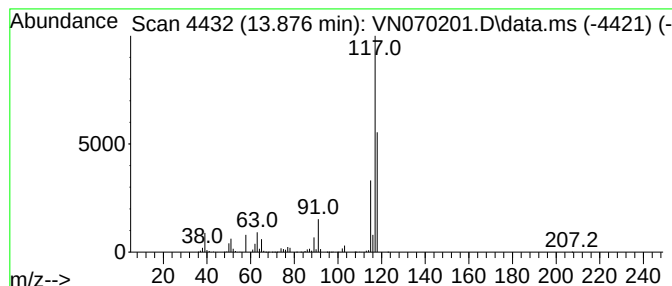
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 trans-Cinnamyl bromide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	65.61 ug/l	9775690	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
2			Deltacyclene	118	C9H10	007785-10-6	53
3			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50
4			Indole	117	C8H7N	000120-72-9	49
5			4-Ethynylaniline	117	C8H7N	014235-81-5	47



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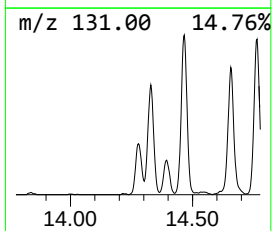
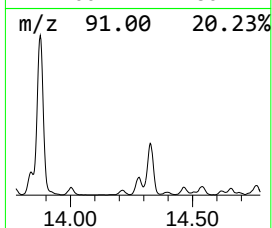
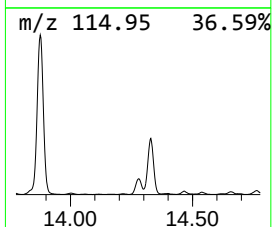
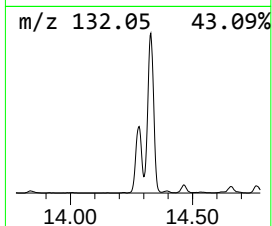
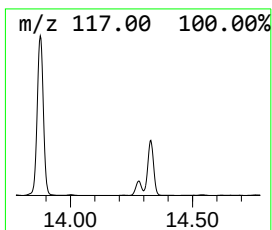
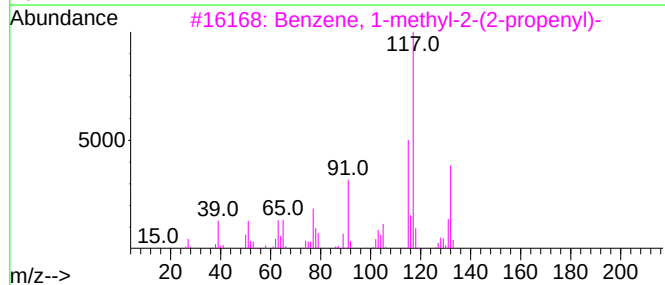
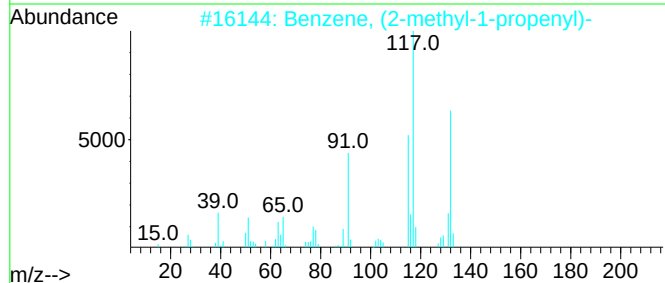
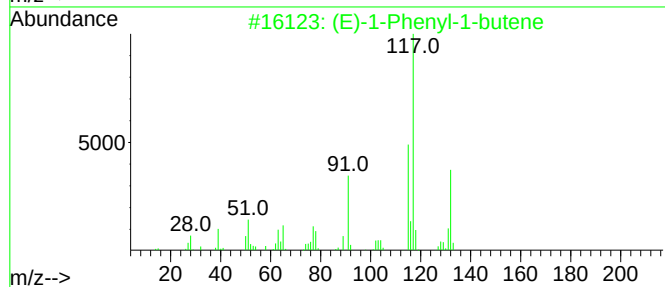
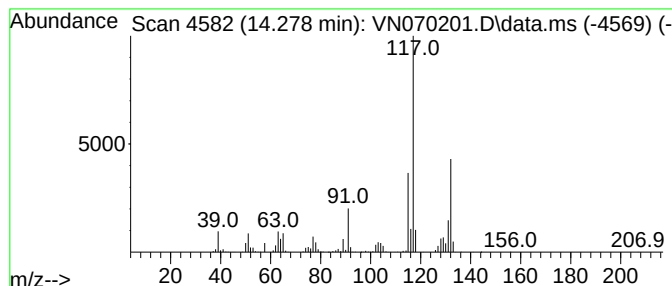
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 3 (E)-1-Phenyl-1-butene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.278	6.88 ug/l	1024830	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	95
