

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
 Data File : VU048727.D
 Acq On : 28 May 2022 05:32
 Operator : SY/MD
 Sample : N3056-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VIBLK

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_U\Method\82U052622W.M
 Title : SW846 8260

Signal : TIC: VU048727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.375	1242	1255	1273	rVB	331410	691195	1.12%	0.278%
2	6.250	1512	1527	1567	rBV	469048	927069	1.50%	0.373%
3	6.764	1667	1687	1710	rBV	366993	760283	1.23%	0.306%
4	7.899	2031	2040	2054	rVB	706858	1227624	1.98%	0.494%
5	9.417	2499	2512	2522	rBV	704360	1166015	1.88%	0.470%
6	9.571	2547	2560	2583	rVV	6251634	9922222	16.04%	3.996%
7	9.693	2587	2598	2613	rVB	666730	1154301	1.87%	0.465%
8	10.102	2713	2725	2754	rVB	706356	1195126	1.93%	0.481%
9	10.484	2831	2844	2878	rVB	2414179	3837650	6.20%	1.546%
10	10.632	2878	2890	2904	rBV	634875	1035637	1.67%	0.417%
11	10.905	2959	2975	2992	rBV	2512158	3883528	6.28%	1.564%
12	11.024	2993	3012	3022	rVV	1359268	2368559	3.83%	0.954%
13	11.089	3022	3032	3049	rVB	1539988	2402948	3.88%	0.968%
14	11.291	3081	3095	3116	rBV	4254887	6742646	10.90%	2.716%
15	11.468	3131	3150	3166	rBV	10691916	16224355	26.22%	6.534%
16	11.745	3221	3236	3244	rBV	769439	1186134	1.92%	0.478%
17	11.809	3244	3256	3270	rVB4	1073343	2062364	3.33%	0.831%
18	11.896	3270	3283	3295	rBV	5246427	8040258	13.00%	3.238%
19	12.095	3330	3345	3363	rBV	14331461	22857735	36.95%	9.206%
20	12.188	3363	3374	3388	rVB4	1230619	2292485	3.71%	0.923%
21	12.465	3449	3460	3466	rBV	998477	1600036	2.59%	0.644%
22	12.497	3466	3470	3480	rVB	678222	890736	1.44%	0.359%
23	12.571	3480	3493	3501	rBV	1805791	2816592	4.55%	1.134%
24	12.684	3515	3528	3548	rBV	5657446	9211739	14.89%	3.710%
25	12.876	3577	3588	3599	rVB	667509	1047680	1.69%	0.422%
26	12.973	3600	3618	3626	rBV	1256411	1897321	3.07%	0.764%
27	13.028	3626	3635	3651	rVB	2514746	3919060	6.33%	1.578%
28	13.294	3701	3718	3730	rBV	4639877	6972471	11.27%	2.808%
29	13.452	3746	3767	3780	rBV3	5541746	9517654	15.38%	3.833%
30	13.629	3810	3822	3842	rVB2	2888206	4704060	7.60%	1.895%
31	13.786	3861	3871	3880	rBV	568661	911554	1.47%	0.367%
32	13.950	3914	3922	3935	rVB3	345940	749780	1.21%	0.302%
33	14.095	3947	3967	3987	rBV2	36007239	61868476	100.00%	24.918%
34	14.683	4136	4150	4156	rBV4	300210	702925	1.14%	0.283%
35	14.809	4178	4189	4203	rVB2	475884	994860	1.61%	0.401%
36	15.224	4306	4318	4344	rVB	6663115	10673566	17.25%	4.299%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Title : SW846 8260

37	15.413	4363	4377	4403	rBV	17862663	28296554	45.74%	11.396%
38	15.954	4527	4545	4556	rBV	1800850	2843233	4.60%	1.145%
39	16.146	4589	4605	4611	rBV	472663	784734	1.27%	0.316%
40	16.262	4627	4641	4666	rVB	949765	1729742	2.80%	0.697%
41	16.407	4667	4686	4694	rBV	1929214	3267013	5.28%	1.316%
42	16.445	4694	4698	4712	rVB	555930	802441	1.30%	0.323%
43	17.095	4887	4900	4918	rBV	1269471	2112675	3.41%	0.851%

