

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
 Data File : VN067506.D
 Acq On : 25 Jun 2021 15:55
 Operator : JC/MD
 Sample : M2806-06 10X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 FD-062121

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: VN067506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.220	74	86	107	rBV	85717	140640	4.86%	0.686%
2	8.021	2227	2249	2260	rBV2	185724	450107	15.55%	2.196%
3	8.083	2260	2272	2300	rVB2	348057	785901	27.15%	3.835%
4	8.437	2383	2404	2431	rBV2	265941	611899	21.14%	2.986%
5	8.968	2583	2602	2633	rBV	567888	1208167	41.74%	5.896%
6	10.443	3131	3152	3183	rBV	956171	1795011	62.01%	8.759%
7	11.747	3620	3638	3662	rBV	836235	1547580	53.46%	7.552%
8	11.846	3662	3675	3683	rVV3	23501	39599	1.37%	0.193%
9	11.961	3698	3718	3721	rBV4	19043	32800	1.13%	0.160%
10	12.256	3813	3828	3839	rBV4	29601	64170	2.22%	0.313%
11	12.455	3894	3902	3913	rVV4	34680	58592	2.02%	0.286%
12	12.581	3936	3949	3974	rVB	688421	1180865	40.79%	5.762%
13	12.733	3991	4006	4023	rBV2	662255	1132124	39.11%	5.524%
14	12.811	4026	4035	4048	rBV6	28886	52533	1.81%	0.256%
15	12.921	4059	4076	4094	rVB	1087745	1875017	64.77%	9.150%
16	13.018	4104	4112	4121	rBV	35650	53929	1.86%	0.263%
17	13.294	4204	4215	4216	rBV5	35661	39206	1.35%	0.191%
18	13.324	4221	4226	4231	rVV2	82464	111100	3.84%	0.542%
19	13.372	4231	4244	4262	rVB	1777271	2894841	100.00%	14.126%
20	13.501	4274	4292	4306	rBV2	255124	565343	19.53%	2.759%
21	13.554	4308	4312	4327	rVB9	20185	33040	1.14%	0.161%
22	13.675	4343	4357	4382	rBV3	714842	1477399	51.04%	7.209%
23	13.774	4382	4394	4405	rBV3	119722	188844	6.52%	0.922%
24	13.841	4407	4419	4424	rBV	260677	392193	13.55%	1.914%
25	13.879	4424	4433	4444	rVB	600495	969346	33.49%	4.730%
26	14.005	4468	4480	4493	rVB4	143911	240508	8.31%	1.174%
27	14.133	4514	4528	4533	rBV2	69239	113363	3.92%	0.553%
28	14.219	4548	4560	4572	rBV2	393083	615754	21.27%	3.005%
29	14.281	4572	4583	4590	rVV2	100619	167743	5.79%	0.819%
30	14.327	4590	4600	4614	rVV4	378496	668364	23.09%	3.261%
31	14.394	4616	4625	4637	rVB9	21395	42236	1.46%	0.206%
32	14.466	4639	4652	4662	rBV3	53726	89707	3.10%	0.438%
33	14.541	4663	4680	4689	rVV2	177505	306044	10.57%	1.493%
34	14.581	4690	4695	4705	rVB	60904	79392	2.74%	0.387%
35	14.812	4772	4781	4792	rBV4	22972	39119	1.35%	0.191%
36	14.922	4807	4822	4839	rBV4	155130	344624	11.90%	1.682%

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FD-062121

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	15.086	4872	4883	4897	rBV2	30698	51872	1.79%	0.253%
38	15.509	5031	5041	5052	rVB2	20347	34019	1.18%	0.166%