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	95
3			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	94
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	94
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	93



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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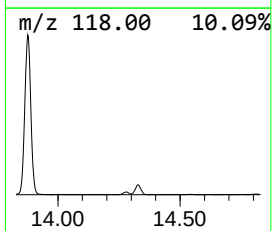
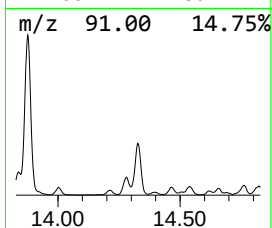
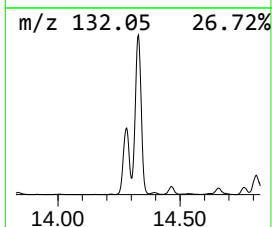
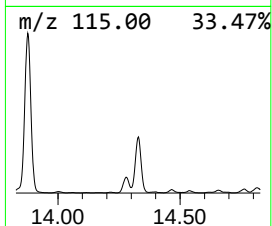
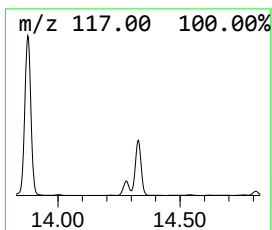
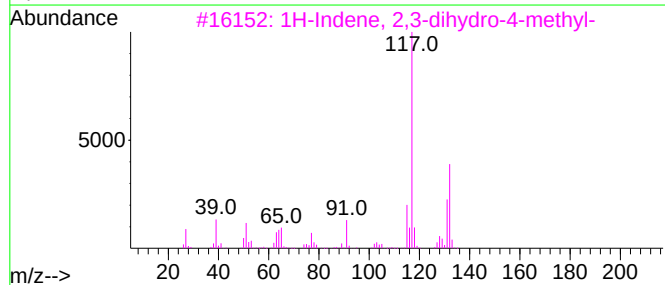
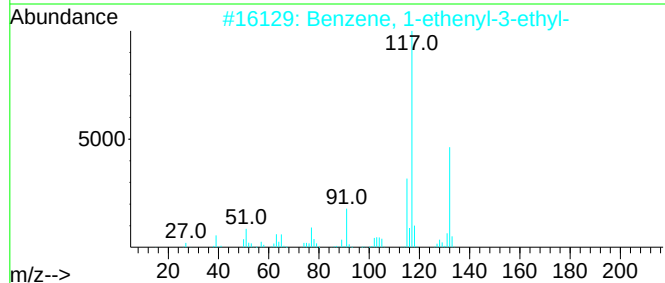
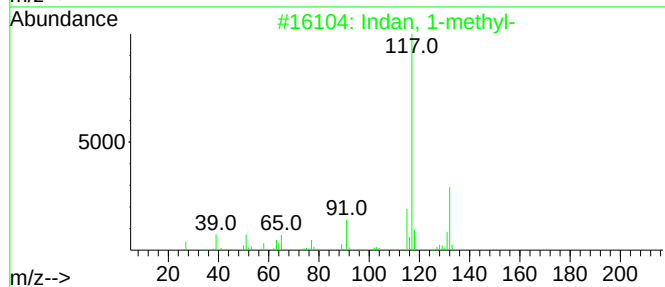
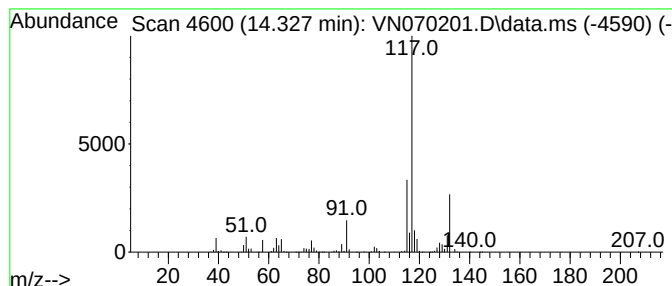
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	21.09 ug/l	3142560	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	86
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	80



