

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
 Data File : VN067503.D
 Acq On : 25 Jun 2021 14:42
 Operator : JC/MD
 Sample : M2806-01 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-1

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\82N062421W.M
 Title : SW846 8260

Signal : TIC: VN067503.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	77	89	109	rBV3	48053	81260	2.68%	0.388%
2	8.024	2227	2250	2261	rBV2	207711	488840	16.10%	2.336%
3	8.086	2262	2273	2298	rVB2	359534	816085	26.88%	3.899%
4	8.440	2382	2405	2432	rBV2	284303	656087	21.61%	3.135%
5	8.968	2584	2602	2637	rBV	607318	1277902	42.09%	6.106%
6	10.443	3131	3152	3184	rBV	985316	1866090	61.47%	8.916%
7	11.746	3621	3638	3661	rBV	840053	1552376	51.13%	7.417%
8	11.846	3664	3675	3697	rVB4	36112	71557	2.36%	0.342%
9	11.966	3703	3720	3723	rBV4	22759	37898	1.25%	0.181%
10	12.256	3811	3828	3839	rBV5	30750	68639	2.26%	0.328%
11	12.310	3843	3848	3866	rVB8	14501	31604	1.04%	0.151%
12	12.457	3895	3903	3912	rVV3	34605	55182	1.82%	0.264%
13	12.583	3936	3950	3970	rVB	712501	1219491	40.17%	5.827%
14	12.733	3992	4006	4024	rBV	627307	1083001	35.67%	5.175%
15	12.814	4026	4036	4049	rBV5	31354	53615	1.77%	0.256%
16	12.924	4058	4077	4095	rBV	1119762	1940623	63.92%	9.272%
17	13.018	4102	4112	4121	rBV2	48326	76322	2.51%	0.365%
18	13.299	4205	4217	4218	rBV7	36709	46602	1.54%	0.223%
19	13.326	4219	4227	4231	rVV2	82465	126925	4.18%	0.606%
20	13.372	4231	4244	4263	rVB	1817991	3035930	100.00%	14.506%
21	13.500	4274	4292	4305	rBV4	255630	568783	18.74%	2.718%
22	13.677	4343	4358	4383	rVB3	699237	1492648	49.17%	7.132%
23	13.774	4383	4394	4406	rBV	116373	182543	6.01%	0.872%
24	13.841	4406	4419	4424	rBV	251387	395698	13.03%	1.891%
25	13.879	4425	4433	4444	rVB	608388	948562	31.24%	4.532%
26	14.005	4468	4480	4497	rVB3	142079	233157	7.68%	1.114%
27	14.133	4512	4528	4533	rBV	68747	116805	3.85%	0.558%
28	14.219	4548	4560	4572	rBV	385432	597019	19.67%	2.853%
29	14.281	4572	4583	4590	rVV2	103449	171256	5.64%	0.818%
30	14.329	4590	4601	4615	rVB3	378400	666692	21.96%	3.185%
31	14.466	4640	4652	4663	rBV3	54679	90217	2.97%	0.431%
32	14.541	4663	4680	4689	rVV	169122	302439	9.96%	1.445%
33	14.579	4690	4694	4705	rVB2	61414	80629	2.66%	0.385%
34	14.812	4771	4781	4792	rVV4	24019	37421	1.23%	0.179%
35	14.922	4807	4822	4840	rBV5	157811	353745	11.65%	1.690%
36	15.085	4872	4883	4895	rVB3	33518	55455	1.83%	0.265%

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Instrument :
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ClientSampleId :
MW-1

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\82N062421W.M
Title : SW846 8260

