

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
 Data File : VN069673.D
 Acq On : 29 Nov 2021 19:09
 Operator : JC/MD
 Sample : M4852-03
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :

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\82N110921W.M
 Title : SW846 8260

Signal : TIC: VN069673.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.150	1900	1924	1954	rVB4	146614	438227	1.69%	0.160%
2	8.024	2228	2250	2260	rBV	1068089	2562351	9.90%	0.938%
3	8.088	2261	2274	2298	rVB3	2539361	6096604	23.55%	2.232%
4	8.442	2387	2406	2435	rVV4	1558184	4523485	17.47%	1.656%
5	8.571	2439	2454	2468	rVV6	177171	467685	1.81%	0.171%
6	8.643	2469	2481	2492	rVV4	157641	357736	1.38%	0.131%
7	8.708	2492	2505	2531	rVB3	229974	526488	2.03%	0.193%
8	8.968	2580	2602	2641	rBV	3170411	6724520	25.97%	2.462%
9	9.459	2750	2785	2826	rBV	2785201	6368539	24.60%	2.331%
10	9.641	2838	2853	2868	rBV3	164123	318540	1.23%	0.117%
11	9.872	2929	2939	2957	rVB4	145955	294540	1.14%	0.108%
12	10.204	3047	3063	3077	rBV6	152479	372927	1.44%	0.137%
13	10.440	3133	3151	3186	rBV	6031312	12377515	47.80%	4.531%
14	10.609	3202	3214	3240	rVB6	467959	1220748	4.71%	0.447%
15	10.781	3264	3278	3295	rVB2	996982	1907855	7.37%	0.698%
16	10.875	3296	3313	3328	rBV4	583747	1193265	4.61%	0.437%
17	11.140	3394	3412	3431	rVB9	73565	269170	1.04%	0.099%
18	11.223	3432	3443	3448	rBV3	197387	324568	1.25%	0.119%
19	11.293	3449	3469	3479	rVV2	1910292	4124935	15.93%	1.510%
20	11.347	3479	3489	3501	rVV	1102854	1974352	7.63%	0.723%
21	11.400	3501	3509	3517	rVV2	187173	288266	1.11%	0.106%
22	11.451	3518	3528	3539	rVB6	228155	390918	1.51%	0.143%
23	11.551	3556	3565	3583	rVB2	513439	961498	3.71%	0.352%
24	11.628	3584	3594	3601	rBV3	186173	303596	1.17%	0.111%
25	11.744	3622	3637	3656	rBV	4950818	9100818	35.15%	3.332%
26	11.838	3661	3672	3682	rBV2	1306156	2186707	8.45%	0.800%
27	11.931	3697	3707	3716	rBV8	205795	468040	1.81%	0.171%
28	11.990	3718	3729	3756	rVB3	1545337	4515841	17.44%	1.653%
29	12.154	3778	3790	3809	rVB2	550315	1120648	4.33%	0.410%
30	12.253	3811	3827	3841	rBV2	1205094	2950737	11.40%	1.080%
31	12.417	3878	3888	3890	rBV4	471164	582442	2.25%	0.213%
32	12.454	3892	3902	3912	rVV2	1912883	3366342	13.00%	1.232%
33	12.578	3936	3948	3970	rVB	8302275	14111314	54.50%	5.166%
34	12.731	3992	4005	4022	rBV	4057933	7058328	27.26%	2.584%
35	12.808	4023	4034	4046	rBV2	900110	1560929	6.03%	0.571%
36	12.918	4058	4075	4089	rBV	9909877	17597095	67.96%	6.442%

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37	12.980	4091	4098	4107	rVB3	439990	600283	2.32%	0.220%
38	13.058	4116	4127	4140	rVB	2828132	4727646	18.26%	1.731%
39	13.219	4171	4187	4202	rBV3	537045	1412582	5.46%	0.517%
40	13.291	4203	4214	4217	rBV5	916009	1326676	5.12%	0.486%
41	13.366	4232	4242	4265	rVB	6884255	11514550	44.47%	4.215%
42	13.498	4275	4291	4303	rBV3	3620286	7474047	28.87%	2.736%
43	13.559	4304	4314	4325	rVB4	815267	1493301	5.77%	0.547%
44	13.675	4344	4357	4362	rBV	4567262	7584274	29.29%	2.776%
45	13.771	4382	4393	4404	rVB	2142411	3293715	12.72%	1.206%
46	13.836	4405	4417	4423	rBV	4517526	7015325	27.09%	2.568%
47	13.876	4424	4432	4443	rVB	8212289	12872106	49.71%	4.712%
48	14.002	4467	4479	4492	rVB2	3049502	4936543	19.07%	1.807%
49	14.069	4495	4504	4514	rVB	719284	1060464	4.10%	0.388%
50	14.131	4518	4527	4532	rBV	769858	1133670	4.38%	0.415%
51	14.217	4547	4559	4571	rBV	10059173	15726465	60.74%	5.757%
52	14.278	4571	4582	4589	rVV	3514771	5682512	21.95%	2.080%
53	14.326	4590	4600	4613	rVB3	9328604	15975929	61.70%	5.848%
54	14.463	4639	4651	4660	rBV3	1790834	2886506	11.15%	1.057%
55	14.538	4661	4679	4689	rBV	5222382	9138480	35.29%	3.345%
56	14.619	4703	4709	4717	rVB2	412647	503906	1.95%	0.184%
57	14.662	4718	4725	4729	rBV2	225123	286460	1.11%	0.105%
58	14.761	4751	4762	4771	rVB4	709824	1213002	4.68%	0.444%
59	14.809	4771	4780	4791	rBV2	1130190	1876965	7.25%	0.687%
60	14.916	4805	4820	4838	rBV3	12671526	25892656	100.00%	9.478%
61	14.984	4839	4845	4860	rVB4	391446	741633	2.86%	0.271%
62	15.083	4872	4882	4895	rVB	860543	1403595	5.42%	0.514%
63	15.195	4916	4924	4931	rVV5	392313	596532	2.30%	0.218%
64	15.236	4933	4939	4950	rVV	532040	769516	2.97%	0.282%
65	15.311	4954	4967	4982	rVB3	943065	2255709	8.71%	0.826%
66	15.450	5011	5019	5027	rBV	188946	293716	1.13%	0.108%
67	15.504	5027	5039	5054	rVB2	1332377	2478329	9.57%	0.907%