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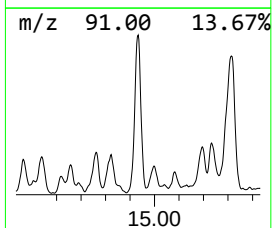
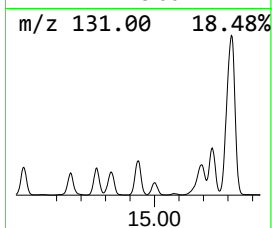
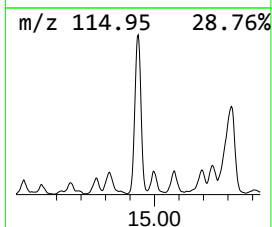
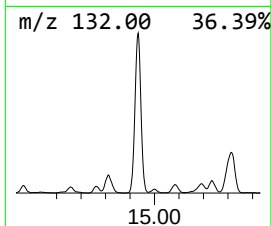
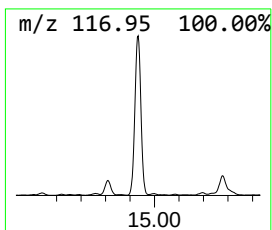
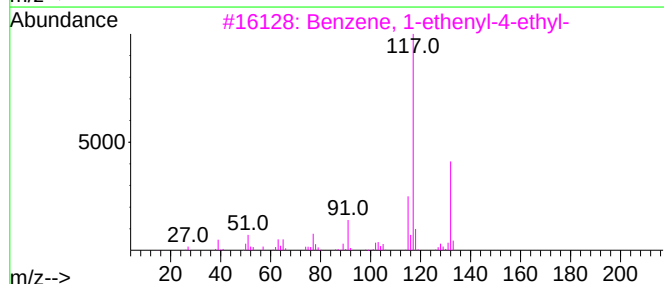
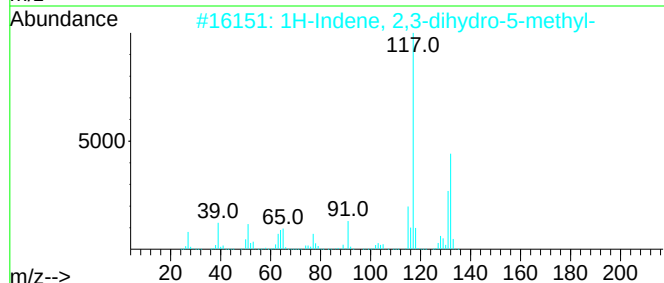
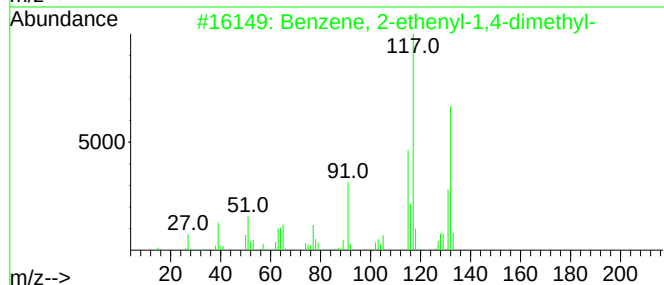
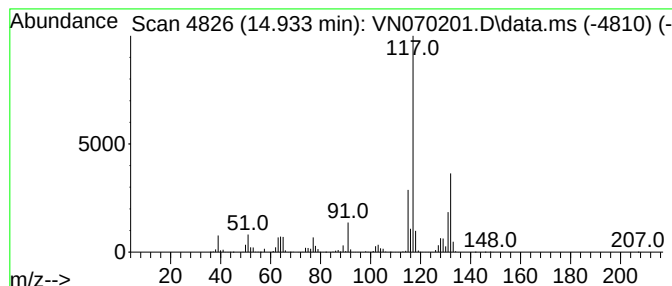
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	18.90 ug/l	2815310	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	95
3			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070201.D
Acq On : 18 Dec 2021 7:57
Operator : JC/MD
Sample : M5115-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

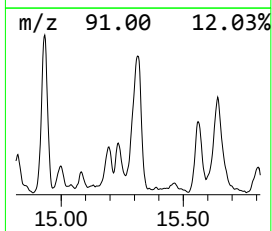
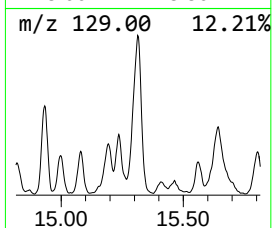
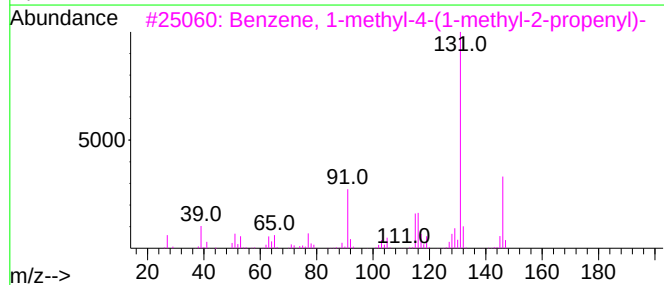
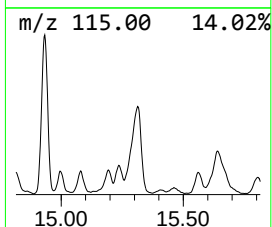
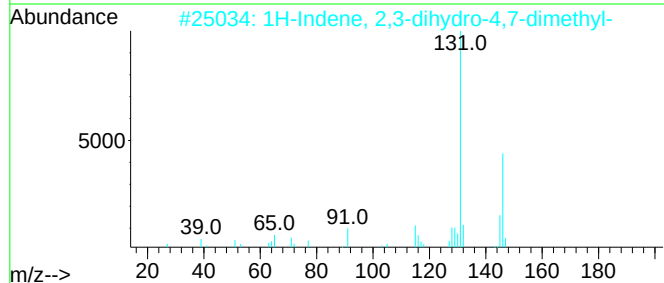
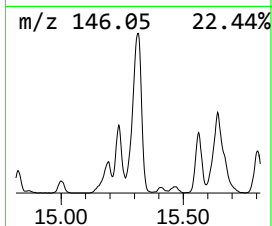
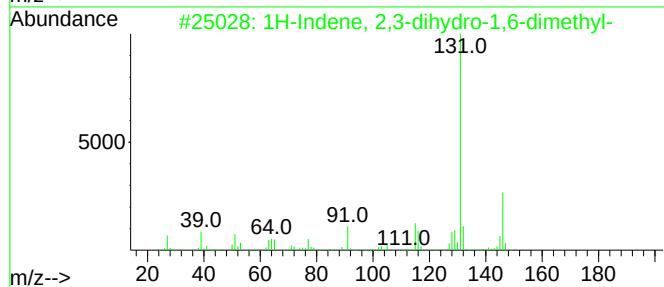