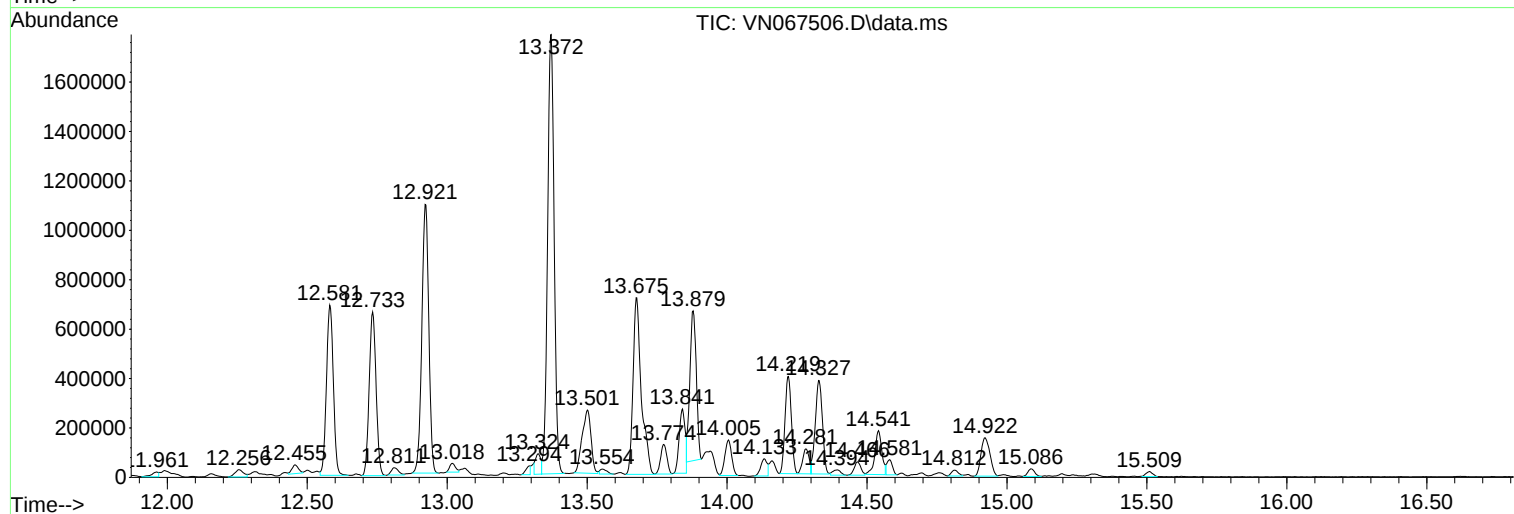
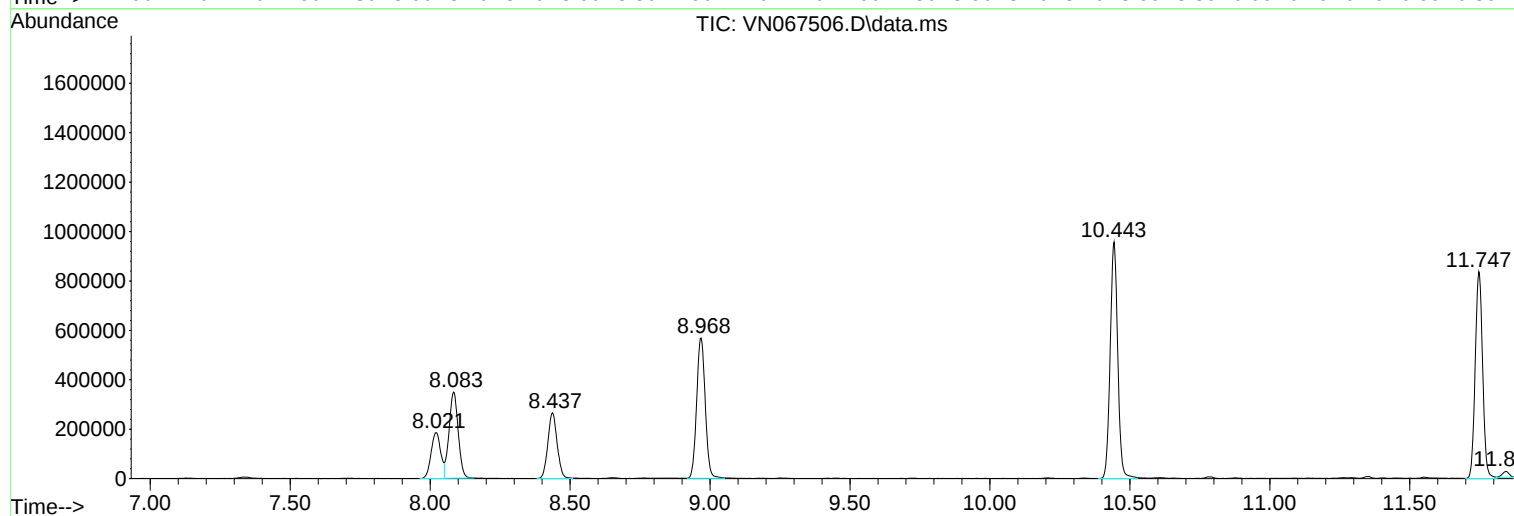
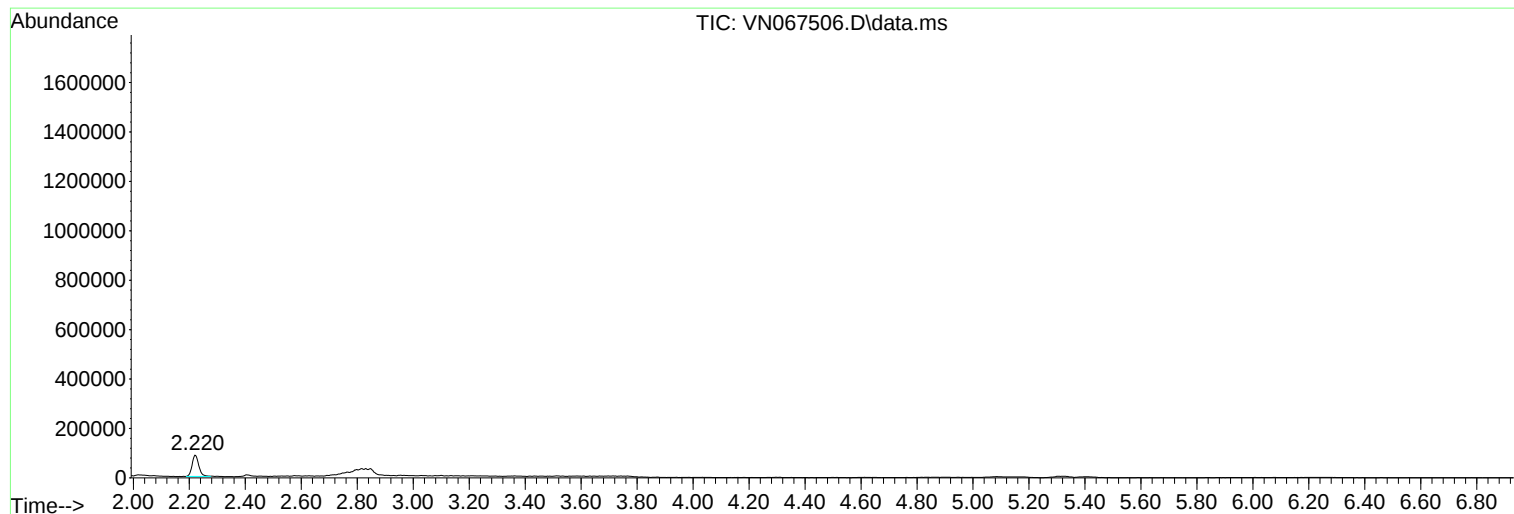
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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 :
MSVOA_N
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FD-062121