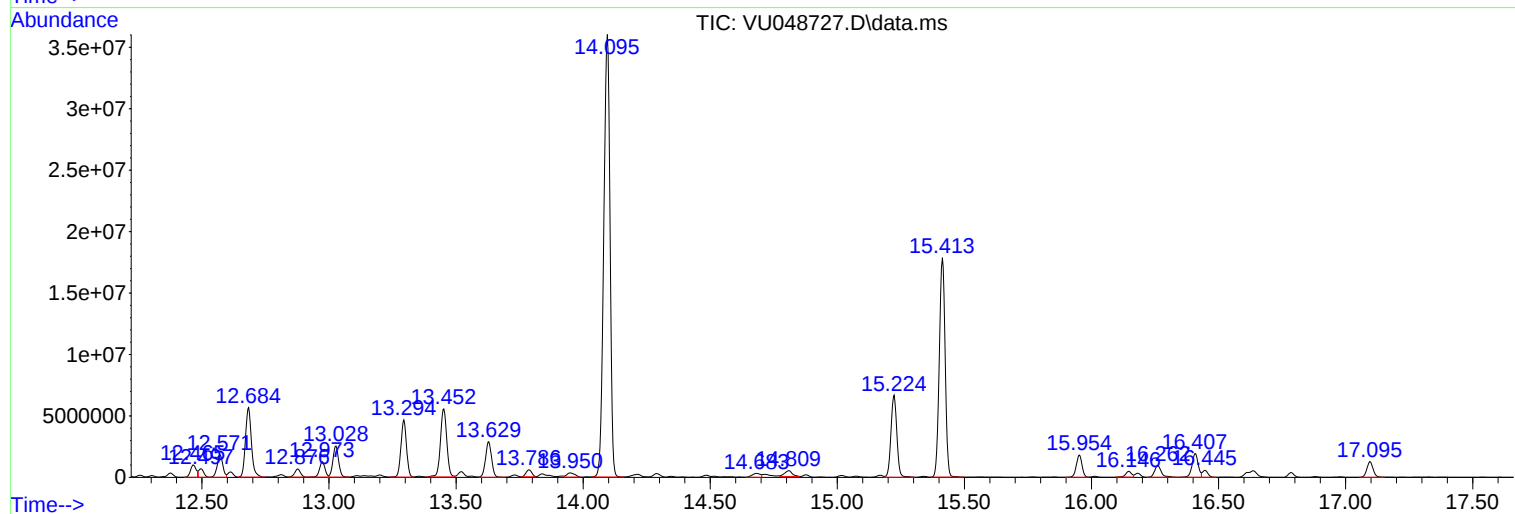
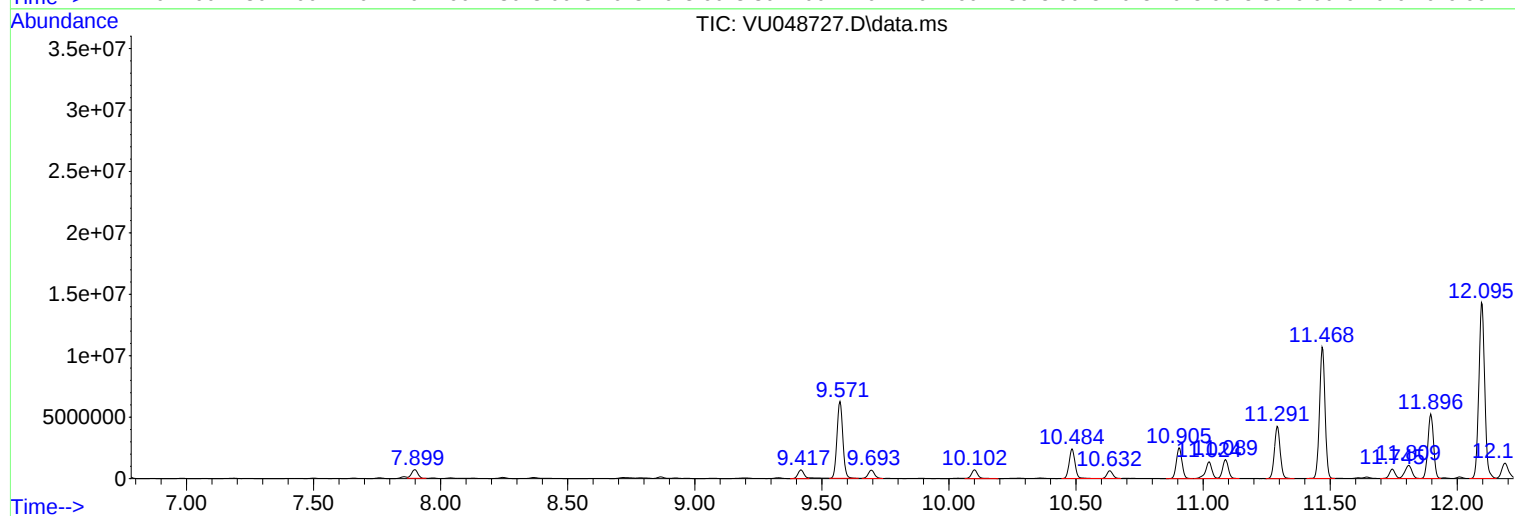
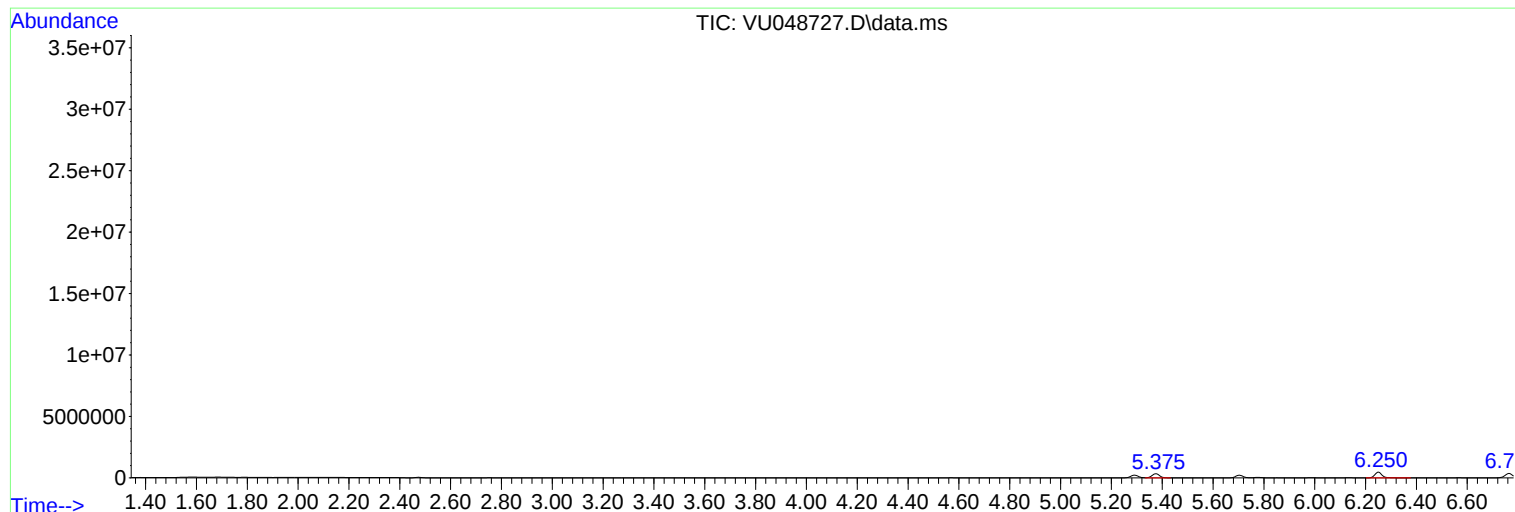
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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



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Sample : N3056-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK

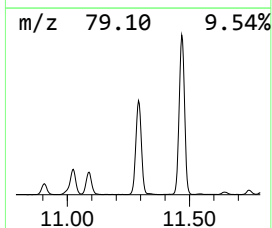
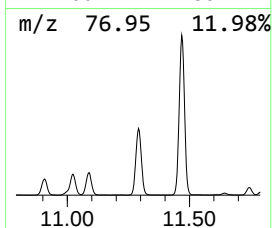
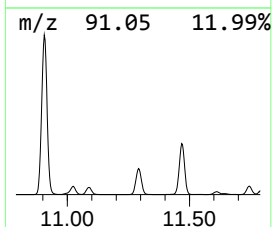
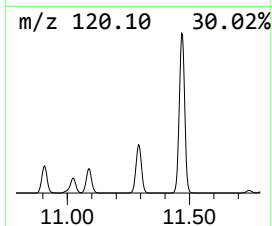
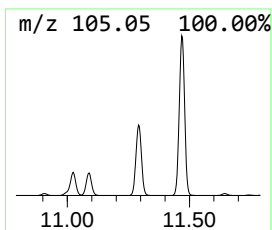
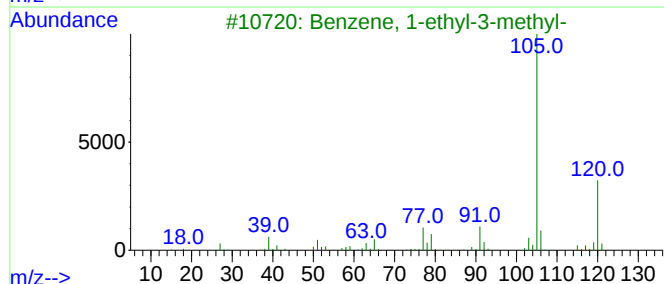
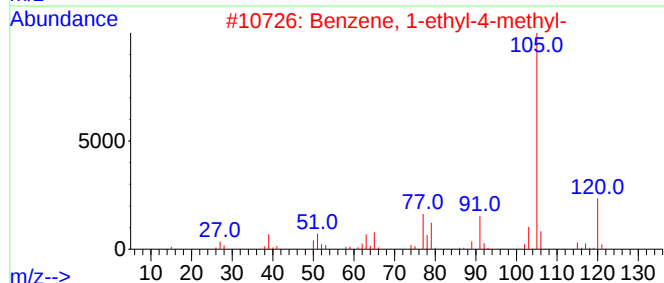
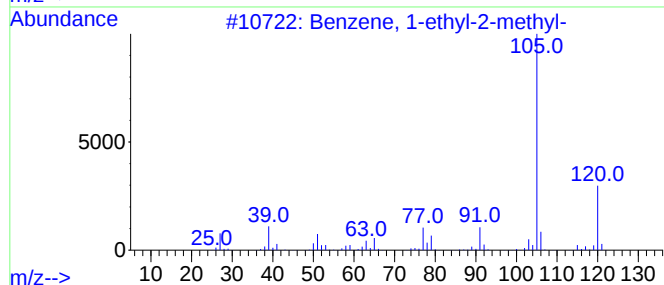
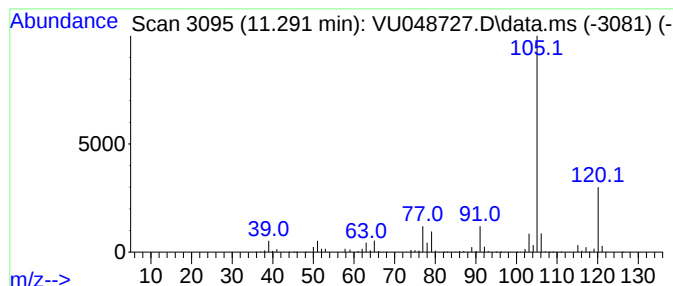
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.291	163.47 ug/l	6742650	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK

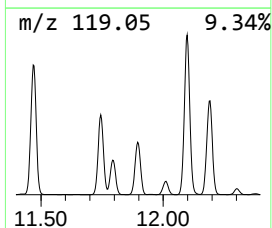
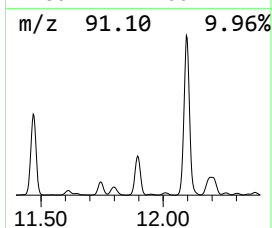
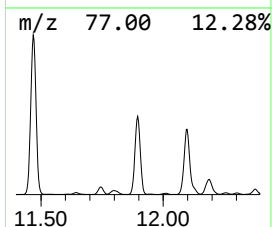
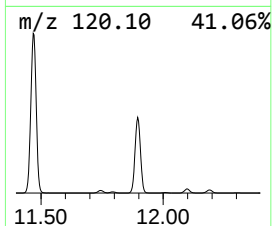
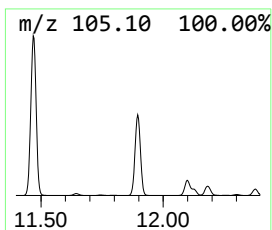
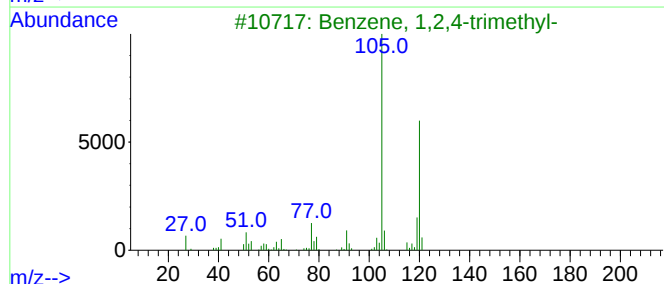
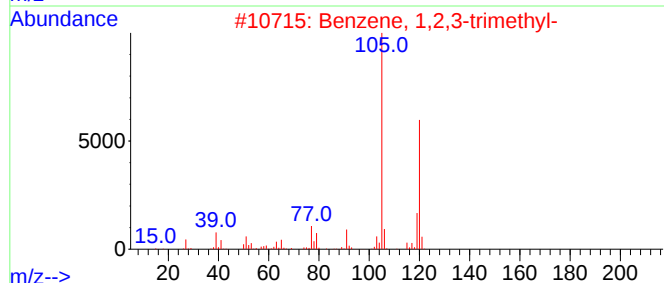
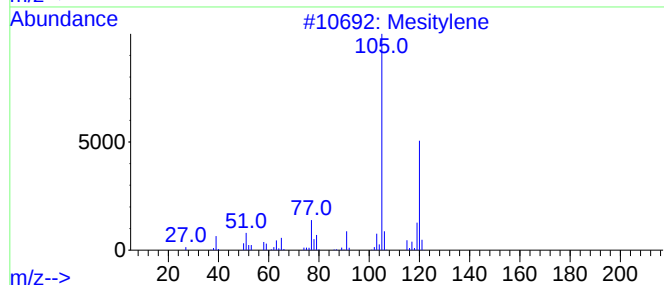
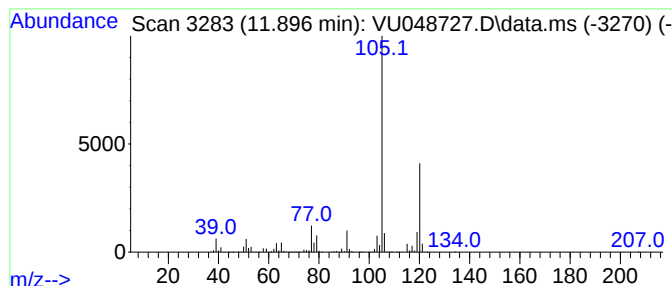
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.896	194.93 ug/l	8040260	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK