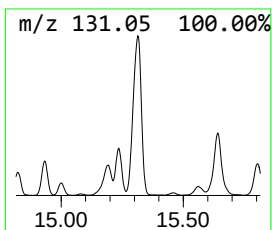
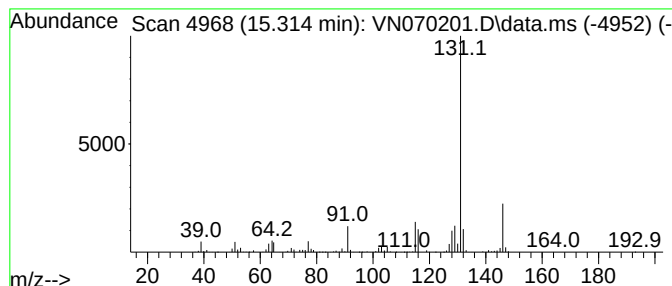
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.314	19.69 ug/l	2934150	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94		
2	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	91		
3	Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	91		
4	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	91		
5	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	91		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070201.D
Acq On : 18 Dec 2021 7:57
Operator : JC/MD
Sample : M5115-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

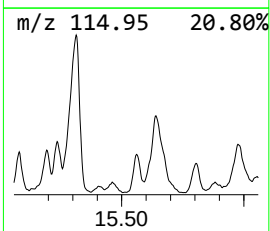
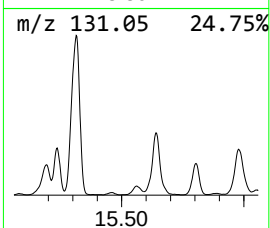
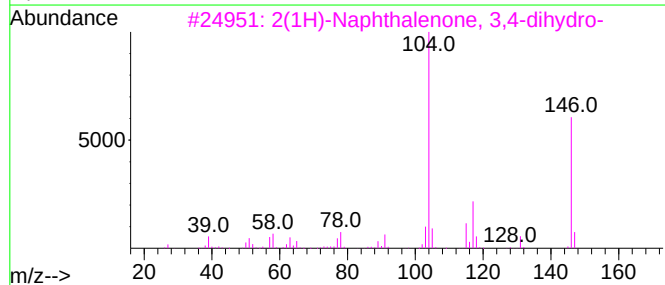
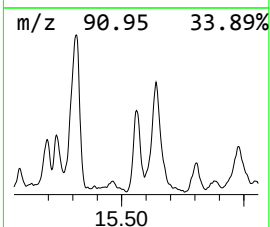
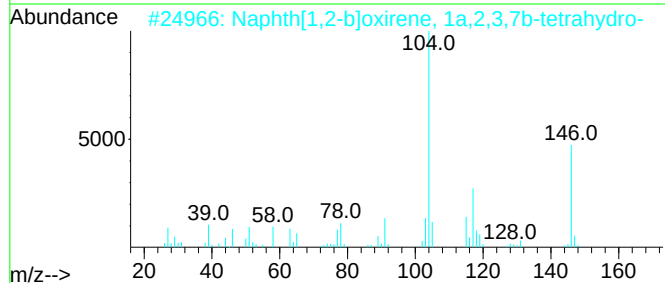
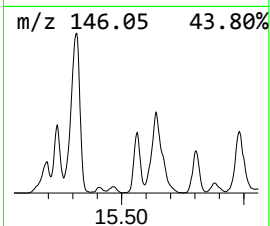
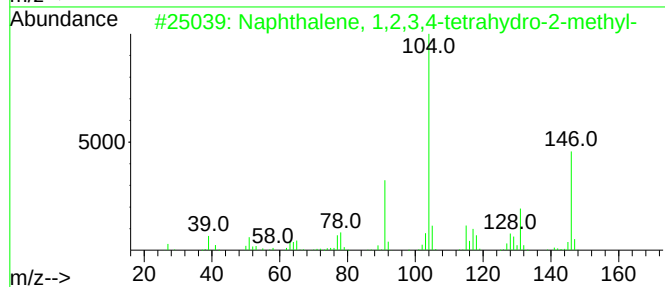
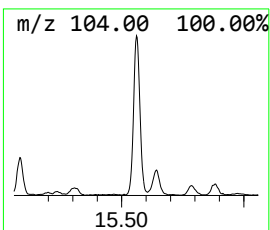
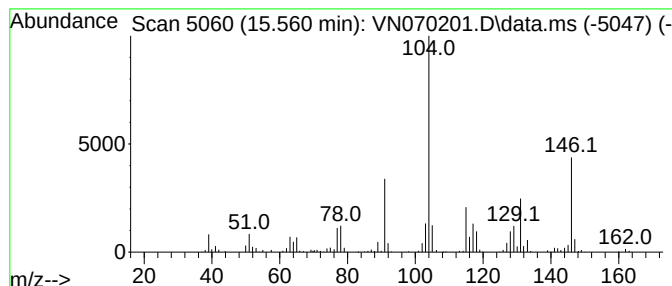