37	15.507	5028	5040	5052	rBV3	27115	50363	1.66%	0.241%
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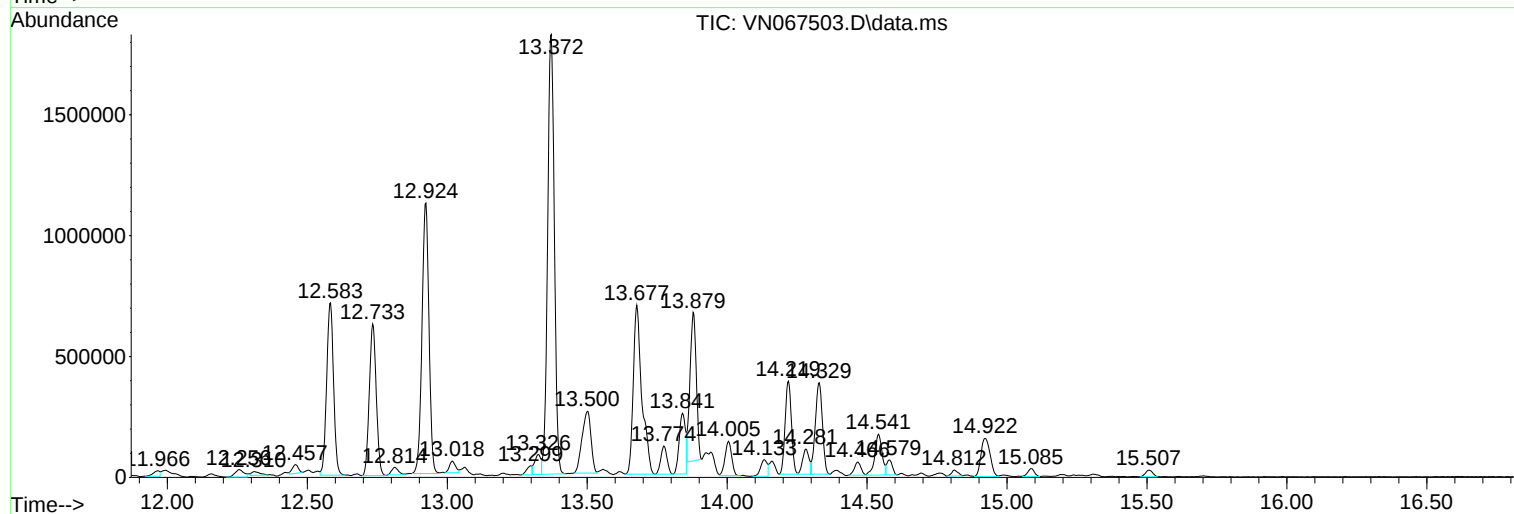
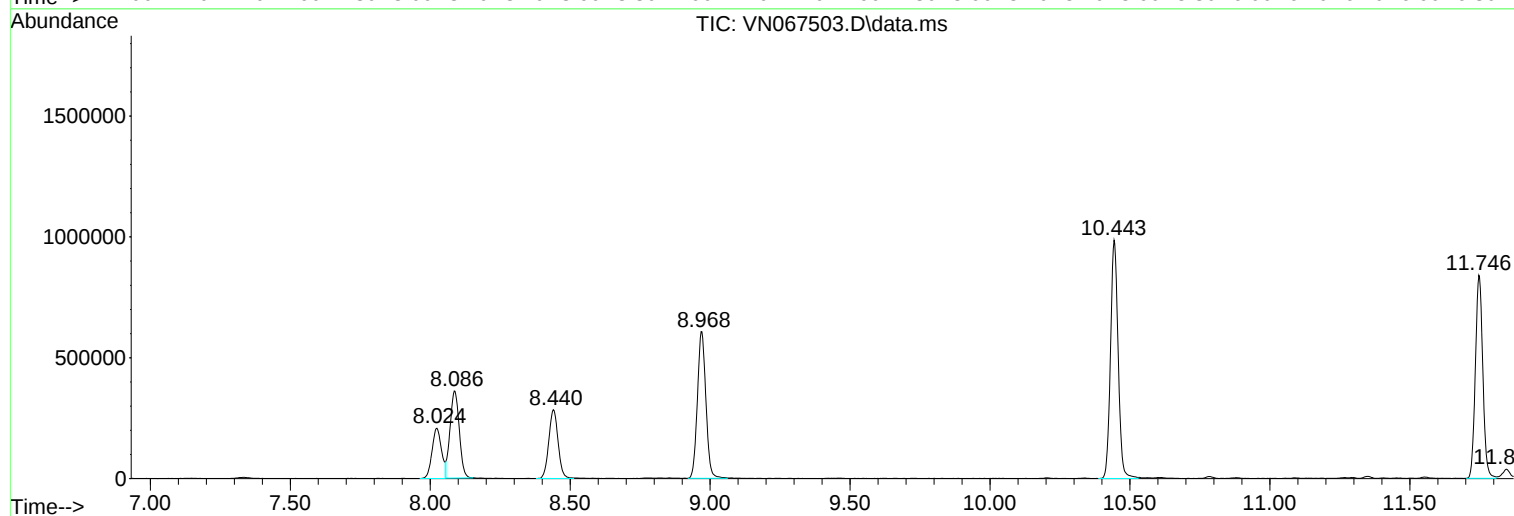
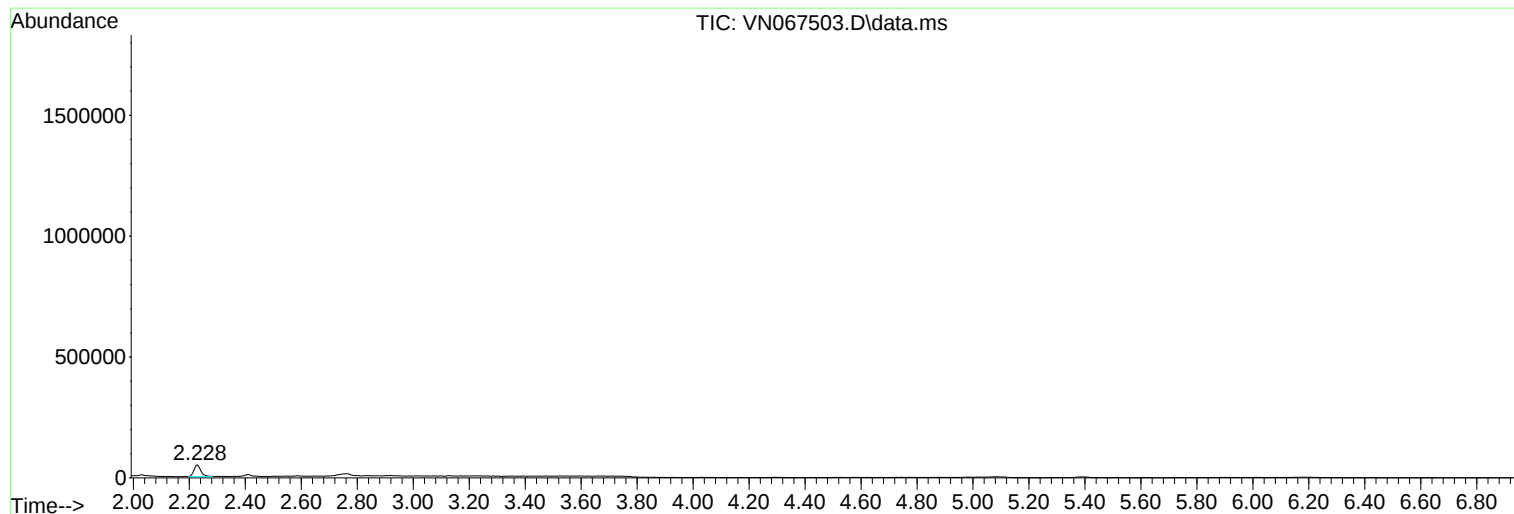
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Misc : 5.00mL/MSVOA_N/WATER
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Instrument :
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ClientSampleId :
MW-1