Sum of corrected areas: 273174662

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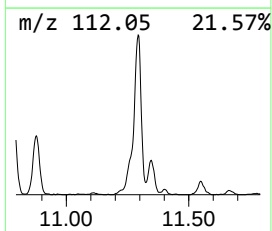
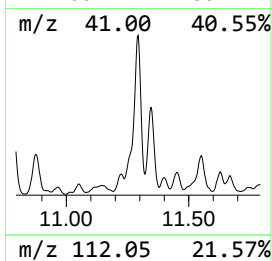
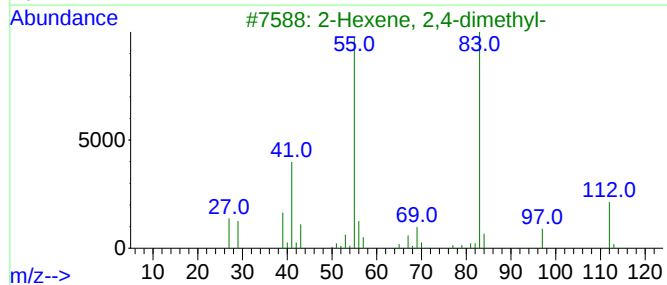
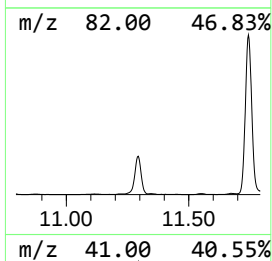
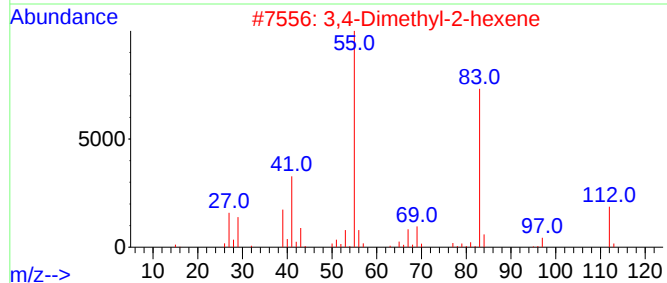
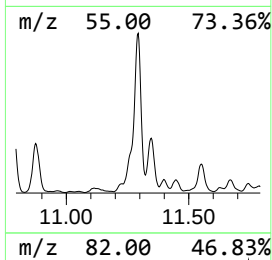
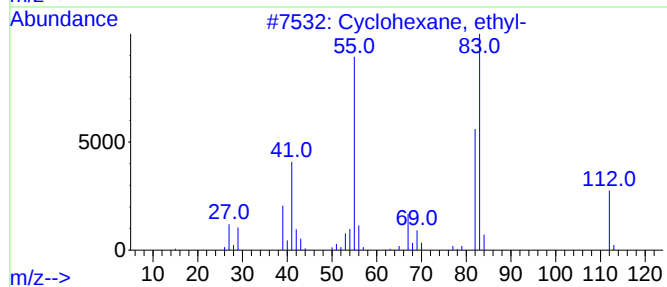
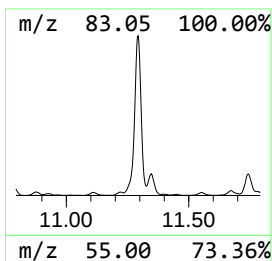
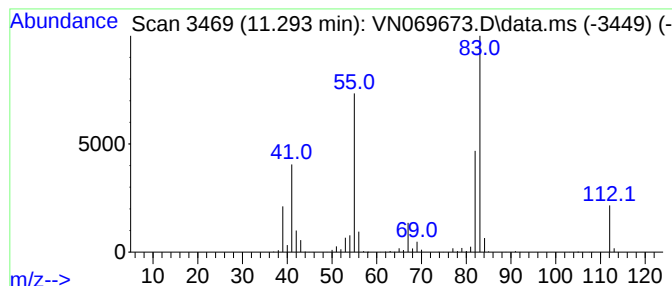
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclohexane, ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.293	22.66 ug/l	4124940	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, ethyl-	112	C8H16	001678-91-7	94
2			3,4-Dimethyl-2-hexene	112	C8H16	002213-37-8	62
3			2-Hexene, 2,4-dimethyl-	112	C8H16	014255-23-3	58
4			2-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-67-7	58
5			Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	53