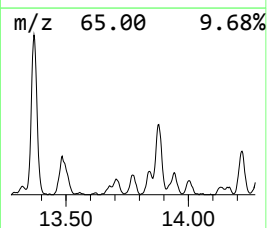
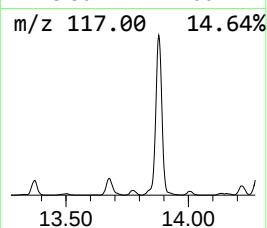
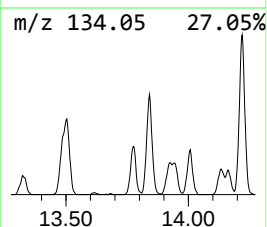
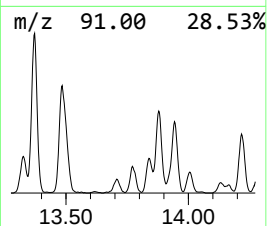
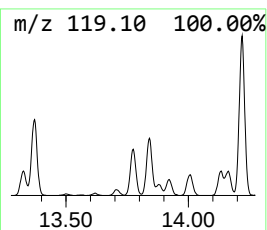
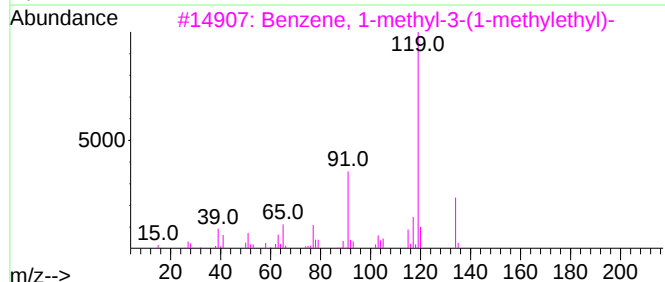
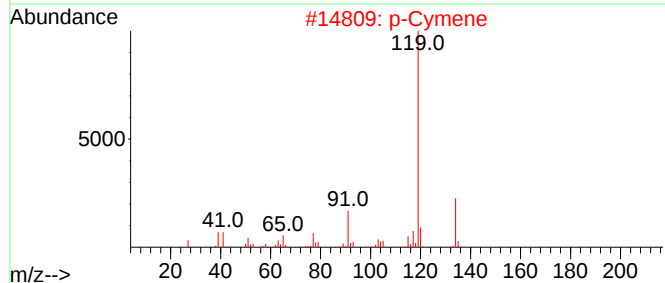
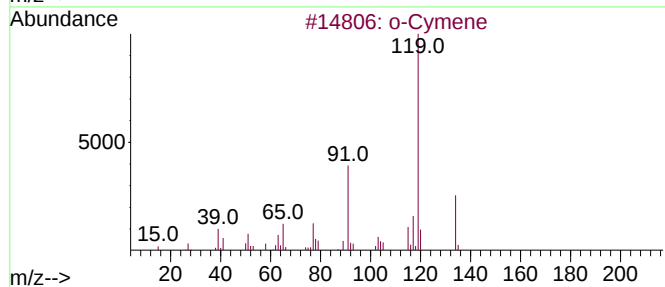
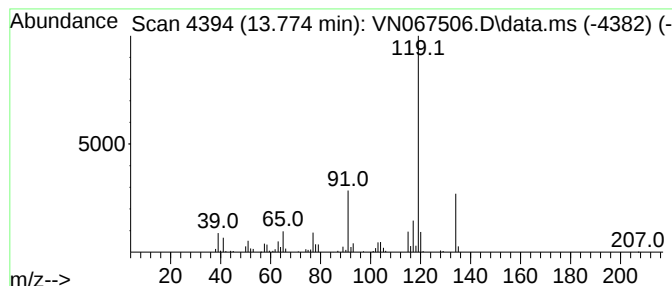
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

Peak Number 2 o-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	6.39 ug/l	188844	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	95
2			p-Cymene	134	C10H14	000099-87-6	93
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	90
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	90



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Sample : M2806-06 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

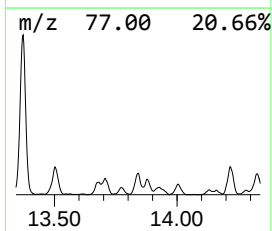
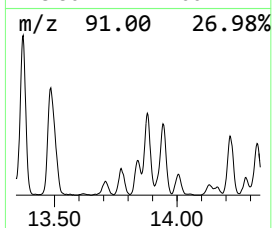
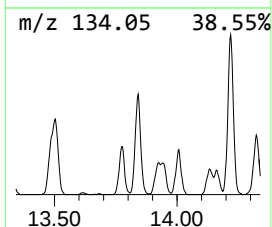
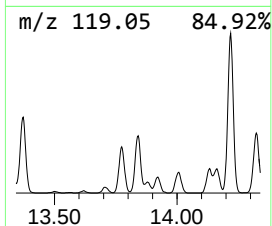
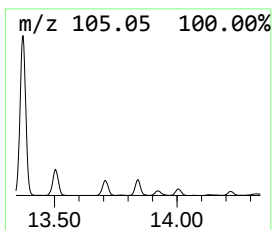
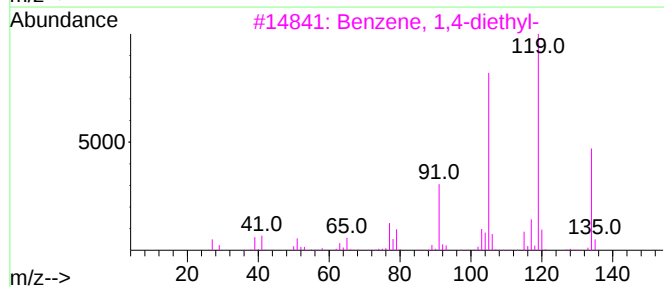
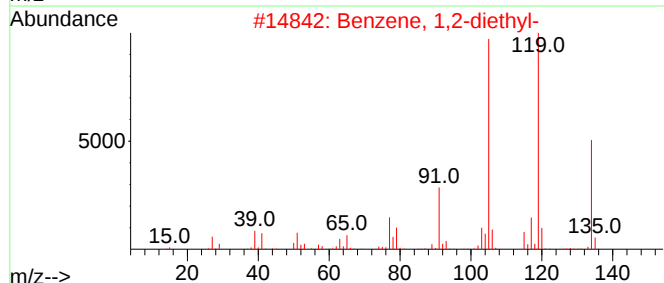
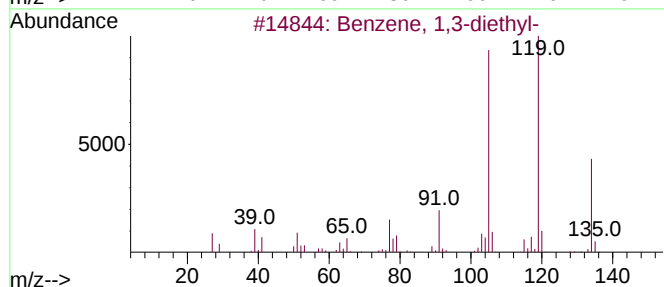
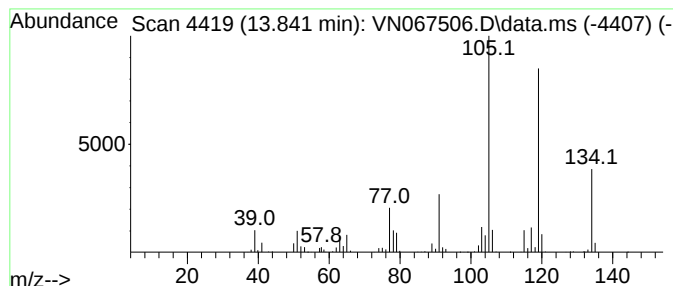
Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.841	13.27 ug/l	392193	1,4-Dichlorobenzene-d4		13.675	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-		134	C10H14	000141-93-5	97
2	Benzene, 1,2-diethyl-		134	C10H14	000135-01-3	96
3	Benzene, 1,4-diethyl-		134	C10H14	000105-05-5	94
4	Benzene, 1-ethyl-3,5-dimethyl-		134	C10H14	000934-74-7	87
5	Benzene, 1-ethyl-2,3-dimethyl-		134	C10H14	000933-98-2	87