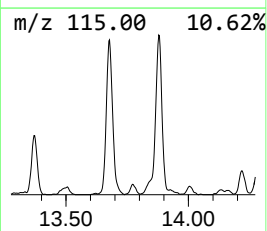
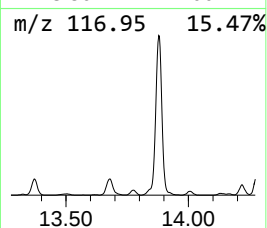
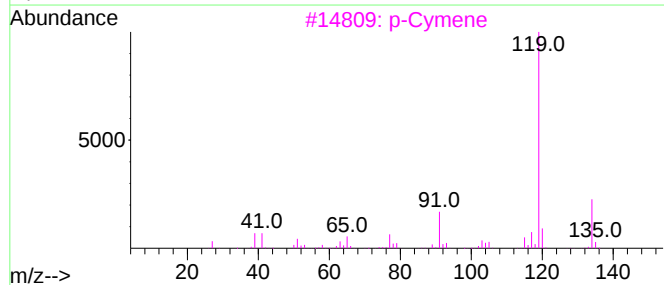
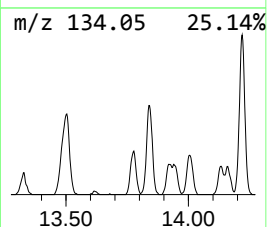
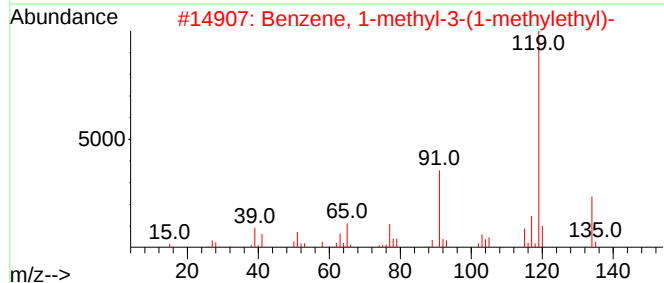
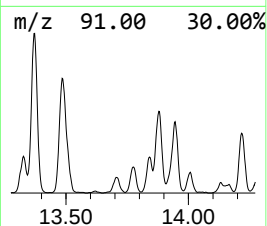
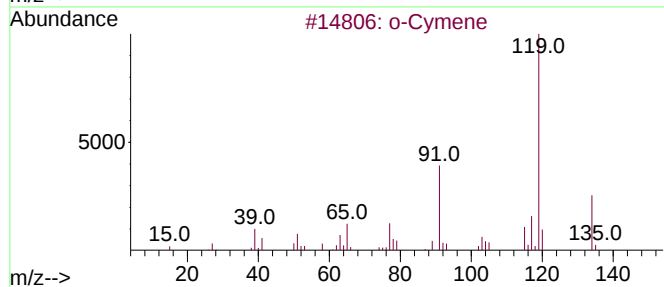
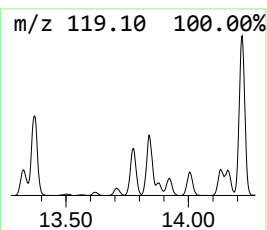
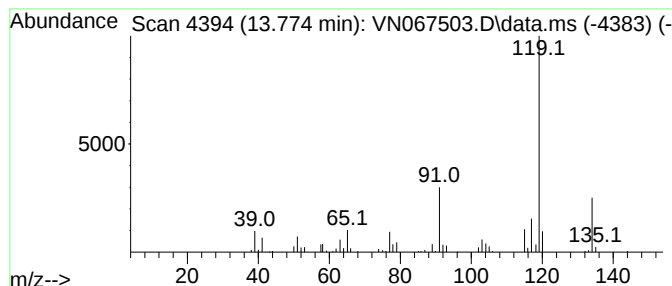
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 o-Cymene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	6.11 ug/l	182543	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			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	94
3			p-Cymene	134	C10H14	000099-87-6	91
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	90
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	90



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Instrument :
MSVOA_N
ClientSampleId :
MW-1

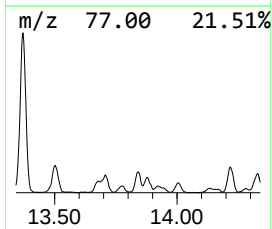
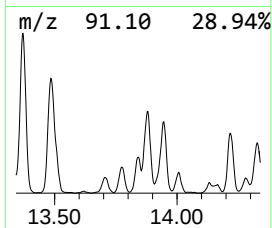
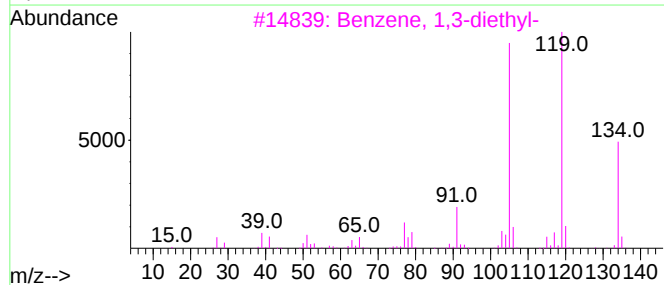
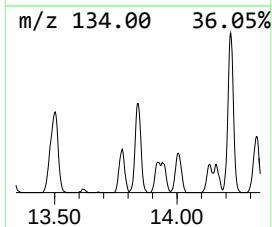
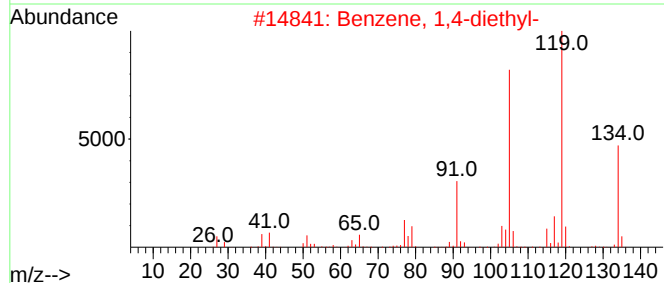
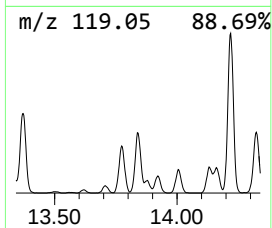
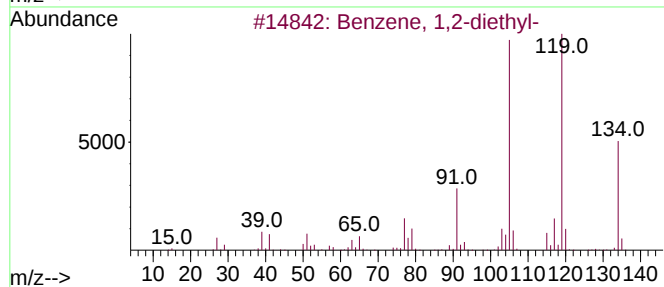
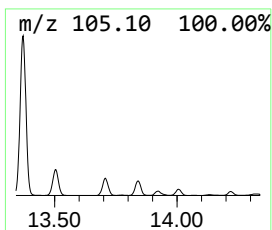
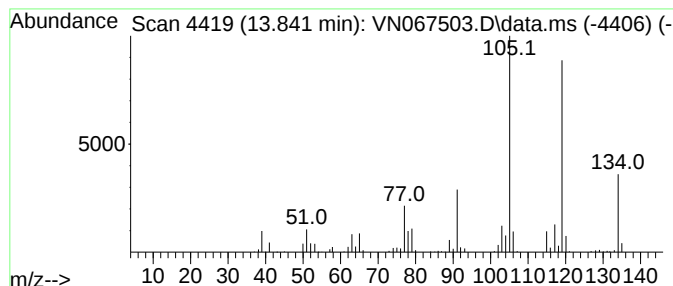
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1,2-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	13.25 ug/l	395698	1,4-Dichlorobenzene-d4	13.677