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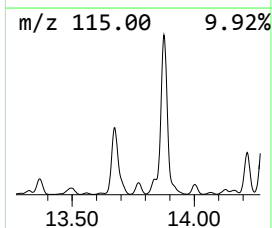
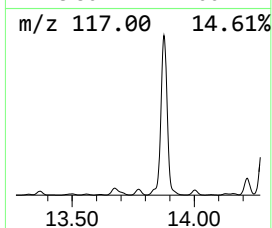
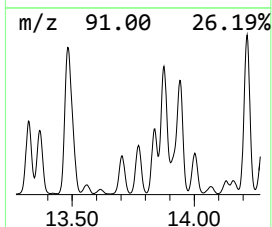
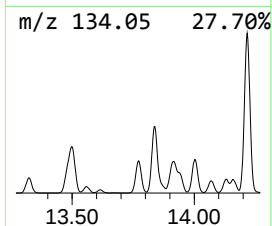
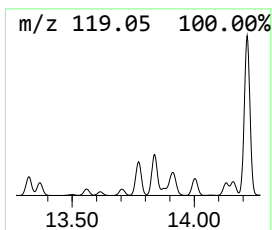
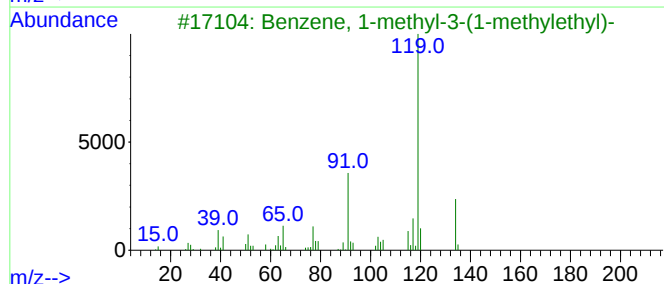
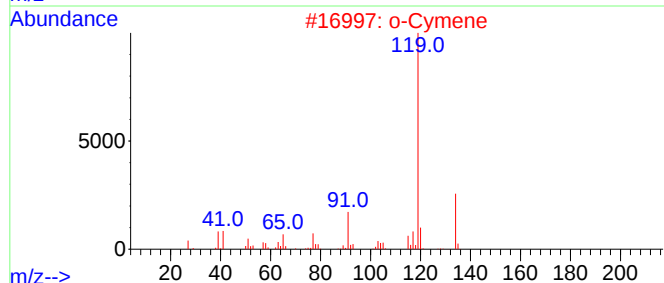
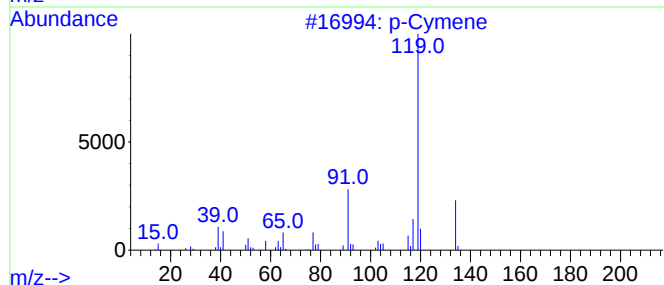
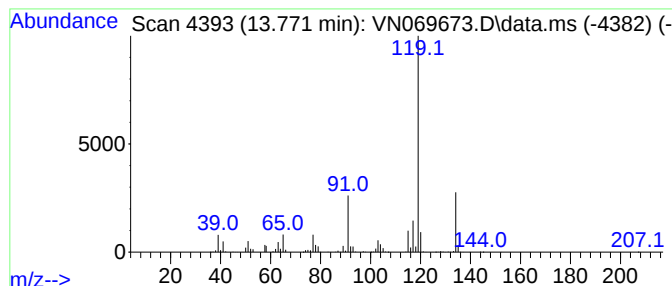
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 p-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.771	21.71 ug/l	3293720	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	97
2			o-Cymene	134	C10H14	000527-84-4	94
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	94
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91



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Misc : 5.00mL/MSVOA_N/WATER
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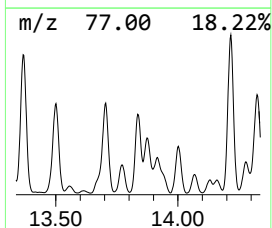
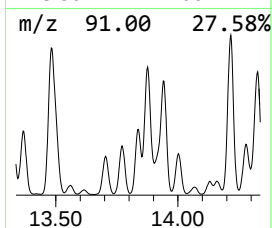
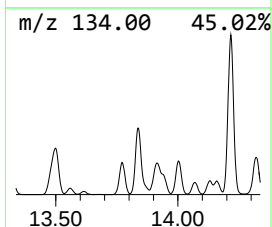
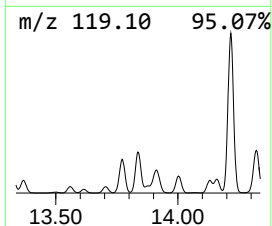
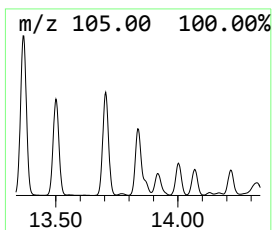
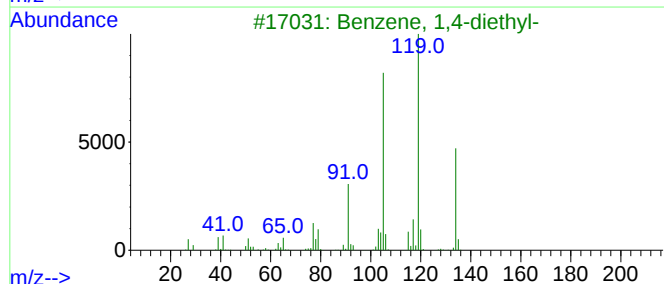
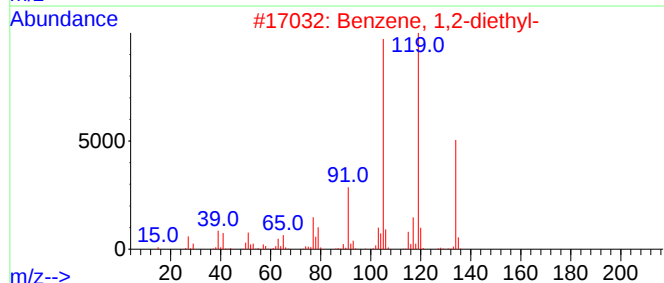
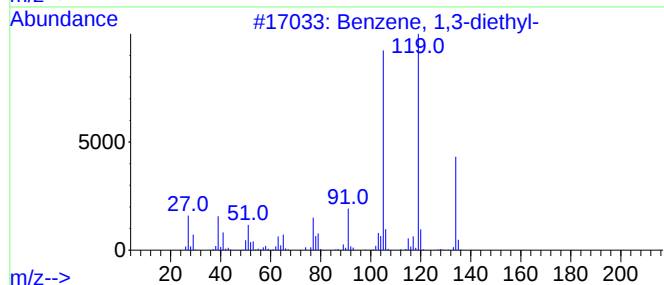
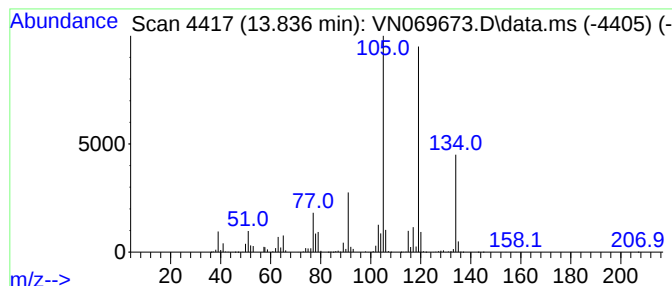
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,3-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.836	46.25 ug/l	7015330	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	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	83