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Acq On : 25 Jun 2021 15:55
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FD-062121

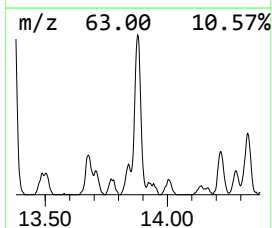
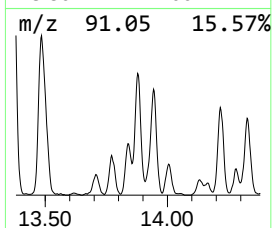
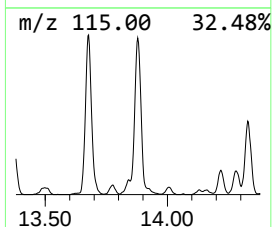
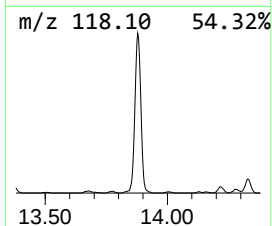
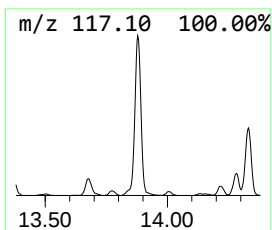
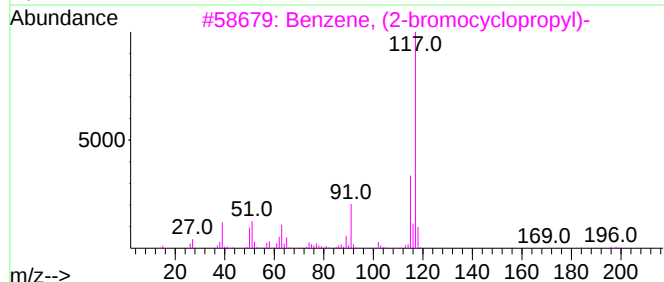
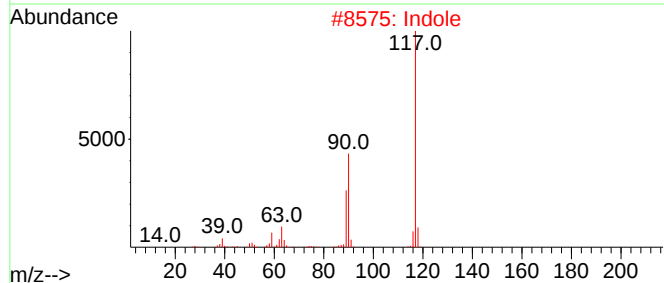
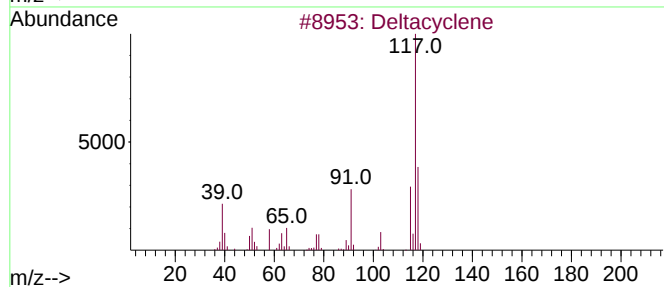
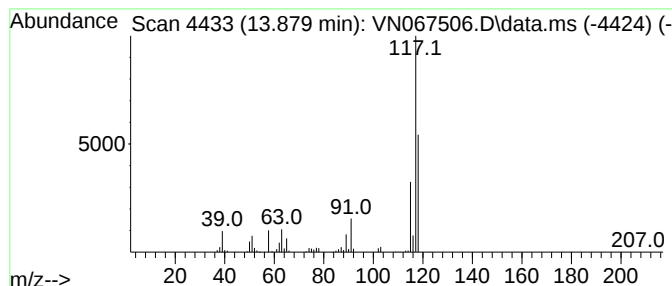
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.879 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.879	32.81 ug/l	969346	1,4-Dichlorobenzene-d4	13.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Deltacyclene	118	C9H10	007785-10-6	59
2		Indole	117	C8H7N	000120-72-9	49
3		Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
4		trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	45
5		Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	37