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	94
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	91
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	90
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	72



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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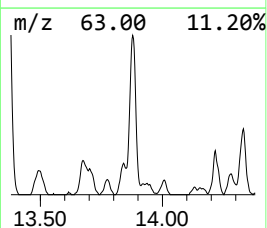
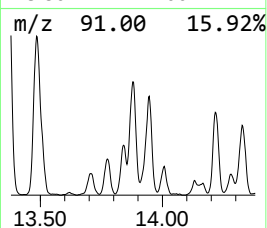
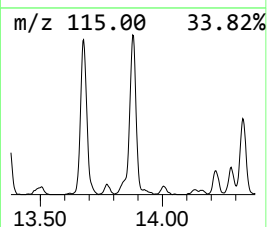
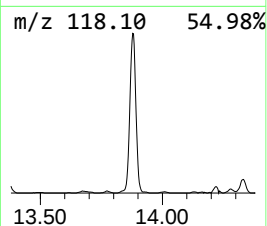
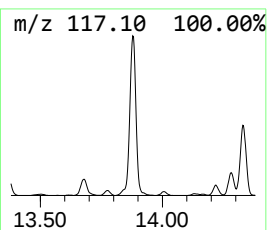
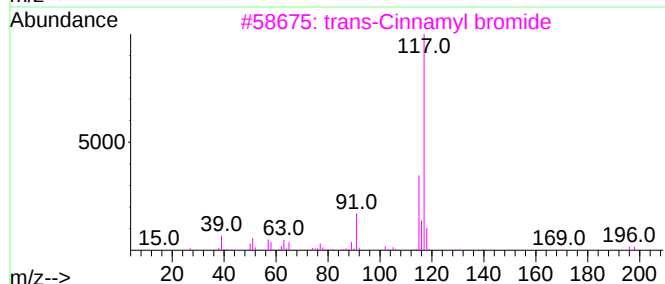
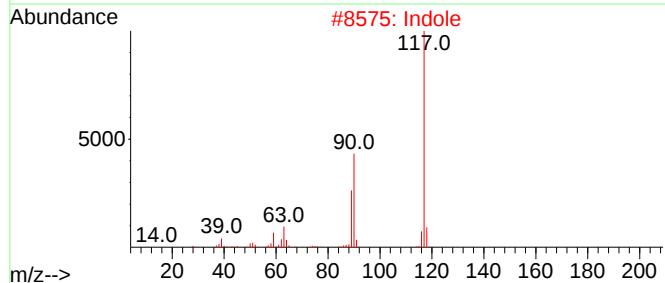
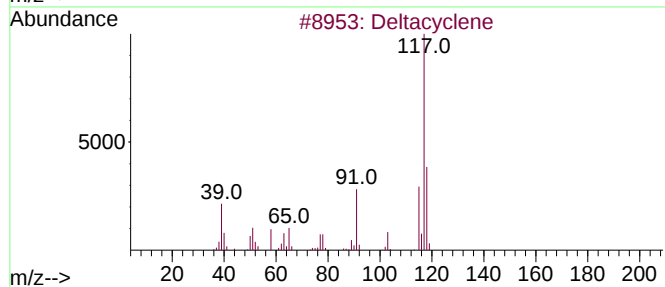
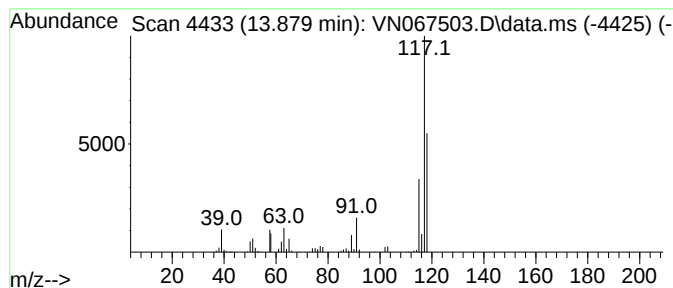
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.879 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.879	31.77 ug/l	948562	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Deltacyclene	118	C9H10	007785-10-6	53
2			Indole	117	C8H7N	000120-72-9	47
3			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	45
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	43
5			Indolizine	117	C8H7N	000274-40-8	37