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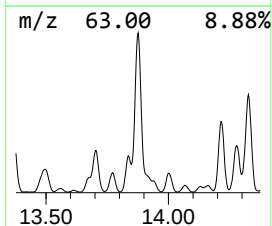
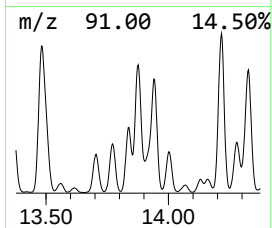
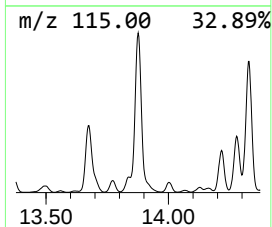
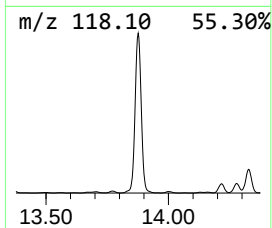
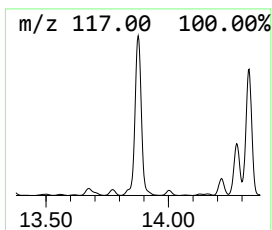
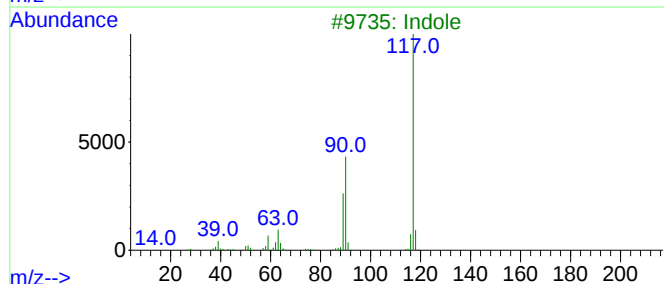
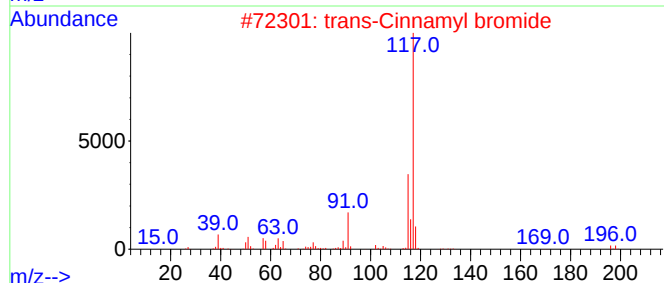
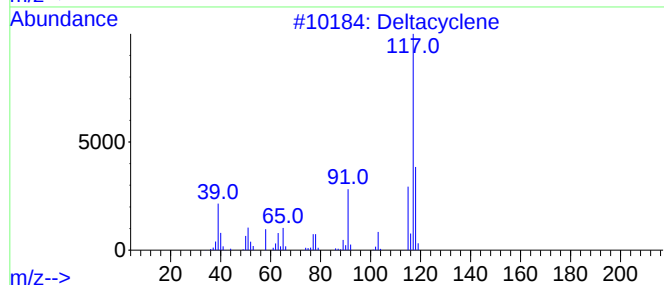
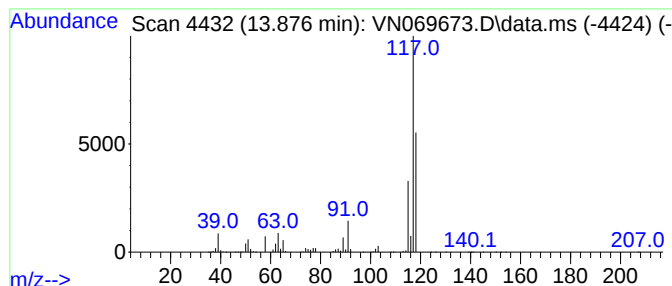
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.M
Quant Title : SW846 8260

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

Peak Number 4 Deltacyclene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	84.86 ug/l	12872100	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Deltacyclene	118	C9H10	007785-10-6	64
2			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53
3			Indole	117	C8H7N	000120-72-9	49
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	43
5			5H-1-Pyridine	117	C8H7N	000270-91-7	37



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ClientSampleId :