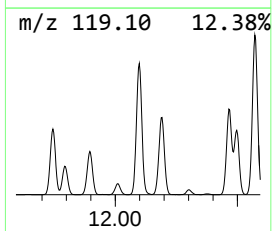
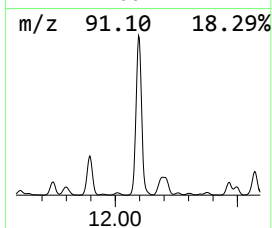
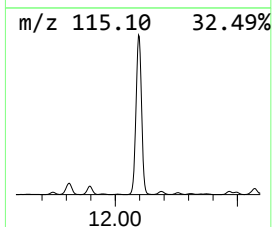
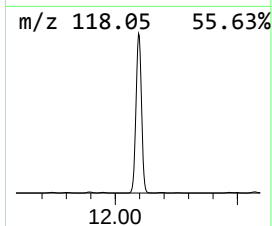
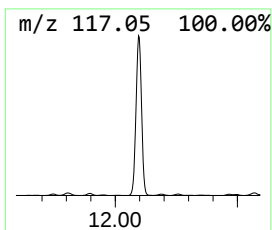
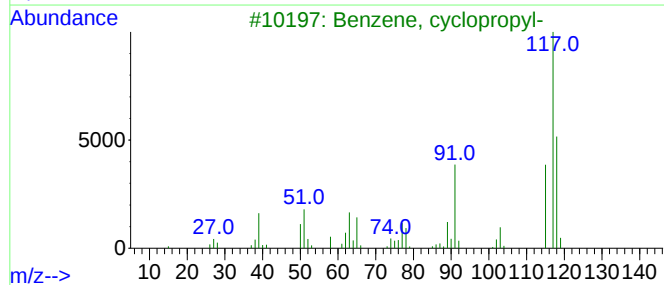
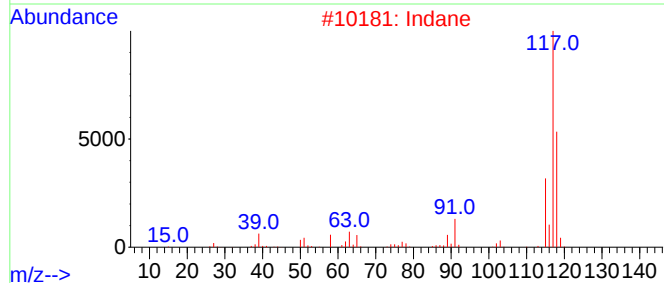
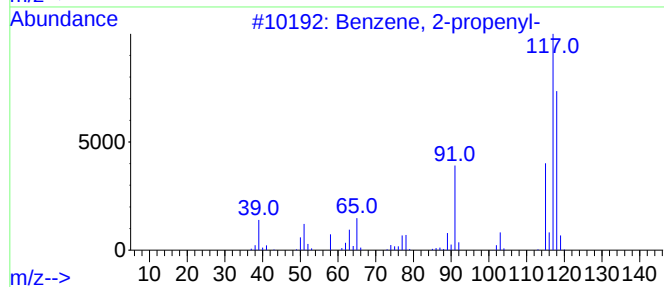
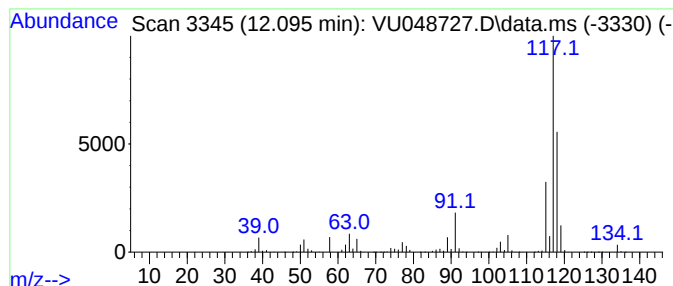
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 2-propenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.095	554.16 ug/l	22857700	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
2			Indane	118	C9H10	000496-11-7	81
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4			Δ-tetralene	118	C9H10	007785-10-6	64
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	49



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VIBLK

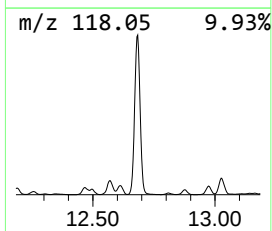
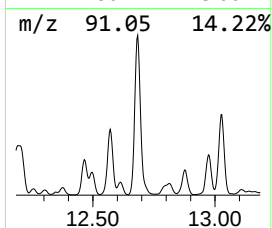
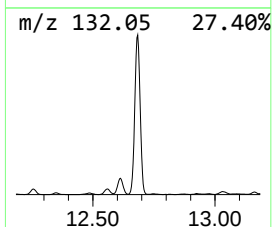
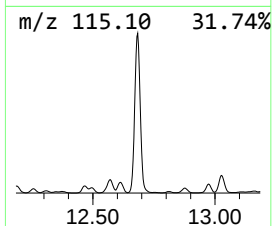
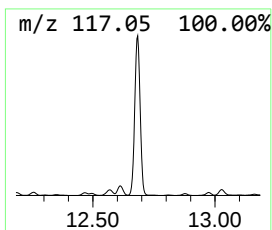
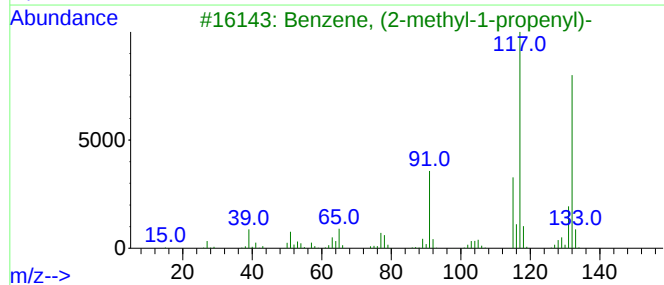
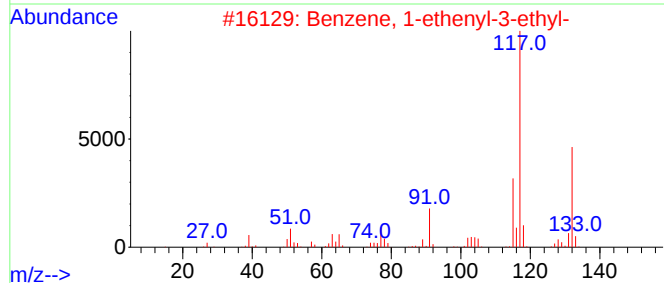
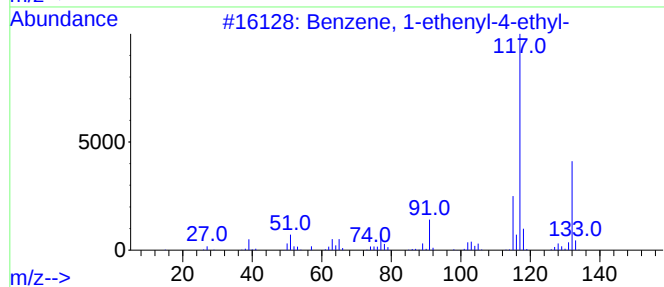
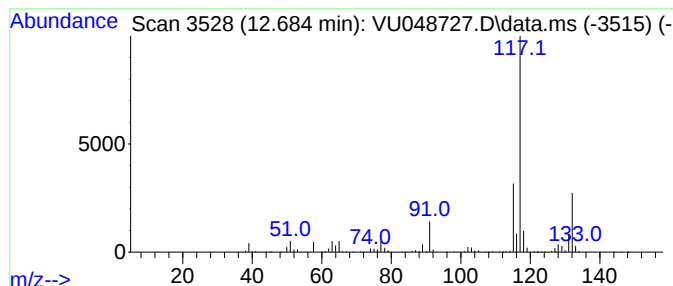
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.684	223.33 ug/l	9211740	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	90
5			Indan, 1-methyl-	132	C10H12	000767-58-8	90