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1

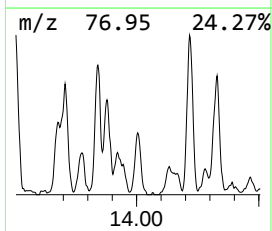
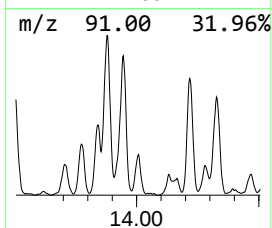
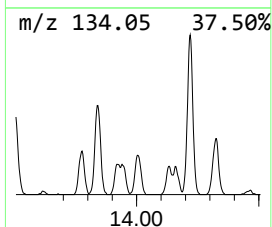
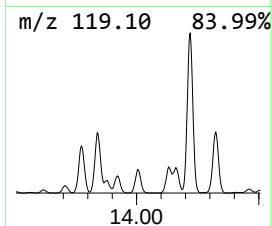
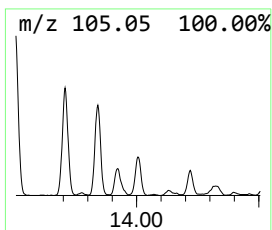
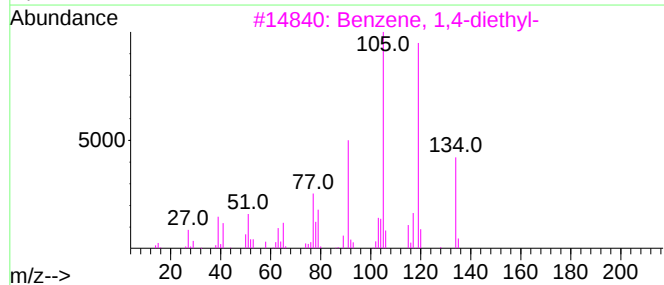
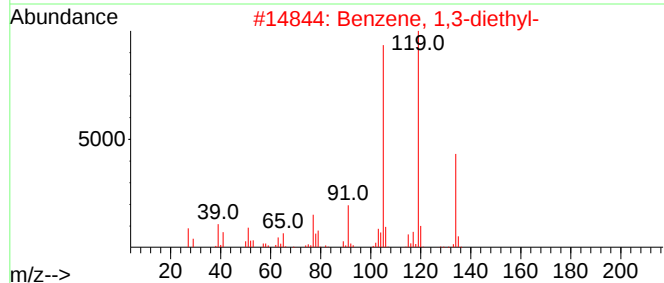
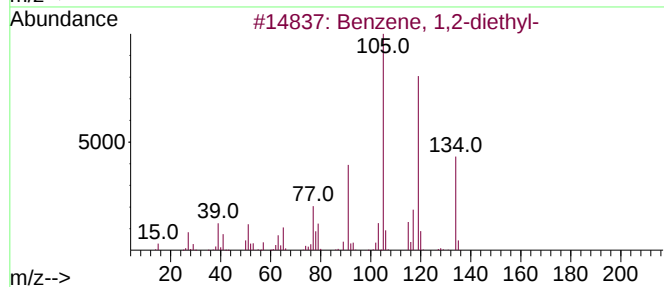
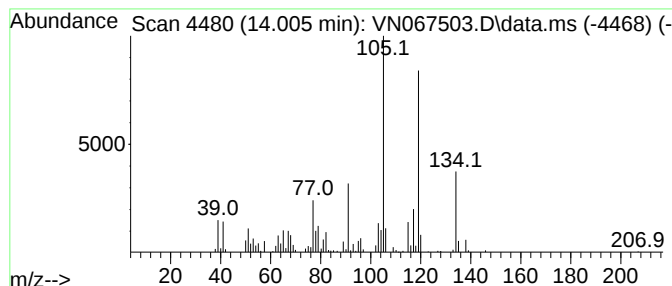
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,3-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.005	7.81 ug/l	233157	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	98
2			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	87
3			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	87
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	74
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	68



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

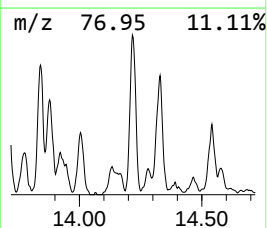
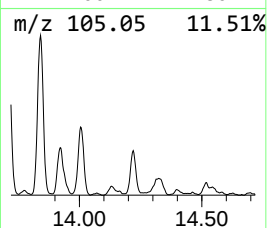
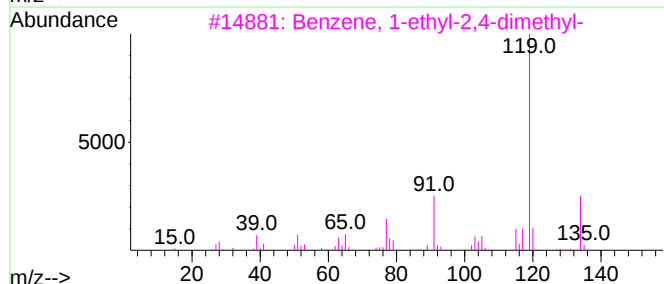
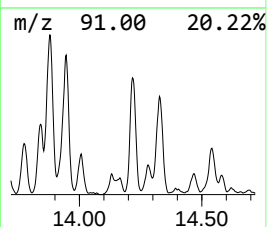
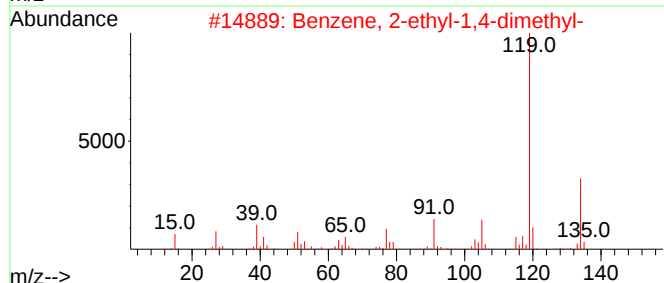
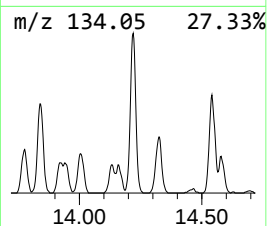
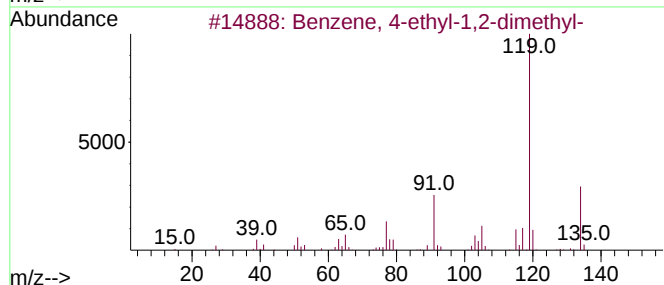
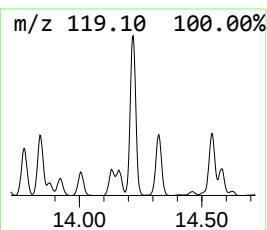
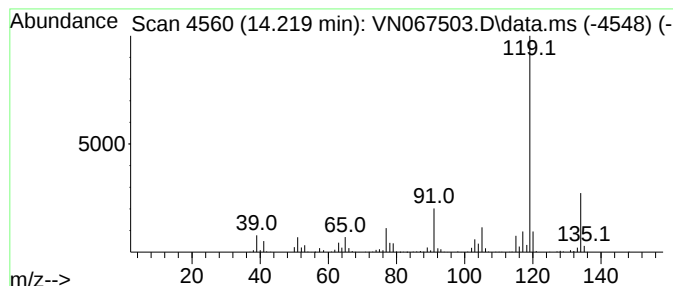
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	20.00 ug/l	597019	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067503.D
Acq On : 25 Jun 2021 14:42
Operator : JC/MD
Sample : M2806-01 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