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.560	5.03 ug/l	748836	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	95
2			Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	70
3			2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	64
4			2-Azetidinone, 4-phenyl-	147	C9H9NO	005661-55-2	43
5			2-Furanone, 4-phenyltetrahydro	162	C10H10O2	1000197-38-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070201.D
Acq On : 18 Dec 2021 7:57
Operator : JC/MD
Sample : M5115-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

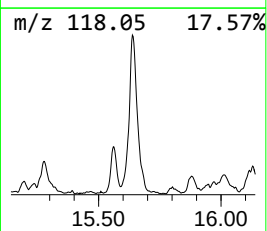
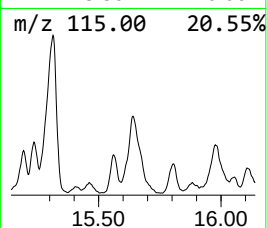
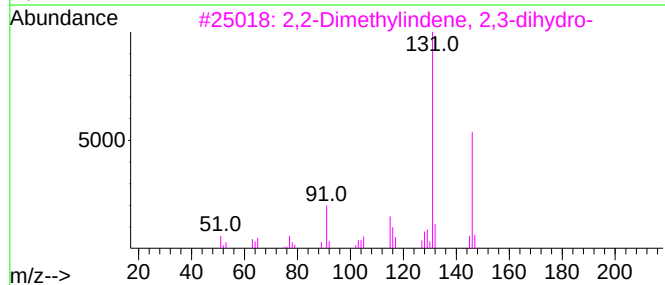
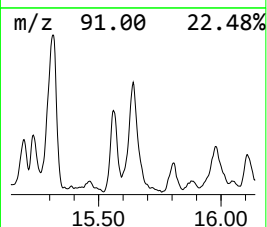
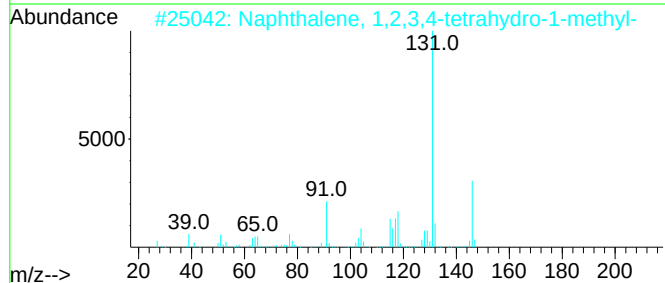
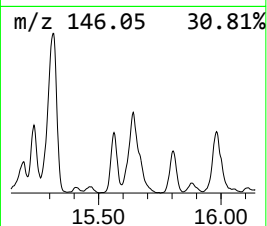
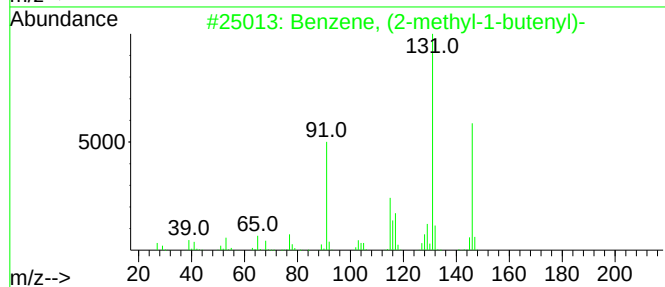
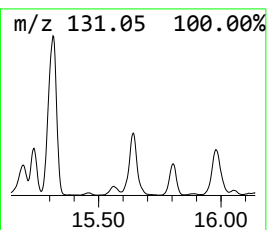
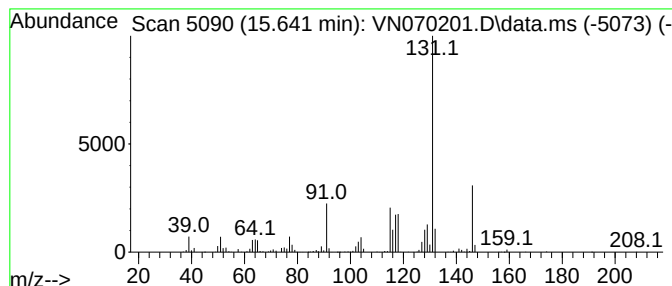