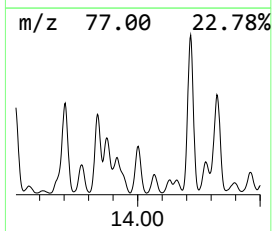
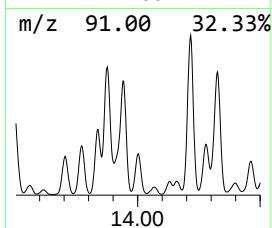
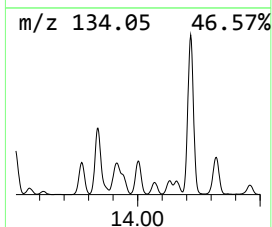
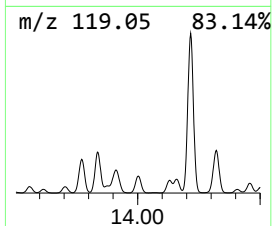
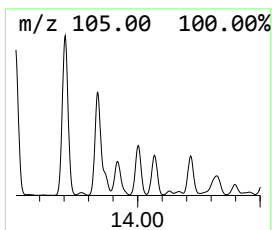
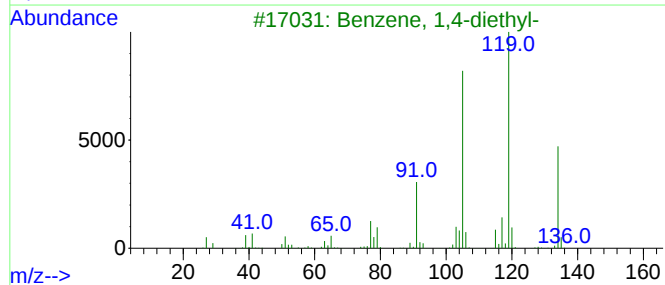
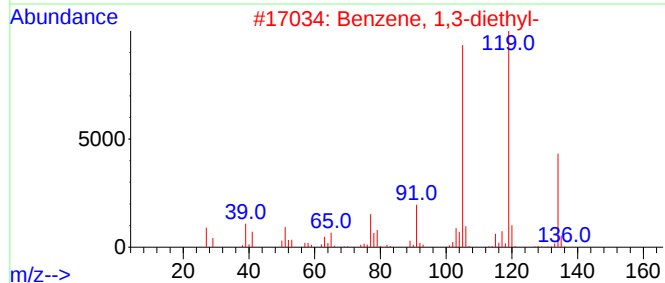
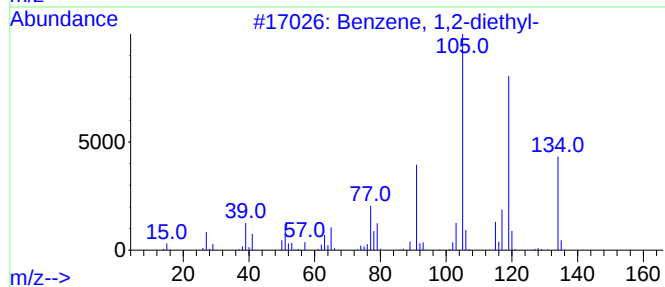
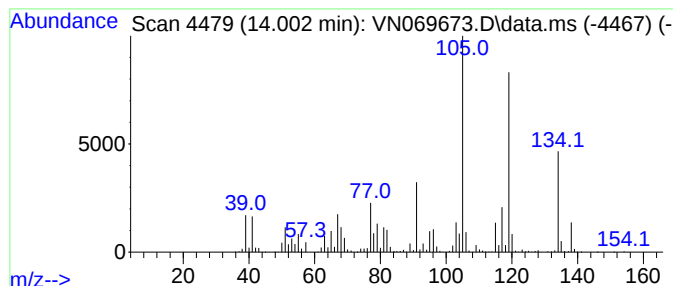
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.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.
14.002	32.54 ug/l	4936540	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, 1,3-diethyl-	134	C10H14	000141-93-5	76
3			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	70
4			2,6-Dimethyl-1,3,5,7-octatetraen...	134	C10H14	000460-01-5	68
5			1,3,8-p-Menthatriene	134	C10H14	018368-95-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069673.D
Acq On : 29 Nov 2021 19:09
Operator : JC/MD
Sample : M4852-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :

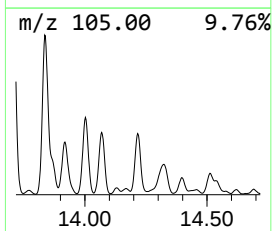
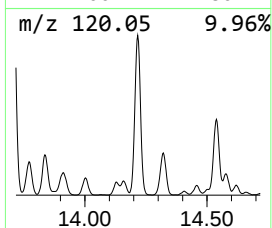
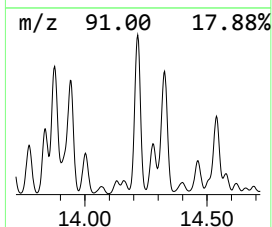
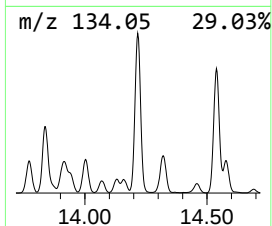
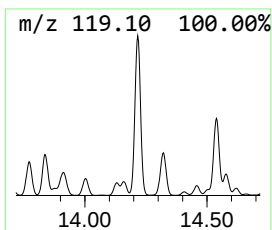
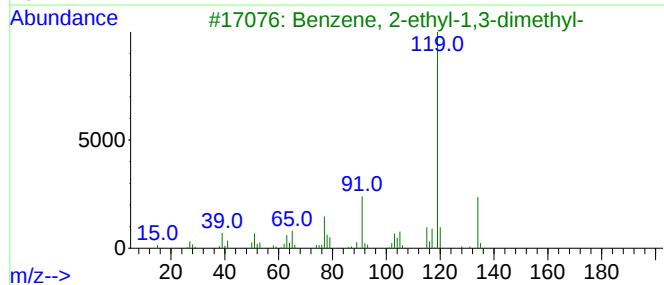
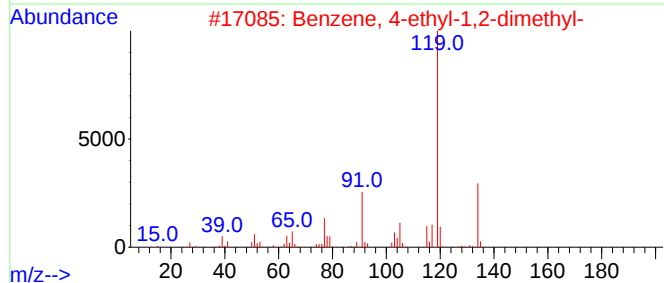
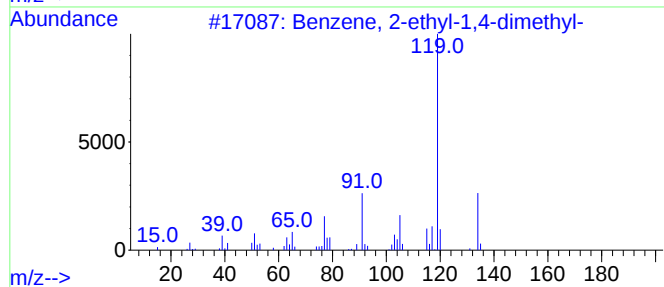
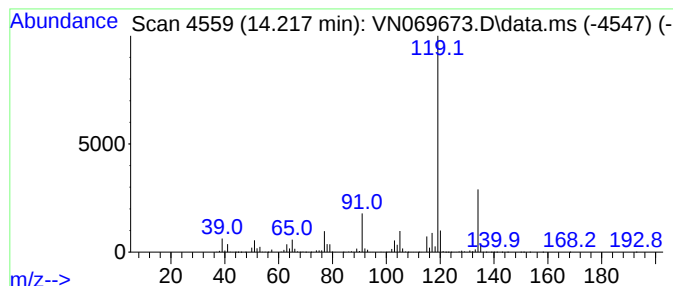
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	103.68 ug/l	15726500	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069673.D
Acq On : 29 Nov 2021 19:09
Operator : JC/MD
Sample : M4852-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :