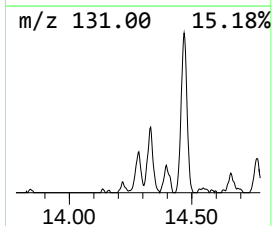
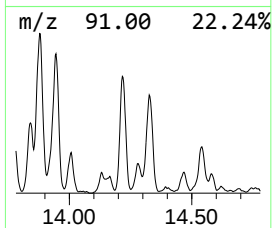
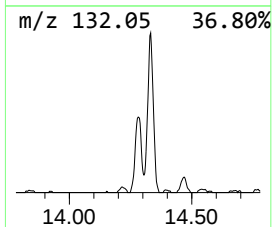
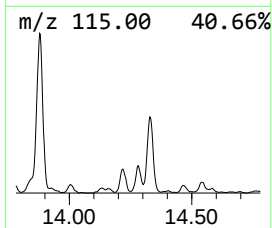
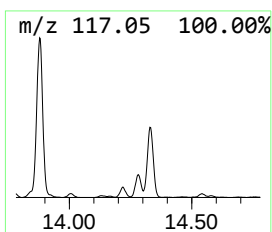
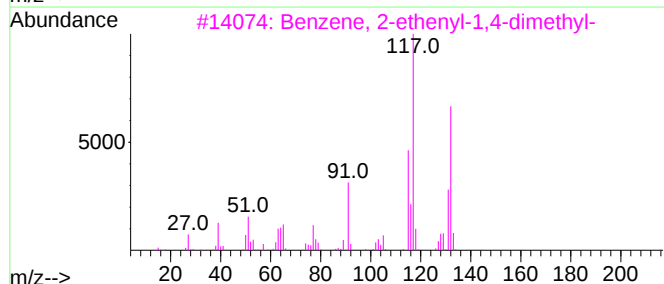
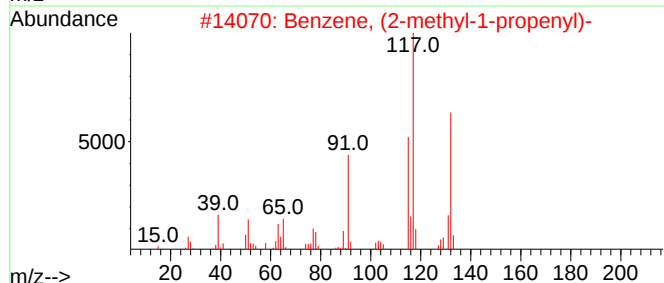
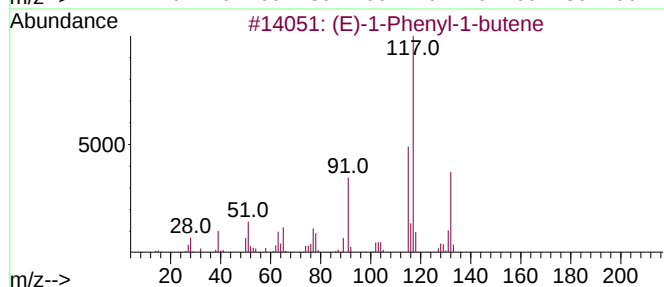
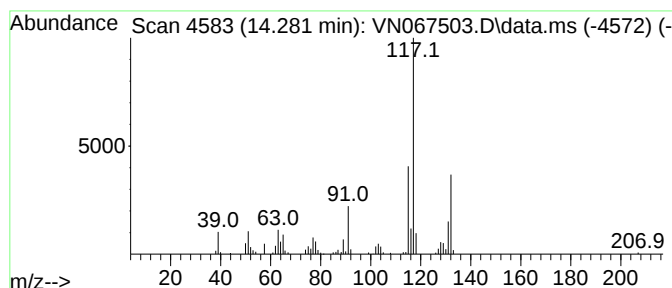
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (E)-1-Phenyl-1-butene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.281	5.74 ug/l	171256	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	94
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	94
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	90
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067503.D
Acq On : 25 Jun 2021 14:42
Operator : JC/MD
Sample : M2806-01 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