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FD-062121

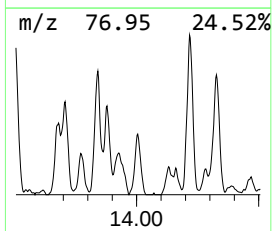
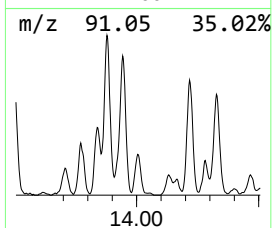
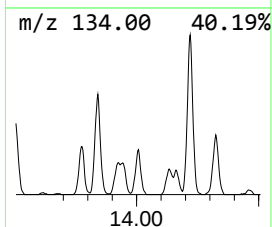
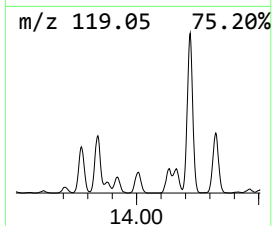
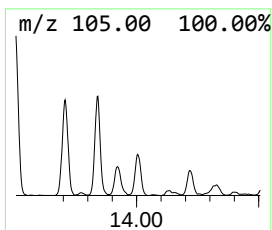
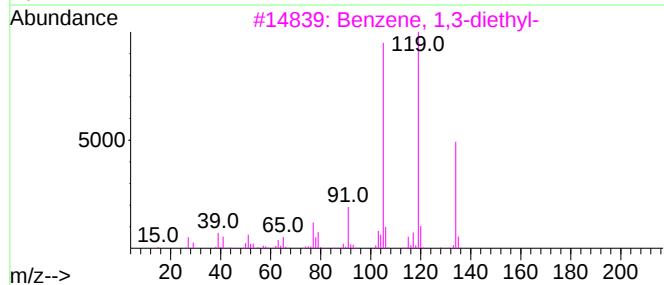
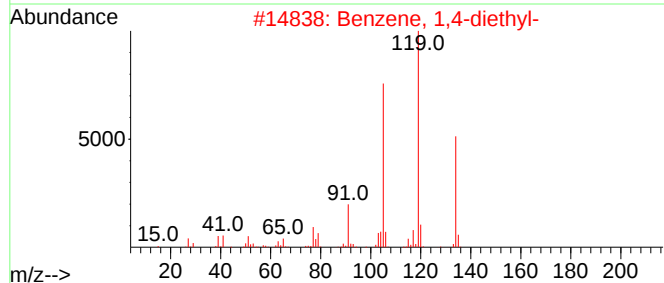
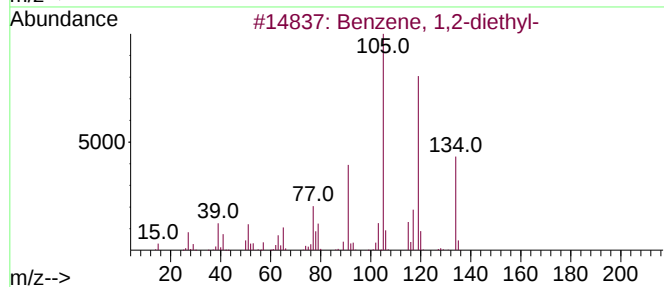
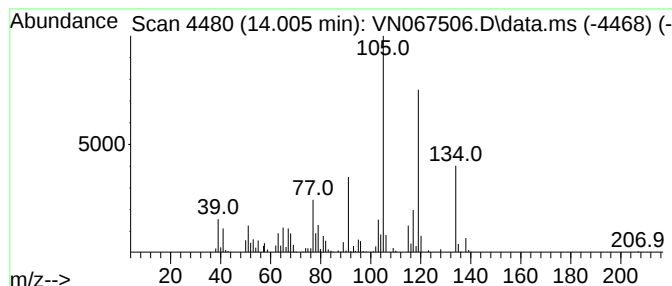
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2-diethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.005	8.14 ug/l	240508	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	98
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	83
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	80
4			Ethanone, 1-(2-methylphenyl)-	134	C9H10O	000577-16-2	52
5			Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	49



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Instrument :
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ClientSampleId :
FD-062121

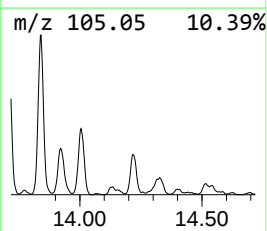
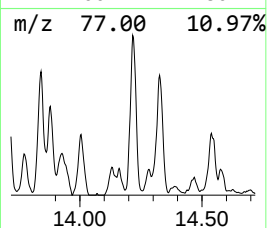
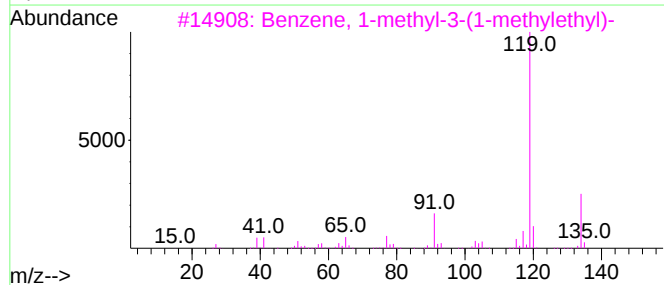
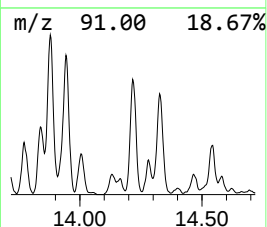
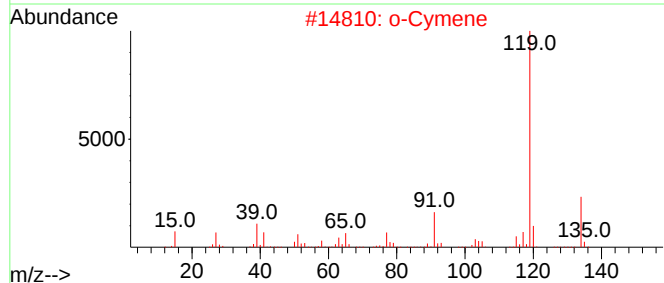
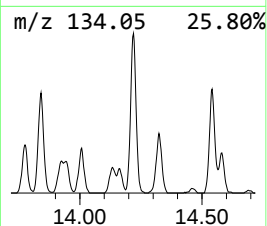
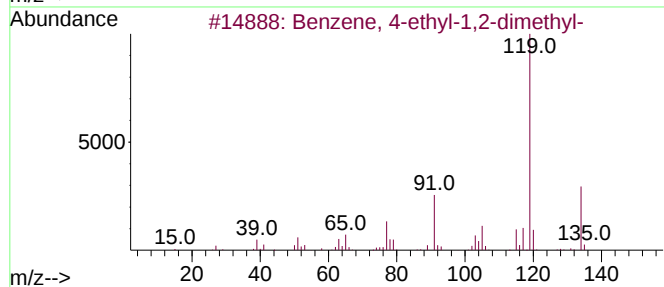
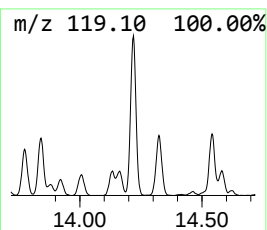
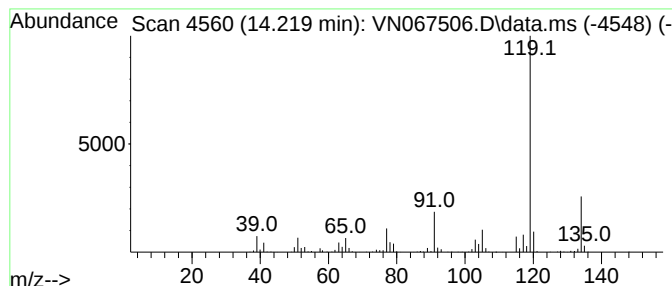
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	20.84 ug/l	615754	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4			p-Cymene	134	C10H14	000099-87-6	95
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067506.D
Acq On : 25 Jun 2021 15:55
Operator : JC/MD
Sample : M2806-06 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FD-062121