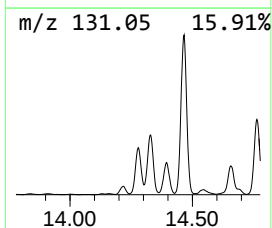
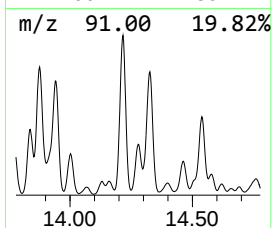
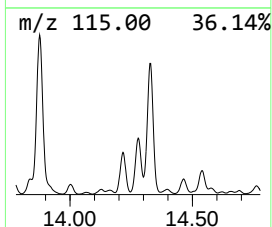
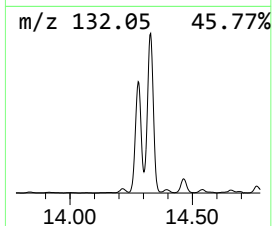
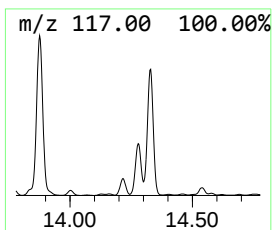
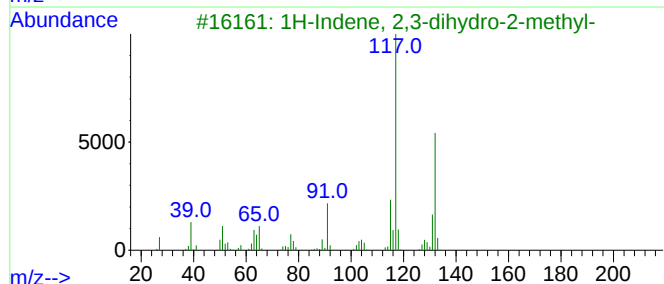
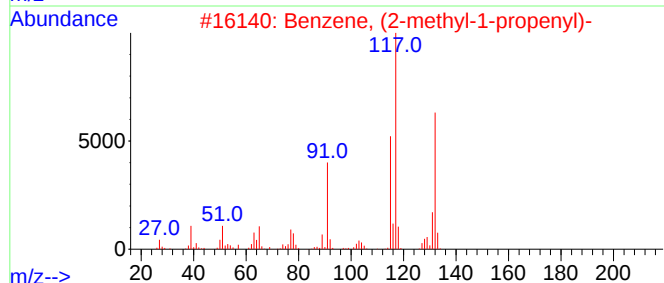
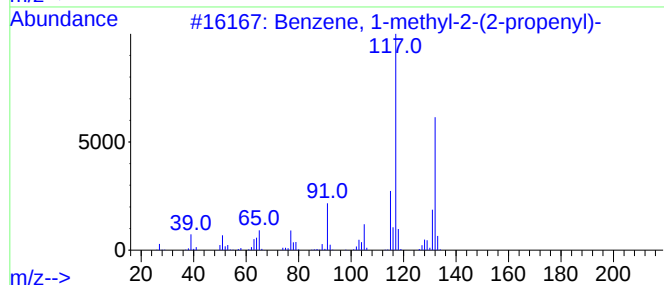
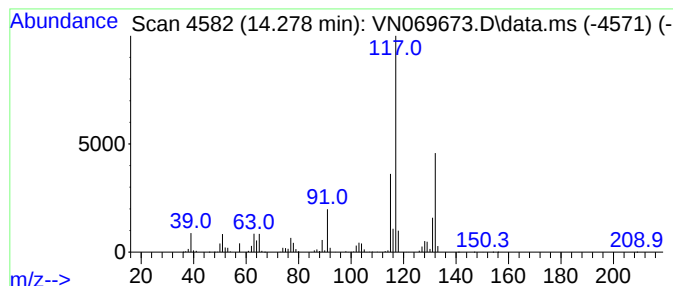
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-methyl-2-(2-prop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.278	37.46 ug/l	5682510	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	94
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	94
3			1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	93
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	91
5			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069673.D
Acq On : 29 Nov 2021 19:09
Operator : JC/MD
Sample : M4852-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :