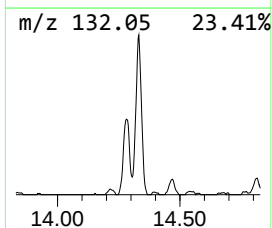
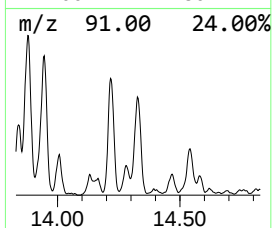
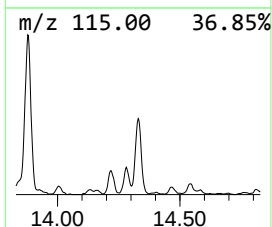
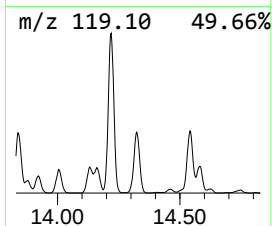
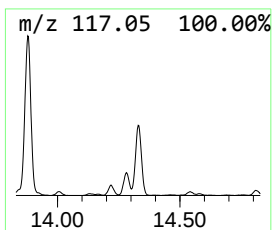
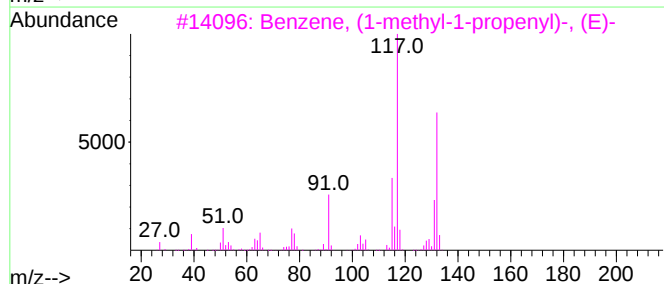
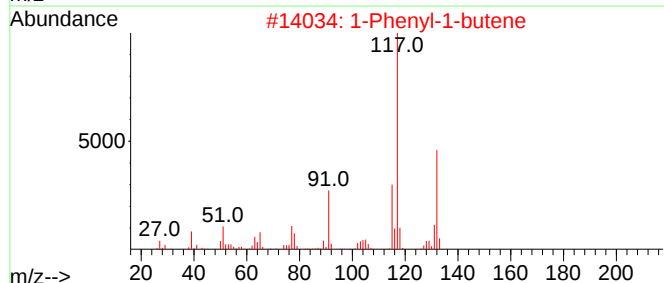
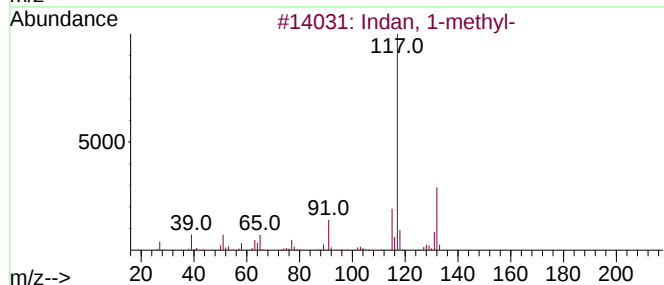
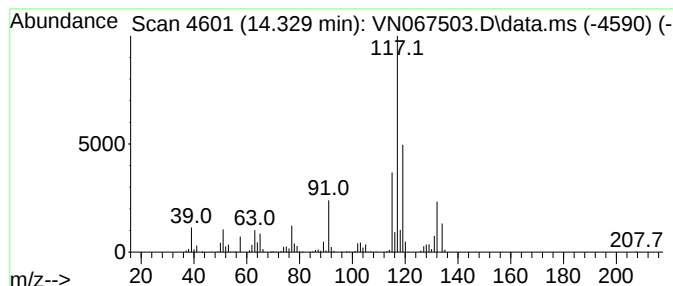
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Indan, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	22.33 ug/l	666692	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	70
2			1-Phenyl-1-butene	132	C10H12	000824-90-8	70
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	62
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067503.D
Acq On : 25 Jun 2021 14:42
Operator : JC/MD
Sample : M2806-01 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

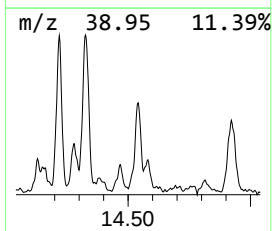
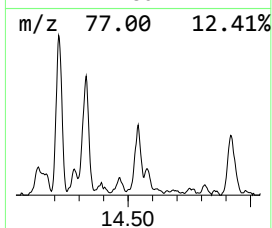
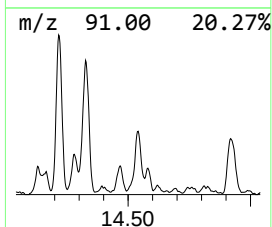
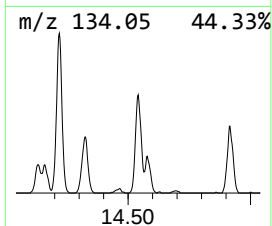
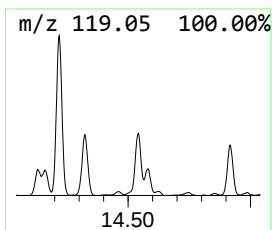
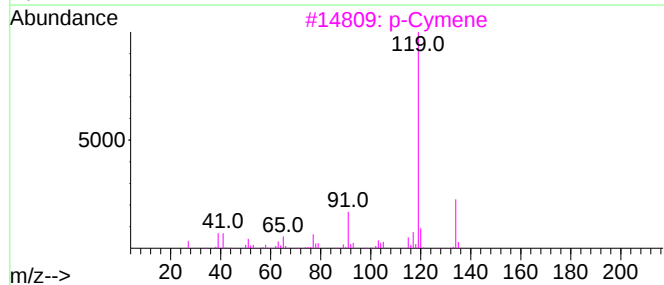
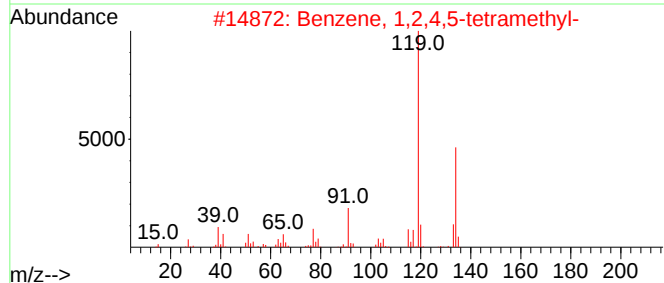
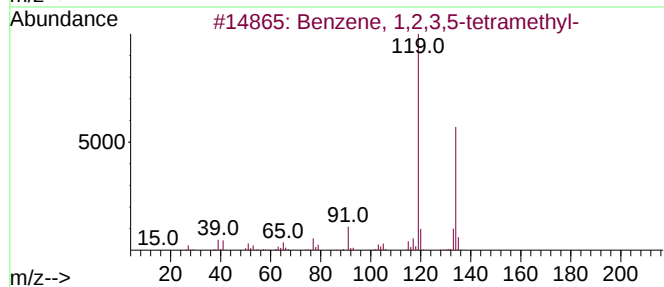
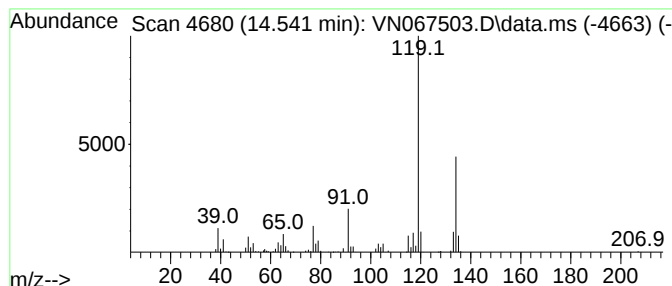
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.541	10.13 ug/l	302439	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3			p-Cymene	134	C10H14	000099-87-6	95
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067503.D
Acq On : 25 Jun 2021 14:42
Operator : JC/MD
Sample : M2806-01 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