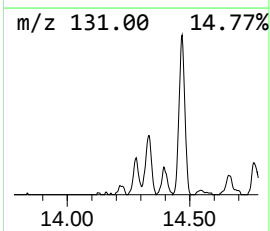
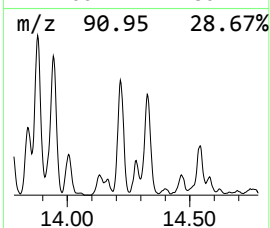
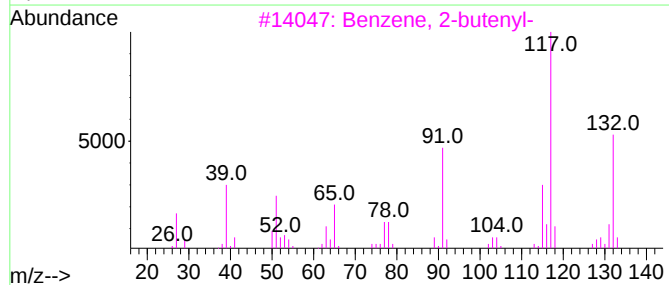
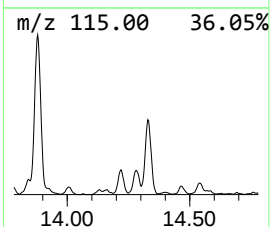
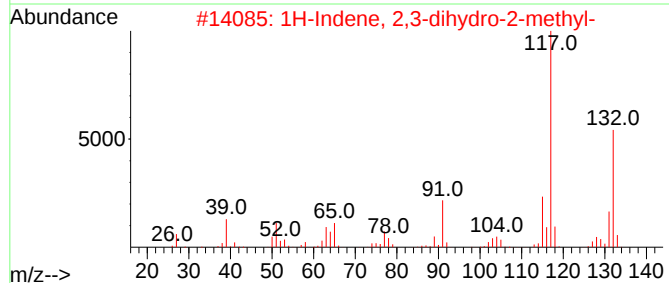
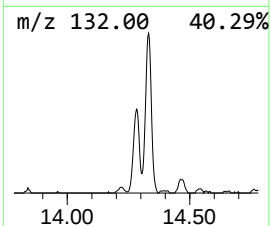
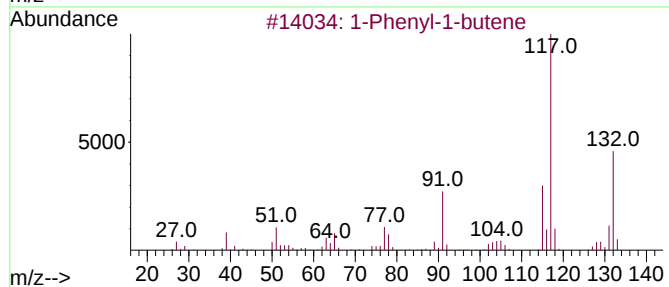
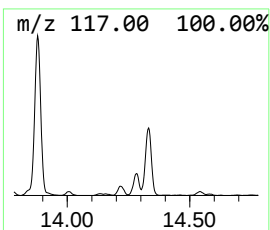
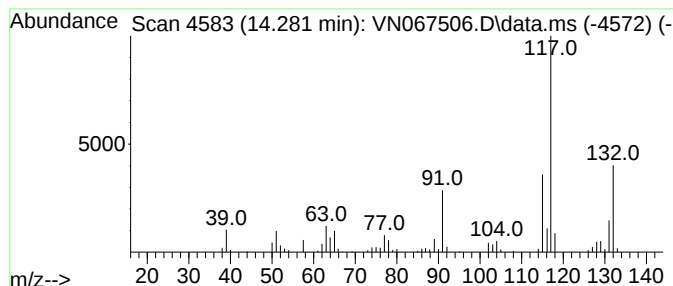
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Quant Title : SW846 8260

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

Peak Number 7 1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.281	5.68 ug/l	167743	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	94
2			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	93
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	91
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	91
5			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067506.D
Acq On : 25 Jun 2021 15:55
Operator : JC/MD
Sample : M2806-06 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FD-062121