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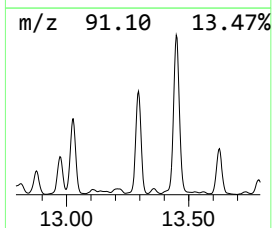
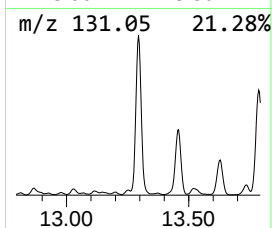
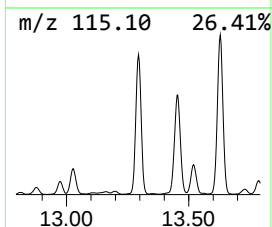
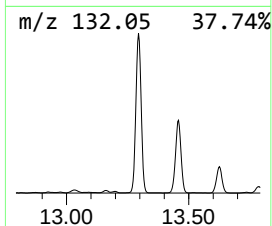
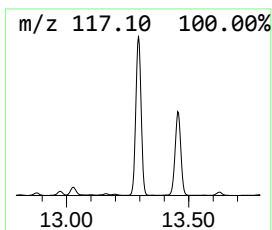
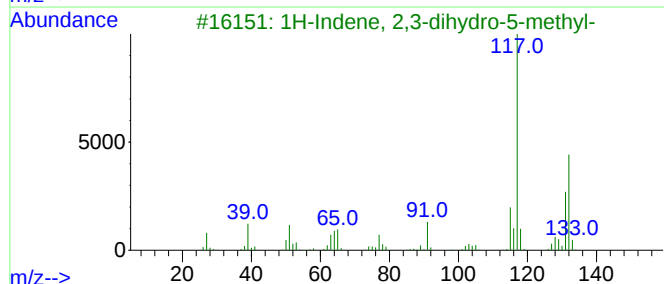
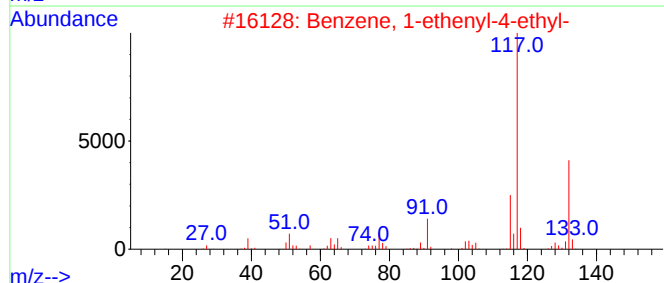
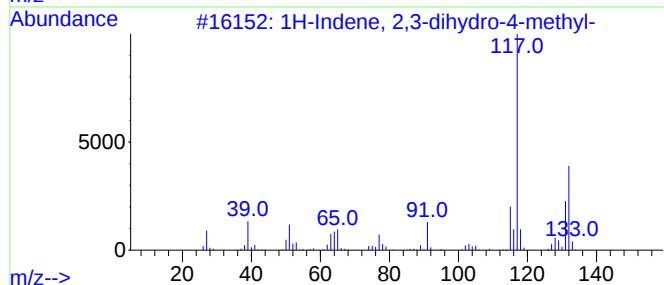
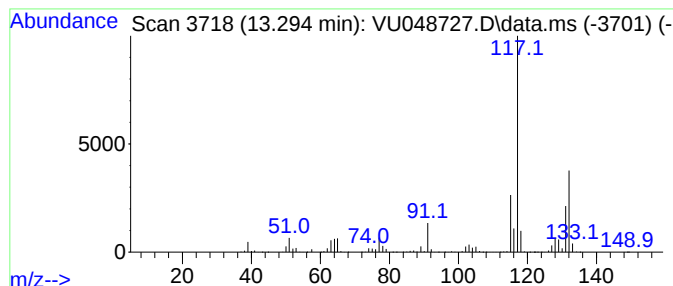
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Quant Title : SW846 8260

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

Peak Number 5 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.294	169.04 ug/l	6972470	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
4			3-Phenylbut-1-ene	132	C10H12	000934-10-1	91
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048727.D
Acq On : 28 May 2022 05:32
Operator : SY/MD
Sample : N3056-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK

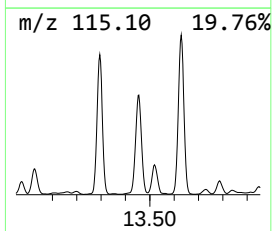
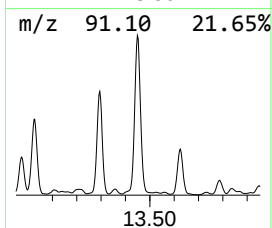
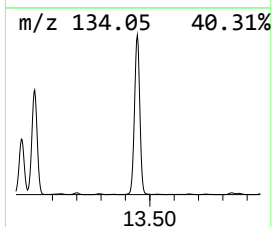
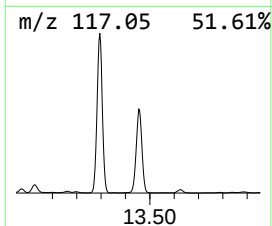
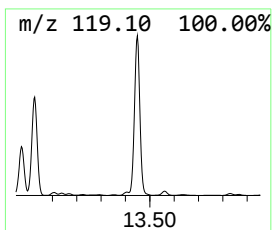
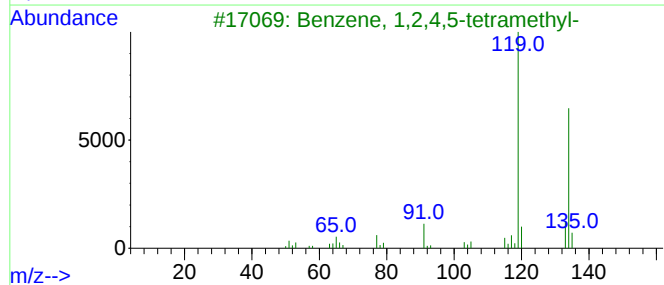
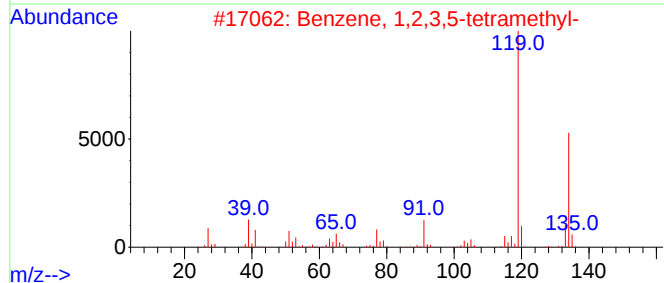
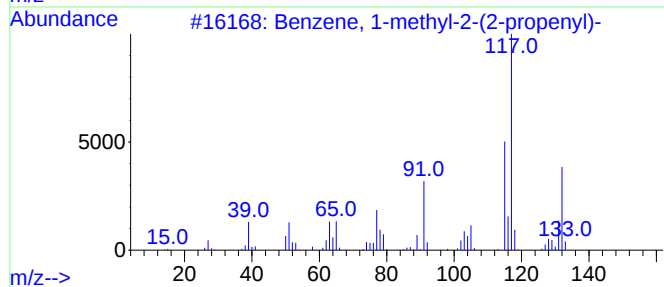
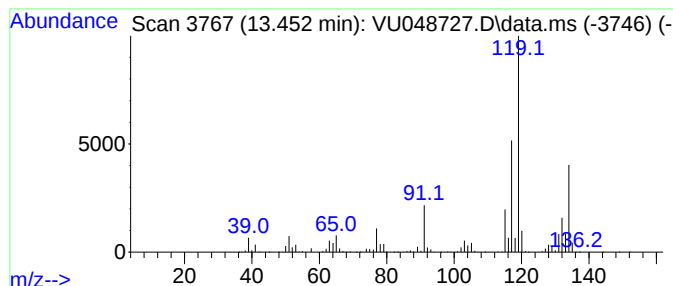
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-methyl-2-(2-prop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.452	230.75 ug/l	9517650	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	70
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	70
4			o-Cymene	134	C10H14	000527-84-4	70
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048727.D
Acq On : 28 May 2022 05:32
Operator : SY/MD
Sample : N3056-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK

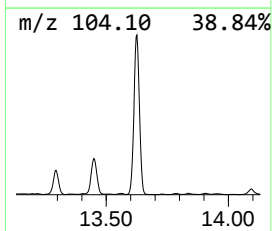
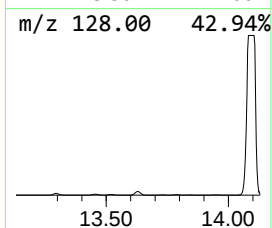
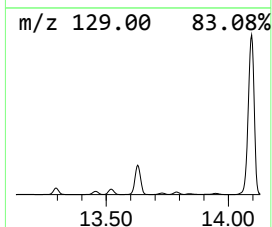
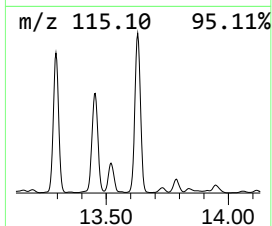
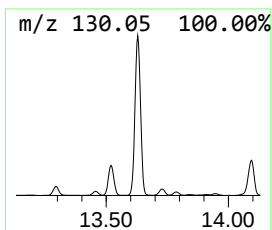
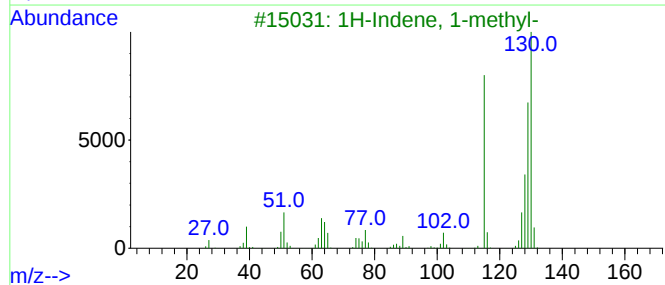
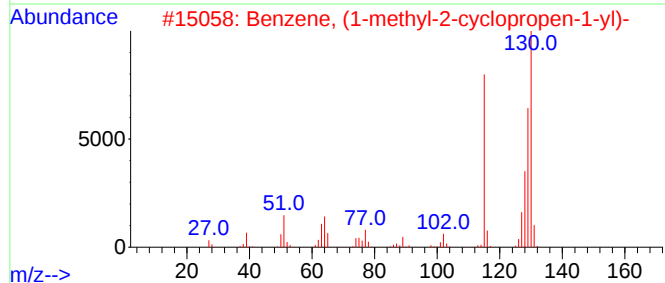
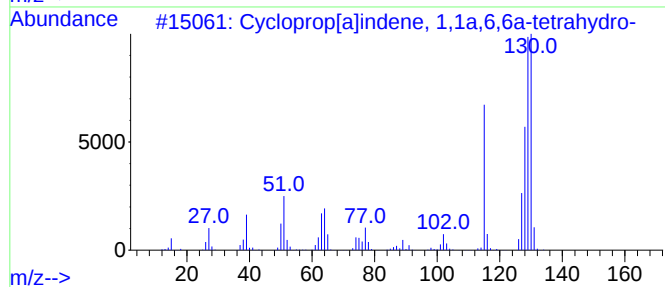
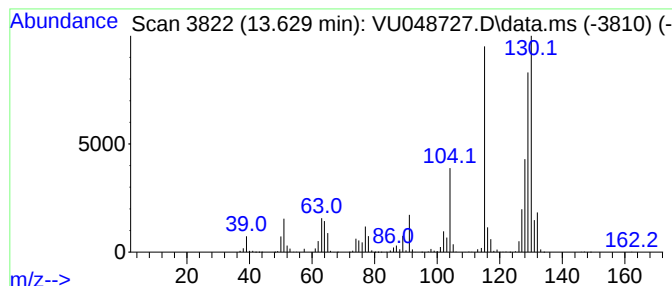
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Quant Title : SW846 8260

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

Peak Number 7 Cycloprop[a]indene, 1,1a,6,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.629	114.05 ug/l	4704060	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	97
2			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
3			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	96
4			2-Methylindene	130	C10H10	002177-47-1	95
5			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048727.D
Acq On : 28 May 2022 05:32
Operator : SY/MD
Sample : N3056-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK