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, (2-methyl-1-butenyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.641	15.33 ug/l	2284650	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	93
3			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	93
4			Benzene, 1-methyl-2-(1-methyl-2-...	146	C11H14	097664-19-2	90
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070201.D
Acq On : 18 Dec 2021 7:57
Operator : JC/MD
Sample : M5115-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

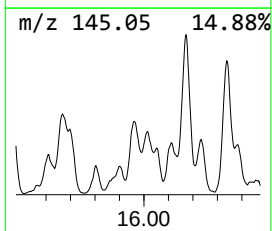
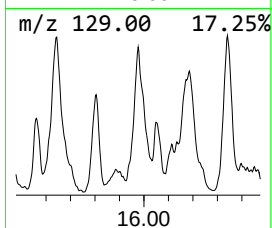
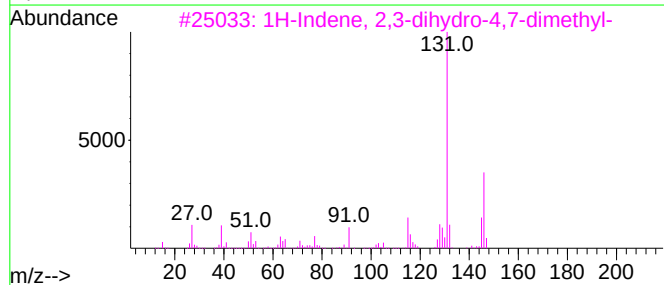
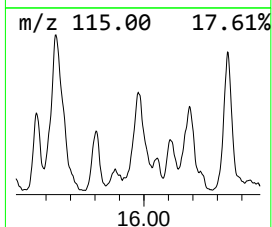
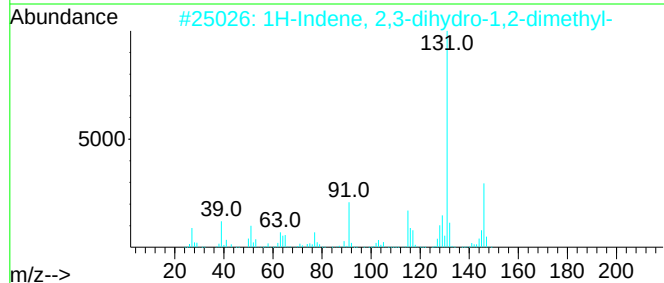
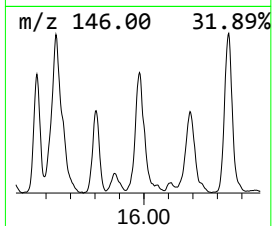
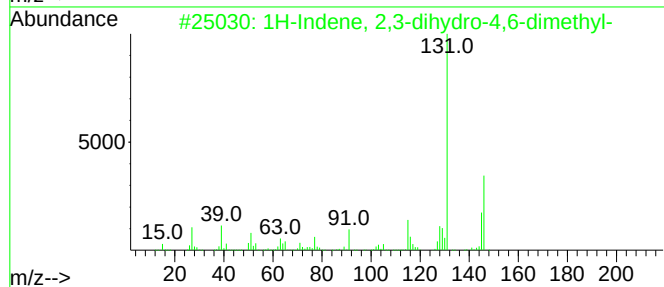
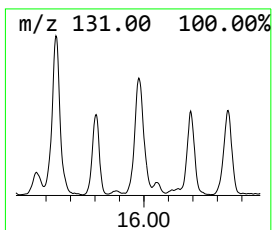
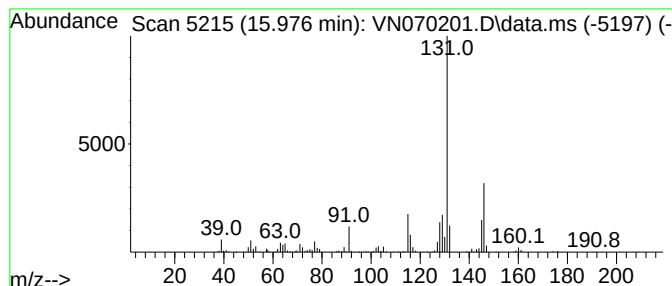
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Quant Title : SW846 8260

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