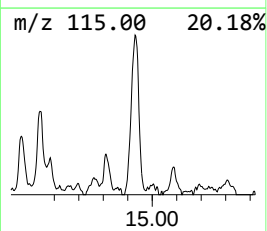
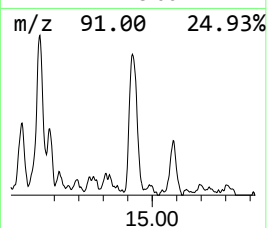
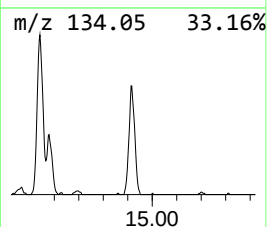
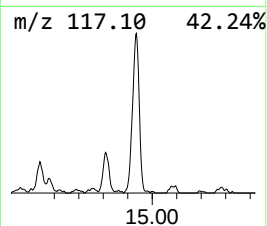
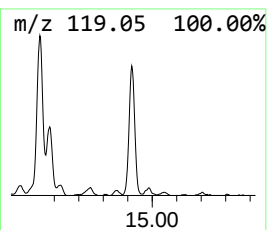
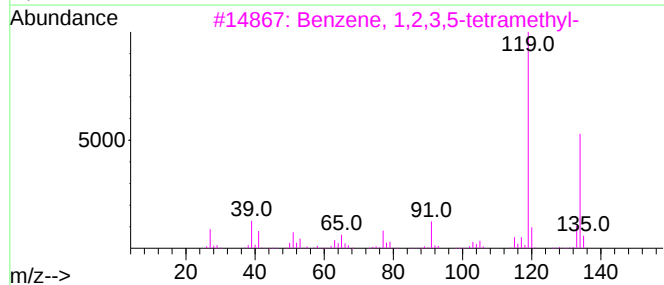
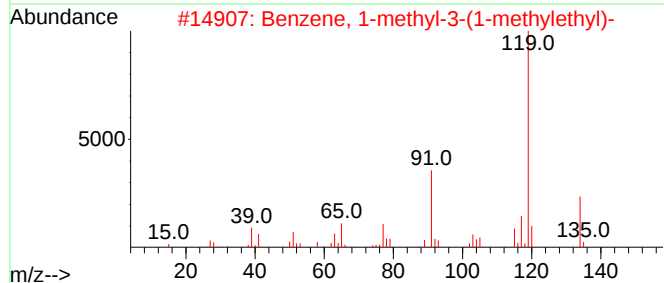
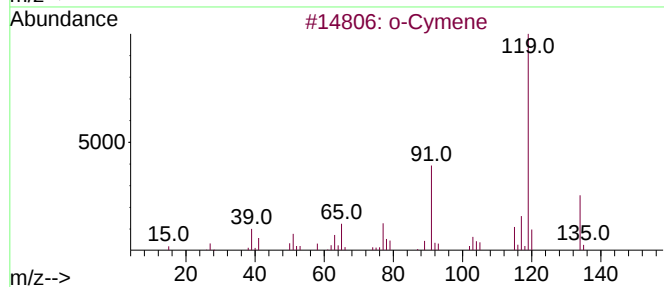
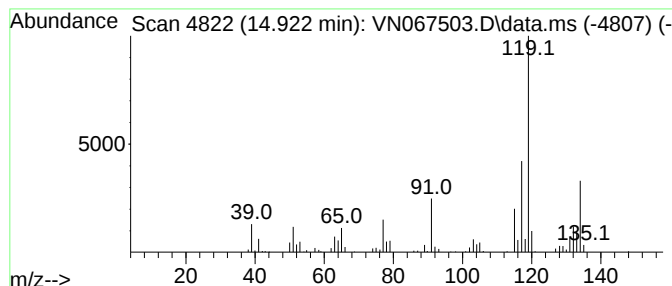
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-methyl-3-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.922	11.85 ug/l	353745	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	64
2			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	64
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
5			p-Cymene	134	C10H14	000099-87-6	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067503.D
Acq On : 25 Jun 2021 14:42
Operator : JC/MD
Sample : M2806-01 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
o-Cymene	13.774	6.1	ug/l	182543	4	13.677	1492650	50.0
Benzene, 1,2-di...	13.841	13.3	ug/l	395698	4	13.677	1492650	50.0
unknown13.879	13.879	31.8	ug/l	948562	4	13.677	1492650	50.0
Benzene, 1,3-di...	14.005	7.8	ug/l	233157	4	13.677	1492650	50.0
Benzene, 4-ethy...	14.219	20.0	ug/l	597019	4	13.677	1492650	50.0
(E)-1-Phenyl-1-...	14.281	5.7	ug/l	171256	4	13.677	1492650	50.0
Indan, 1-methyl-	14.329	22.3	ug/l	666692	4	13.677	1492650	50.0
Benzene, 1,2,3,...	14.541	10.1	ug/l	302439	4	13.677	1492650	50.0
Benzene, 1-meth...	14.922	11.9	ug/l	353745	4	13.677	1492650	50.0