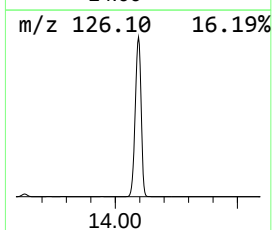
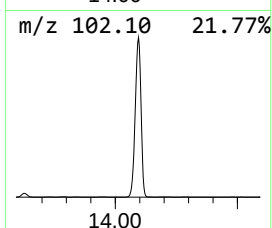
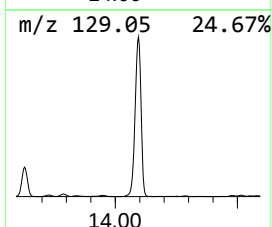
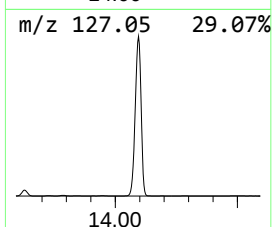
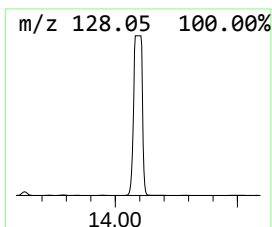
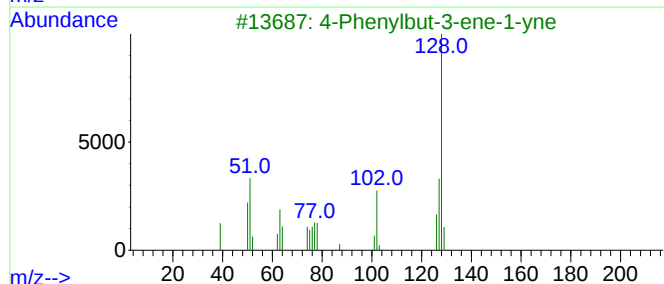
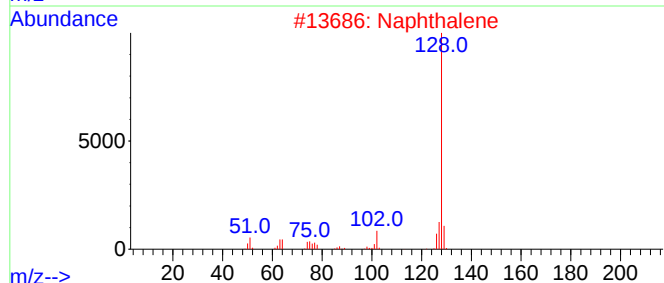
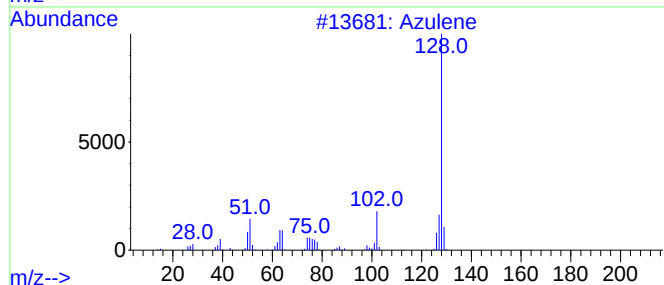
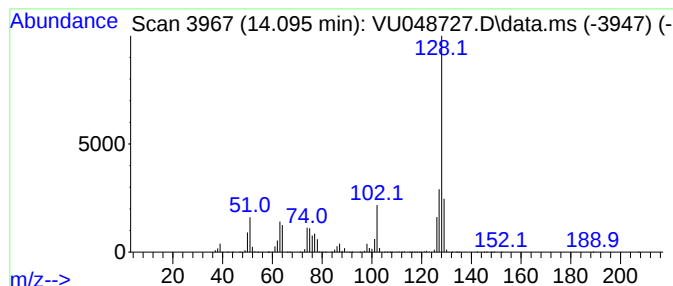
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Quant Title : SW846 8260

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

Peak Number 8 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.095	1499.94 ug/l	61868500	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azulene	128	C10H8	000275-51-4	87
2			Naphthalene	128	C10H8	000091-20-3	87
3			4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	74
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	74
5			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048727.D
Acq On : 28 May 2022 05:32
Operator : SY/MD
Sample : N3056-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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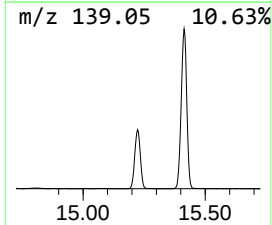
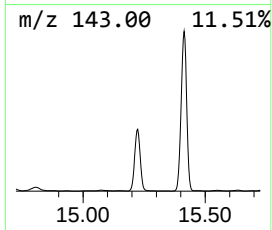
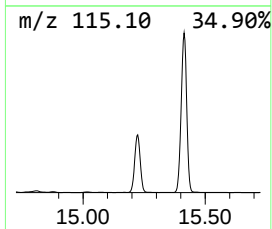
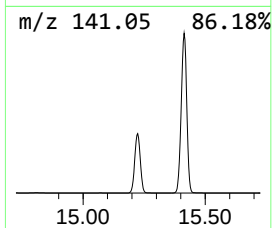
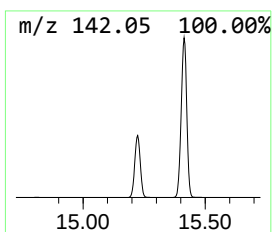
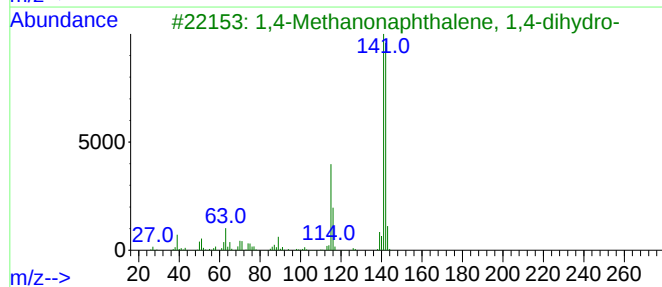
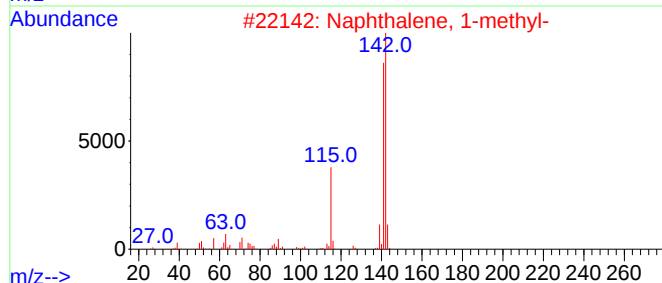
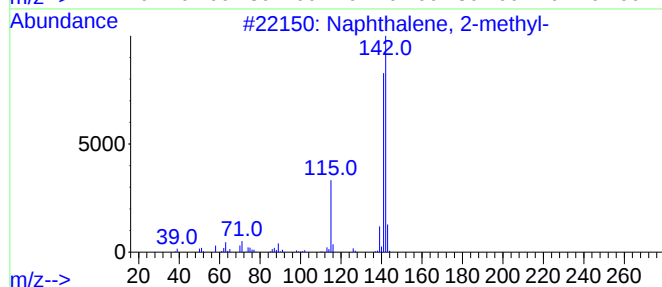
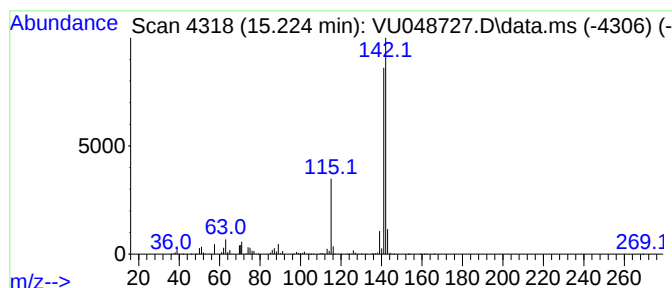
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Quant Title : SW846 8260