Peak Number 9 1H-Indene, 2,3-dihydro-4,6-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.976	7.04 ug/l	1049510	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	94		
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	91		
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	91		
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91		
5	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	91		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070201.D
Acq On : 18 Dec 2021 7:57
Operator : JC/MD
Sample : M5115-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

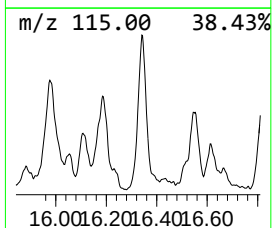
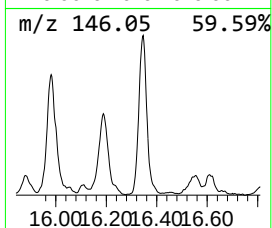
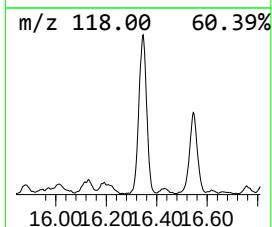
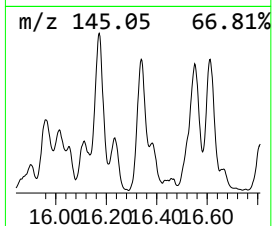
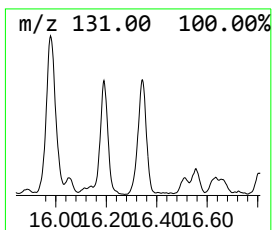
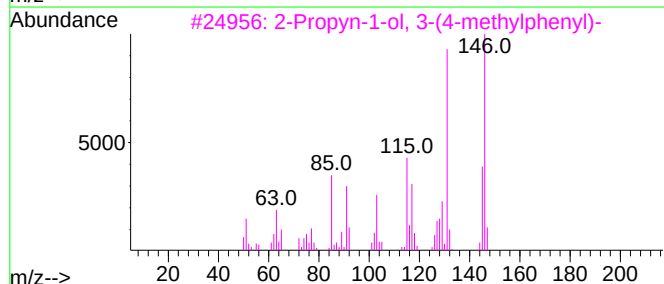
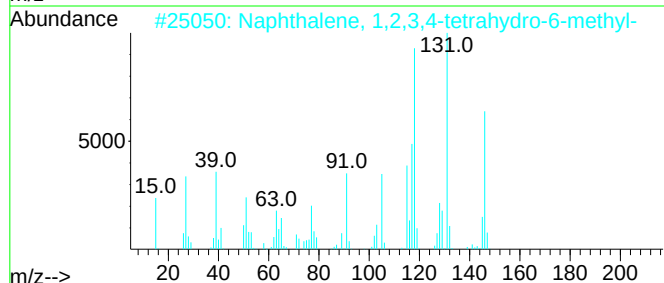
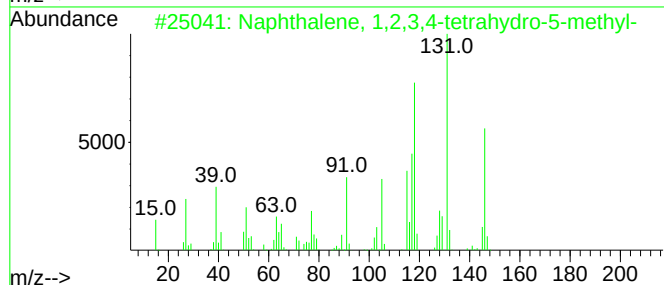
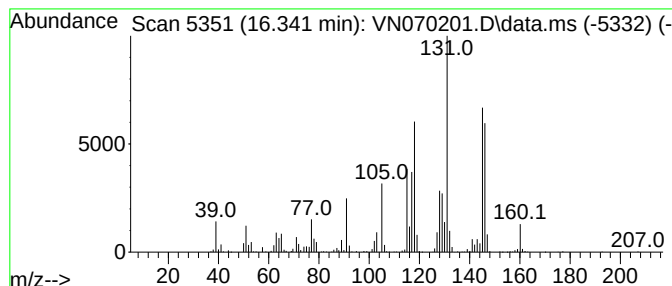
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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.