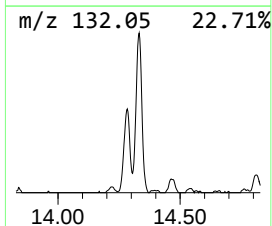
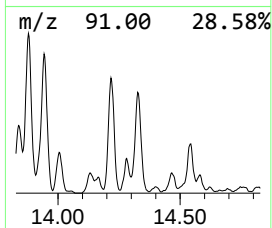
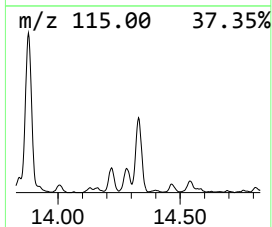
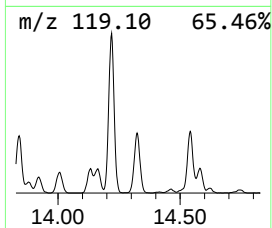
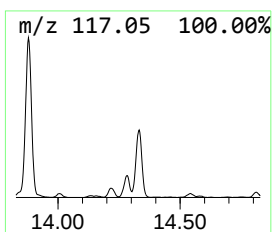
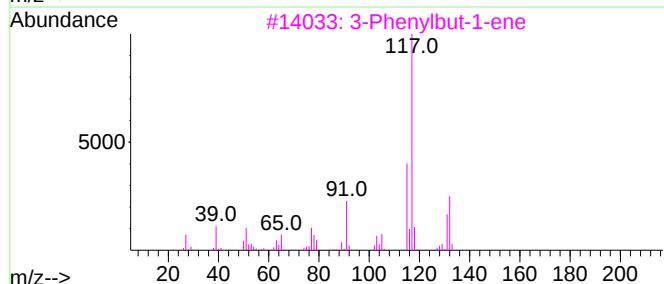
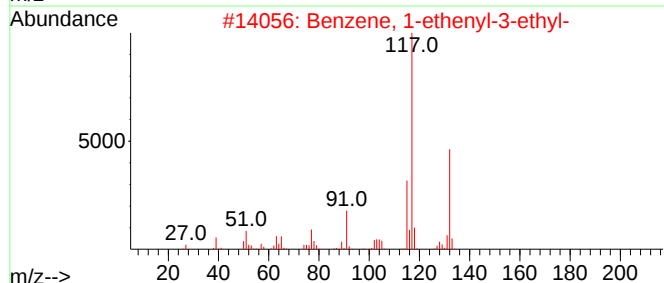
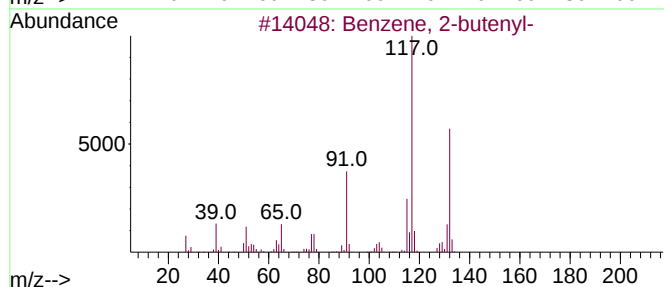
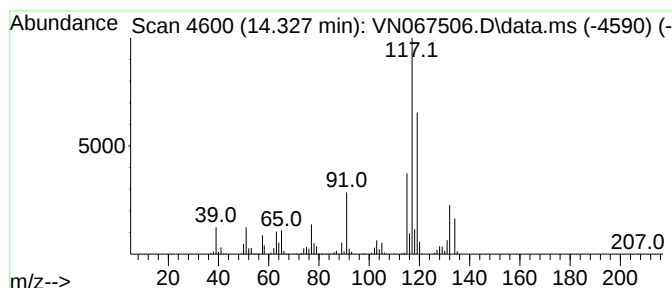
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-butenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	22.62 ug/l	668364	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	70
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067506.D
Acq On : 25 Jun 2021 15:55
Operator : JC/MD
Sample : M2806-06 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FD-062121

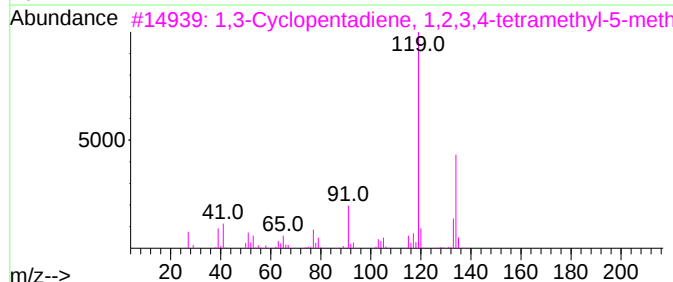
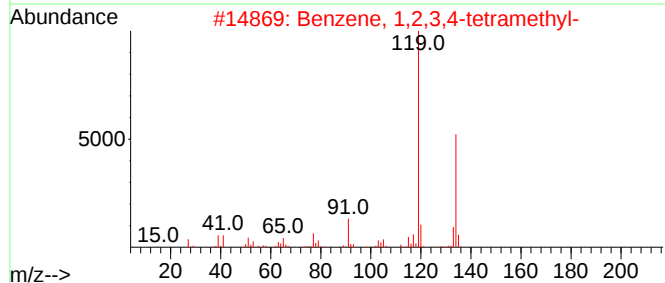
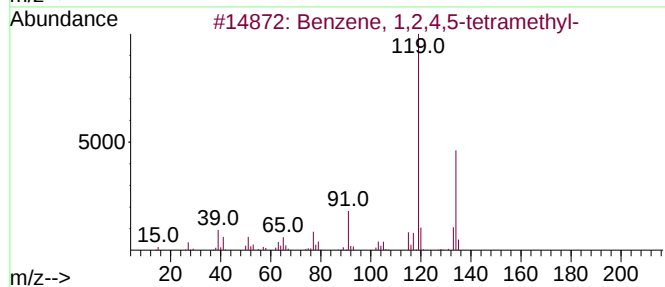
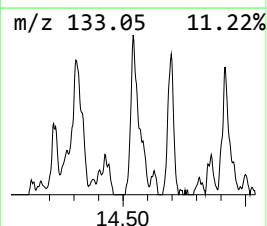
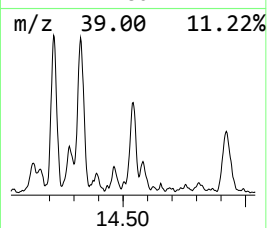
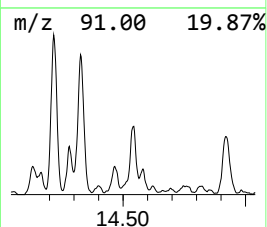
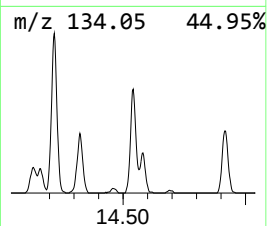
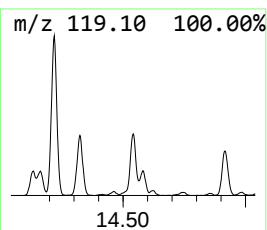
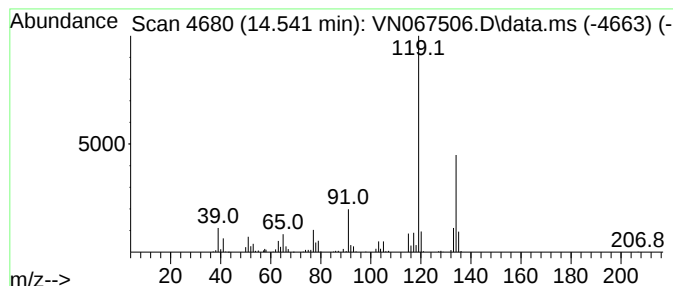
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.541	10.36 ug/l	306044	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	93
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067506.D
Acq On : 25 Jun 2021 15:55
Operator : JC/MD
Sample : M2806-06 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FD-062121