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

Peak Number 9 1,4-Methanonaphthalene, 1,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.224	258.77 ug/l	10673600	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048727.D
Acq On : 28 May 2022 05:32
Operator : SY/MD
Sample : N3056-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

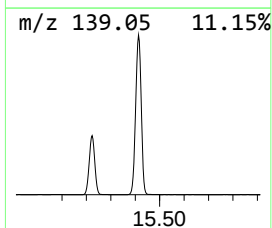
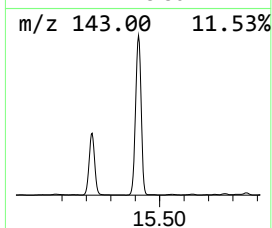
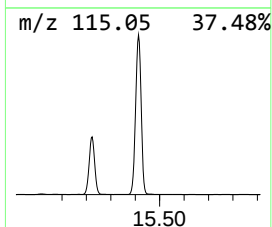
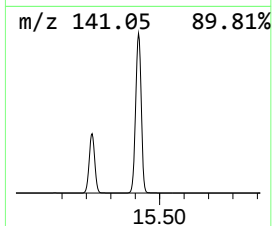
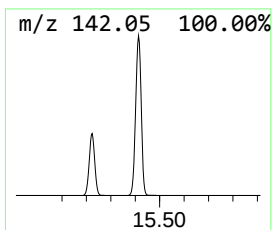
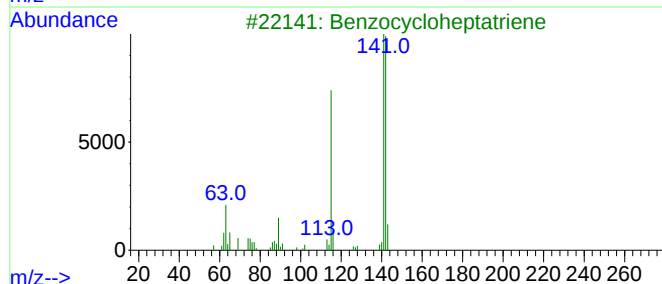
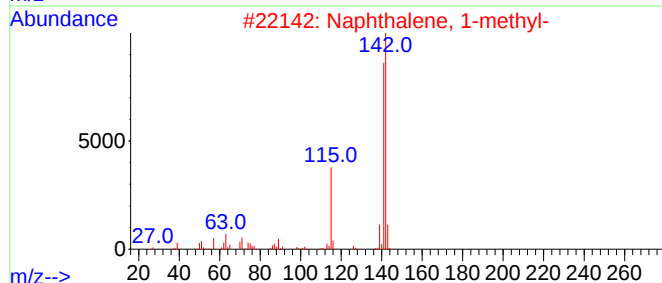
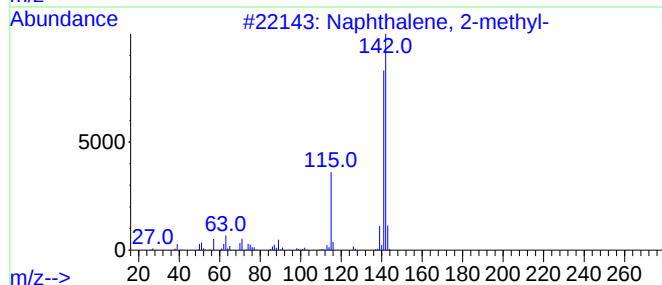
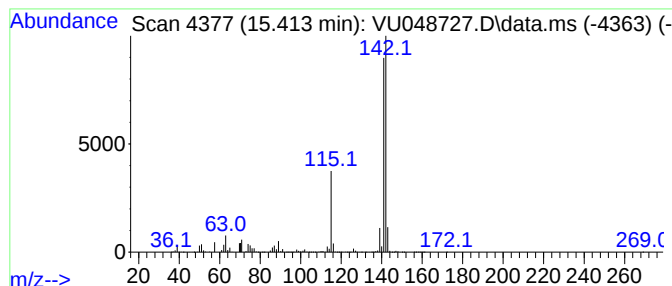
Instrument :
MSVOA_U
ClientSampleId :
VIBLK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 10 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.413	686.02 ug/l	28296600	1,4-Dichlorobenzene-d4	11.812	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048727.D
Acq On : 28 May 2022 05:32
Operator : SY/MD
Sample : N3056-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.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
Benzene, 1-ethy...	11.291	163.5	ug/l	6742650	4	11.812	2062360	50.0
Benzene, 1,2,3-...	11.896	194.9	ug/l	8040260	4	11.812	2062360	50.0
Benzene, 2-prop...	12.095	554.2	ug/l	22857700	4	11.812	2062360	50.0
Benzene, 1-ethe...	12.684	223.3	ug/l	9211740	4	11.812	2062360	50.0
1H-Indene, 2,3-...	13.294	169.0	ug/l	6972470	4	11.812	2062360	50.0
Benzene, 1-meth...	13.452	230.8	ug/l	9517650	4	11.812	2062360	50.0
Cycloprop[a]ind...	13.629	114.1	ug/l	4704060	4	11.812	2062360	50.0
Azulene	14.095	1499.9	ug/l	61868500	4	11.812	2062360	50.0
1,4-Methanonaph...	15.224	258.8	ug/l	10673600	4	11.812	2062360	50.0
Benzocyclohepta...	15.413	686.0	ug/l	28296600	4	11.812	2062360	50.0