16.341	10.64 ug/l	1584620	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	81
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	70
3			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	68
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	64
5			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070201.D
Acq On : 18 Dec 2021 7:57
Operator : JC/MD
Sample : M5115-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

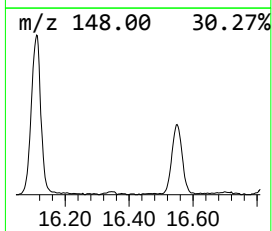
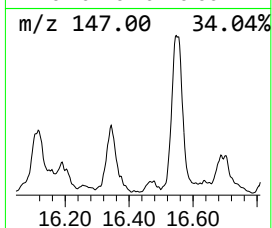
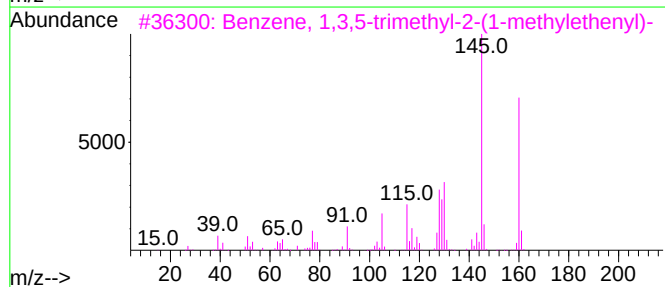
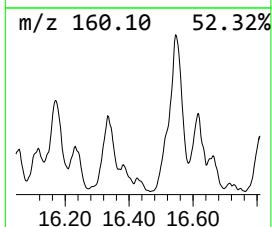
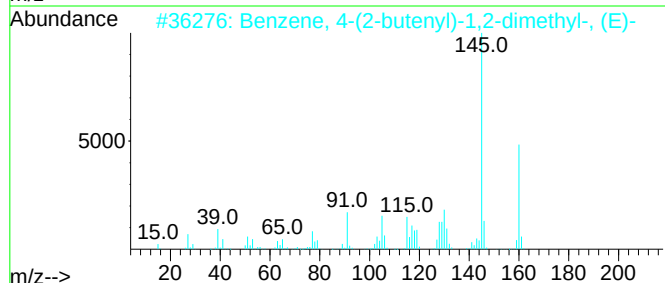
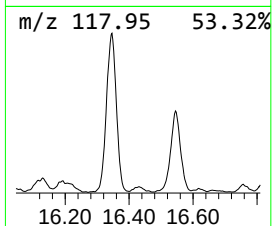
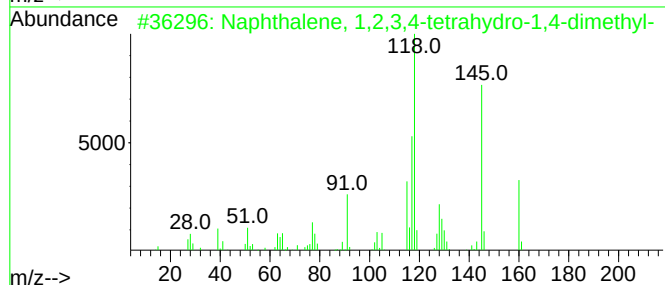
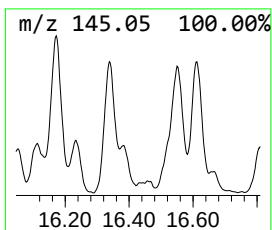
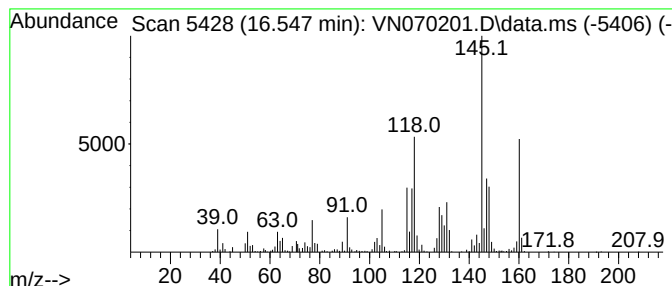
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Quant Title : SW846 8260

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

Peak Number 11 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.547	6.36 ug/l	947800	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	94
2			Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	83
3			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	70
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	70
5			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070201.D
Acq On : 18 Dec 2021 7:57
Operator : JC/MD
Sample : M5115-09
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 51 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.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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trans-Cinnamyl ...	13.876	65.6	ug/l	9775690	4	13.675	7449840	50.0
(E)-1-Phenyl-1-...	14.278	6.9	ug/l	1024830	4	13.675	7449840	50.0
Indan, 1-methyl-	14.327	21.1	ug/l	3142560	4	13.675	7449840	50.0
Benzene, 2-ethe...	14.933	18.9	ug/l	2815310	4	13.675	7449840	50.0
1H-Indene, 2,3-...	15.314	19.7	ug/l	2934150	4	13.675	7449840	50.0
Naphthalene, 1,...	15.560	5.0	ug/l	748836	4	13.675	7449840	50.0
Benzene, (2-met...	15.641	15.3	ug/l	2284650	4	13.675	7449840	50.0
1H-Indene, 2,3-...	15.976	7.0	ug/l	1049510	4	13.675	7449840	50.0
Naphthalene, 1,...	16.341	10.6	ug/l	1584620	4	13.675	7449840	50.0
Naphthalene, 1,...	16.547	6.4	ug/l	947800	4	13.675	7449840	50.0