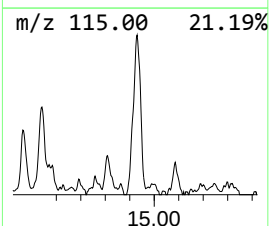
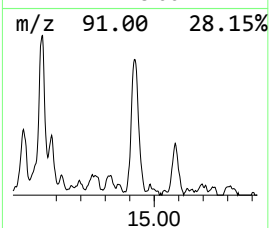
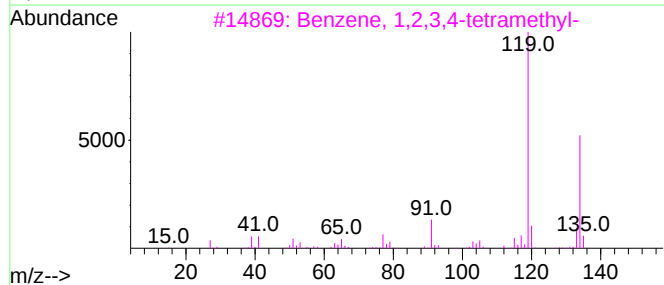
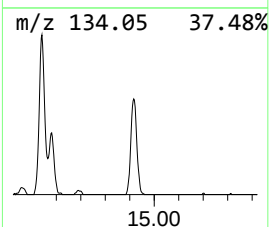
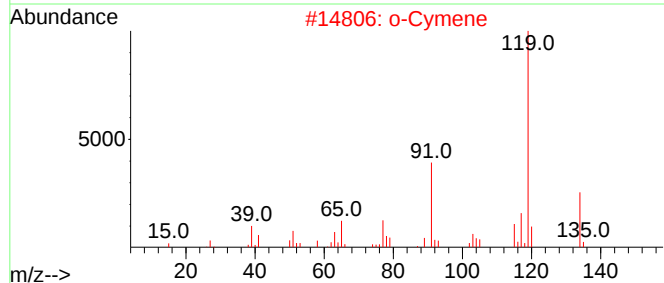
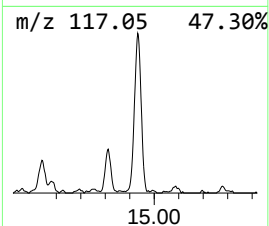
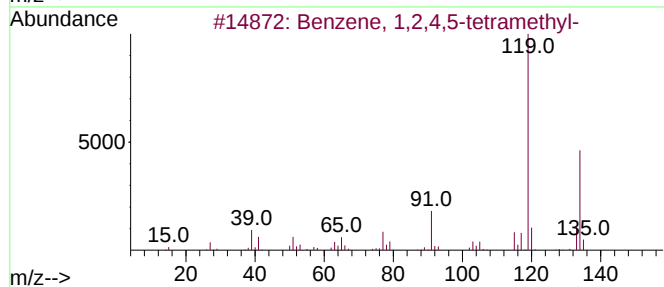
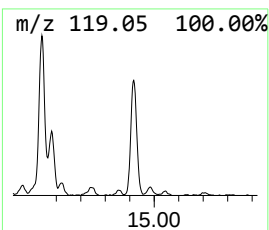
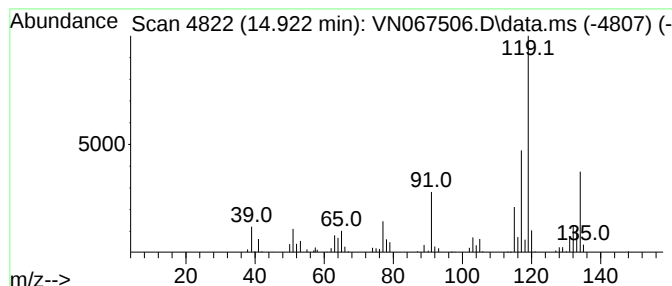
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062421W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.922	11.66 ug/l	344624	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
2			o-Cymene	134	C10H14	000527-84-4	64
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	64
4			p-Cymene	134	C10H14	000099-87-6	60
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062521\
Data File : VN067506.D
Acq On : 25 Jun 2021 15:55
Operator : JC/MD
Sample : M2806-06 10X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
FD-062121

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
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Benzene, 1,3-di...	13.841	13.3	ug/l	392193	4	13.675	1477400	50.0
unknown13.879	13.879	32.8	ug/l	969346	4	13.675	1477400	50.0
Benzene, 1,2-di...	14.005	8.1	ug/l	240508	4	13.675	1477400	50.0
Benzene, 4-ethy...	14.219	20.8	ug/l	615754	4	13.675	1477400	50.0
1-Phenyl-1-butene	14.281	5.7	ug/l	167743	4	13.675	1477400	50.0
Benzene, 2-bute...	14.327	22.6	ug/l	668364	4	13.675	1477400	50.0
Benzene, 1,2,4,...	14.541	10.4	ug/l	306044	4	13.675	1477400	50.0
Benzene, 1,2,3,...	14.922	11.7	ug/l	344624	4	13.675	1477400	50.0