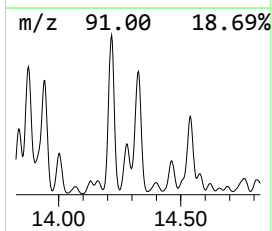
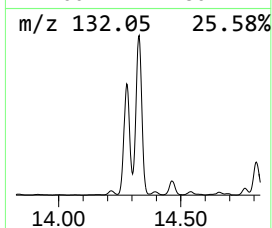
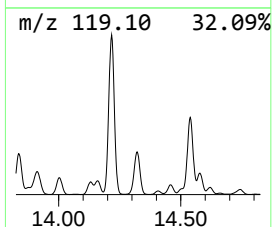
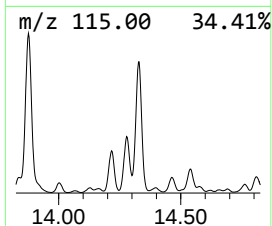
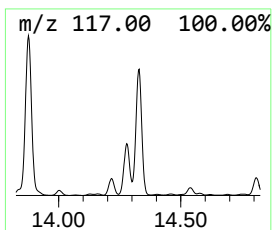
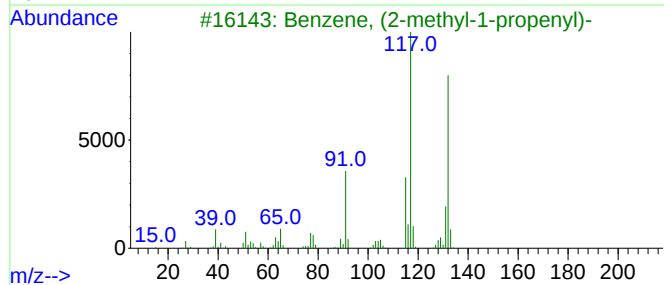
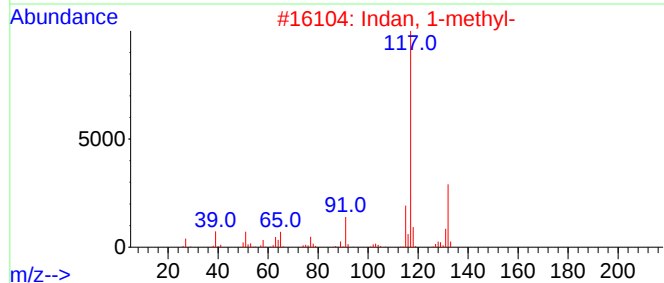
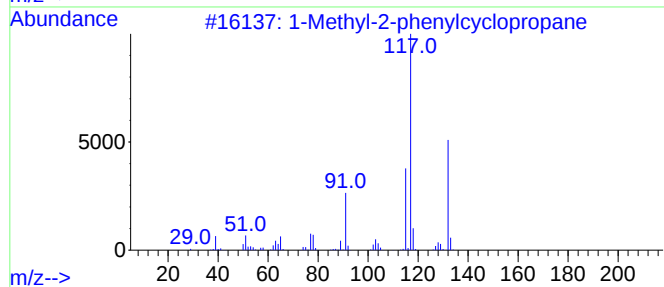
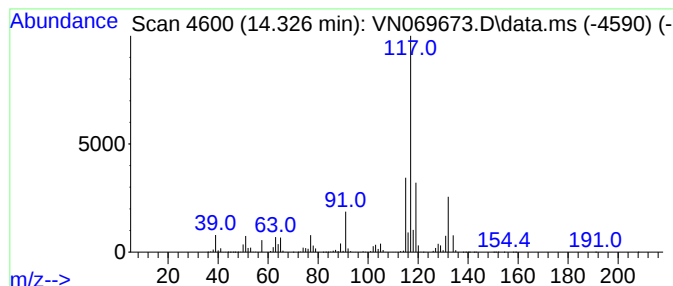
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Quant Title : SW846 8260

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

Peak Number 8 1-Methyl-2-phenylcyclopropane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.326	105.32 ug/l	15975900	1,4-Dichlorobenzene-d4	13.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	76
2		Indan, 1-methyl-	132	C10H12	000767-58-8	76
3		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	68
4		Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
5		3-Phenylbut-1-ene	132	C10H12	000934-10-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069673.D
Acq On : 29 Nov 2021 19:09
Operator : JC/MD
Sample : M4852-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :

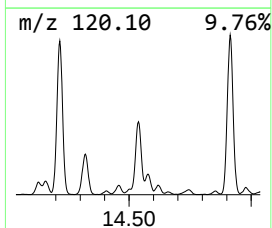
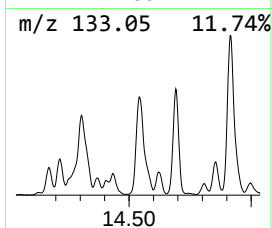
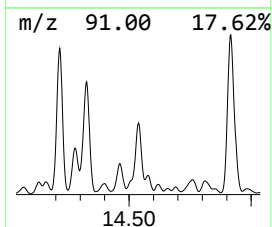
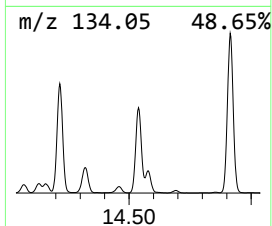
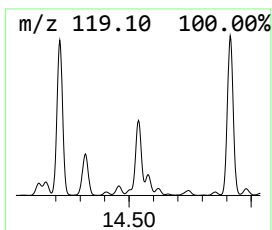
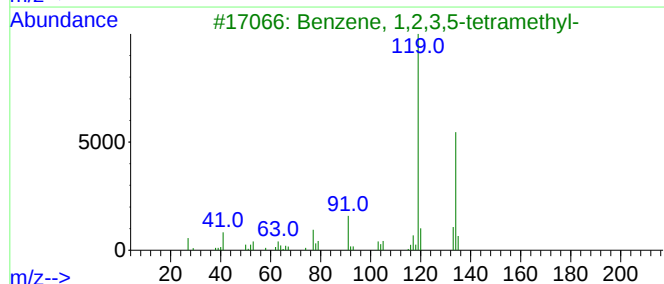
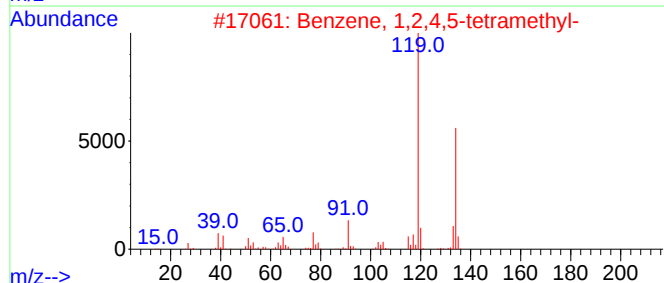
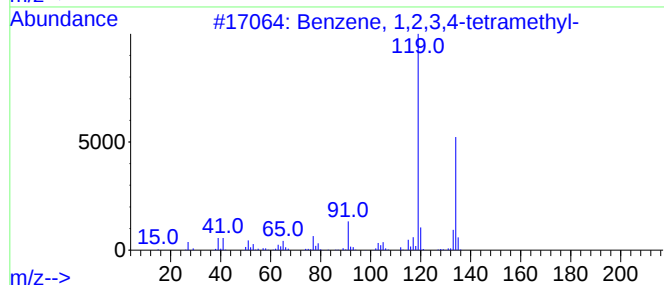
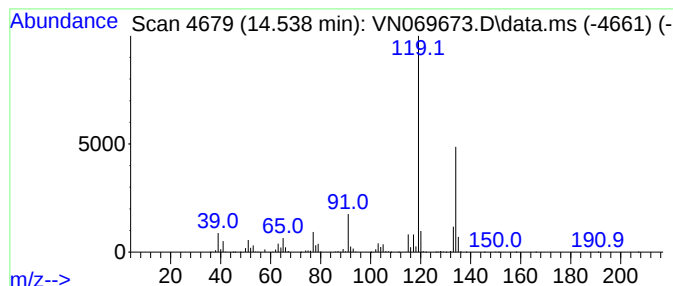
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.538	60.25 ug/l	9138480	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			o-Cymene	134	C10H14	000527-84-4	95
5			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069673.D
Acq On : 29 Nov 2021 19:09
Operator : JC/MD
Sample : M4852-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :

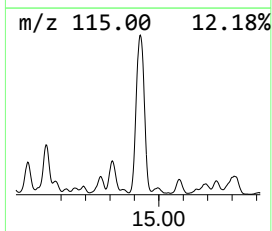
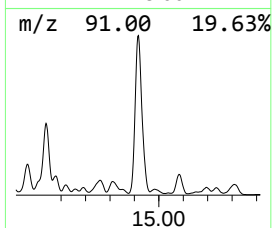
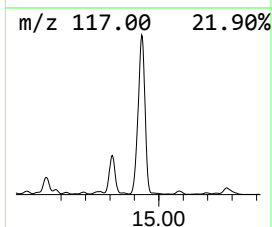
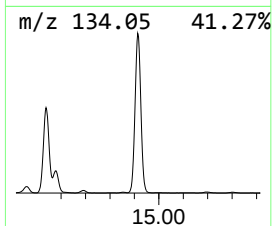
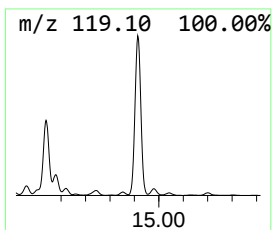
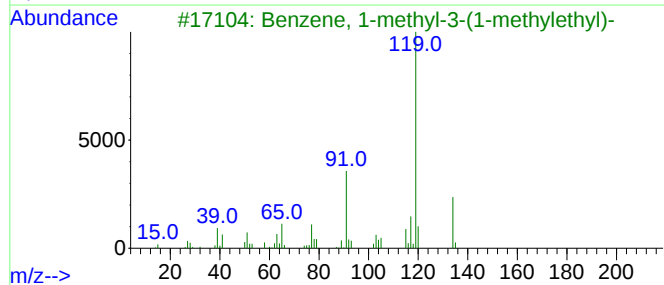
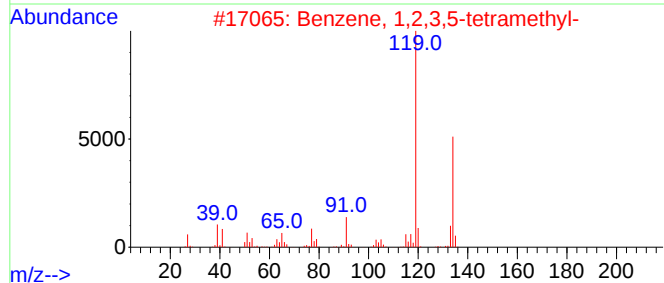
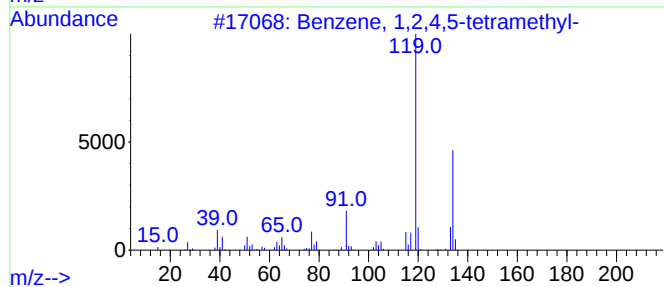
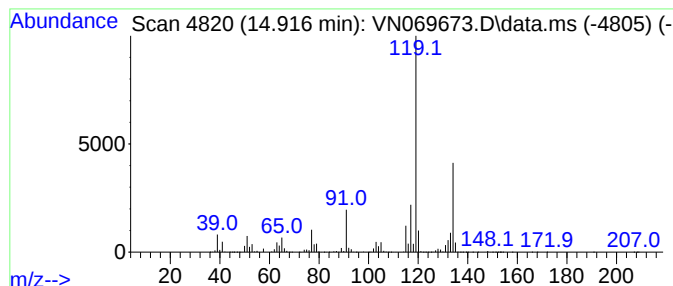
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	170.70 ug/l	25892700	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	94
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	90
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	90
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	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112921\
Data File : VN069673.D
Acq On : 29 Nov 2021 19:09
Operator : JC/MD
Sample : M4852-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110921W.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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p-Cymene	13.771	21.7	ug/l	3293720	4	13.675	7584270	50.0
Benzene, 1,3-di...	13.836	46.3	ug/l	7015330	4	13.675	7584270	50.0
Deltacyclene	13.876	84.9	ug/l	12872100	4	13.675	7584270	50.0
Benzene, 1,2-di...	14.002	32.5	ug/l	4936540	4	13.675	7584270	50.0
Benzene, 2-ethy...	14.217	103.7	ug/l	15726500	4	13.675	7584270	50.0
Benzene, 1-meth...	14.278	37.5	ug/l	5682510	4	13.675	7584270	50.0
1-Methyl-2-phen...	14.326	105.3	ug/l	15975900	4	13.675	7584270	50.0
Benzene, 1,2,3,...	14.538	60.3	ug/l	9138480	4	13.675	7584270	50.0
Benzene, 1,2,4,...	14.916	170.7	ug/l	25892700	4	13.675	7584270	50.0