

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
 Data File : VU048728.D
 Acq On : 28 May 2022 05:55
 Operator : SY/MD
 Sample : N3033-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 53 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 TW-2

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: VU048728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.472	32	41	56	rBV	173243	403358	30.91%	3.447%
2	2.626	390	400	410	rBV	8012	13166	1.01%	0.113%
3	2.752	430	439	451	rBV	8709	16673	1.28%	0.142%
4	5.292	1211	1229	1242	rBV	209671	447934	34.33%	3.828%
5	5.375	1242	1255	1277	rVB	316049	651545	49.94%	5.568%
6	5.703	1339	1357	1380	rBV2	210498	431058	33.04%	3.684%
7	6.250	1510	1527	1559	rBV	448373	849307	65.09%	7.258%
8	7.899	2023	2040	2058	rBV	634274	1092456	83.73%	9.336%
9	9.417	2499	2512	2531	rBV	662597	1091627	83.67%	9.329%
10	9.571	2550	2560	2573	rVB2	26490	42760	3.28%	0.365%
11	9.694	2582	2598	2614	rVB4	8784	16329	1.25%	0.140%
12	10.632	2877	2890	2916	rBV	589763	954573	73.16%	8.158%
13	10.909	2965	2976	2990	rBV2	9080	14922	1.14%	0.128%
14	11.295	3086	3096	3106	rBV	10387	16084	1.23%	0.137%
15	11.468	3137	3150	3167	rBV	31077	50302	3.86%	0.430%
16	11.812	3244	3257	3274	rBV	811369	1304736	100.00%	11.150%
17	11.896	3275	3283	3292	rVB3	12117	19712	1.51%	0.168%
18	12.095	3334	3345	3364	rVB2	42662	69568	5.33%	0.595%
19	12.684	3515	3528	3542	rBV2	14085	23173	1.78%	0.198%
20	13.295	3708	3718	3729	rBV2	14951	24534	1.88%	0.210%
21	13.449	3757	3766	3779	rVB3	17286	28134	2.16%	0.240%
22	13.629	3812	3822	3833	rBV3	11355	18155	1.39%	0.155%
23	14.086	3949	3964	3981	rBV	415443	688449	52.77%	5.884%
24	14.221	3995	4006	4017	rVB6	7400	14097	1.08%	0.120%
25	15.224	4304	4318	4337	rBV	320773	513381	39.35%	4.387%
26	15.407	4363	4375	4399	rBV	635443	1036215	79.42%	8.856%
27	15.954	4532	4545	4558	rBV	211464	334090	25.61%	2.855%
28	16.147	4592	4605	4611	rBV	51612	84189	6.45%	0.719%
29	16.182	4612	4616	4627	rVV2	30022	42011	3.22%	0.359%
30	16.262	4630	4641	4662	rVB	102518	189845	14.55%	1.622%
31	16.410	4672	4687	4694	rBV	212845	360631	27.64%	3.082%
32	16.446	4694	4698	4711	rVB2	68153	100990	7.74%	0.863%
33	16.639	4740	4758	4779	rBV2	70860	197447	15.13%	1.687%
34	16.787	4794	4804	4814	rBV	57064	92956	7.12%	0.794%
35	16.883	4826	4834	4848	rVB4	15623	26634	2.04%	0.228%
36	17.095	4888	4900	4914	rBV	264192	440226	33.74%	3.762%

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Instrument :
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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

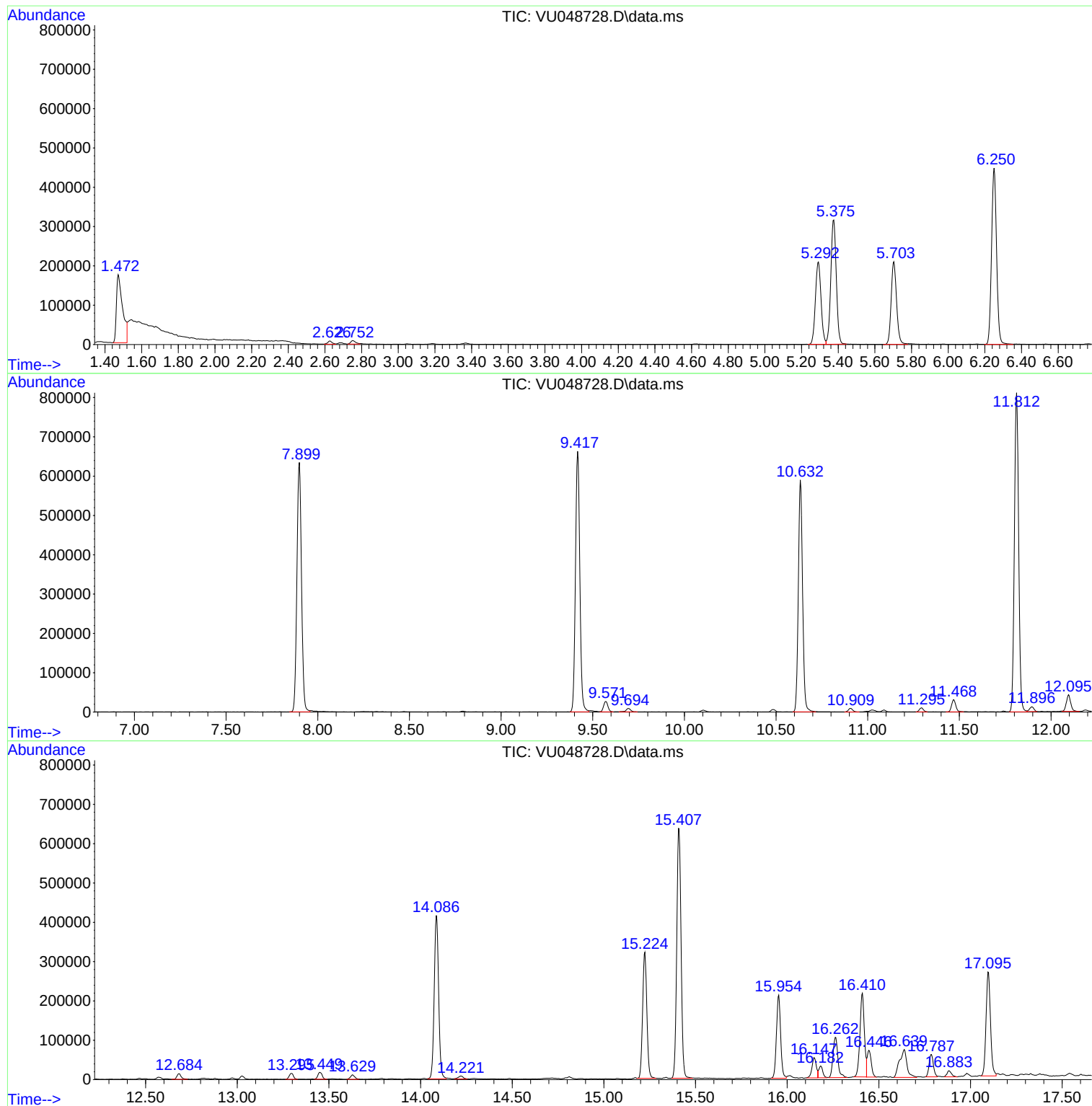
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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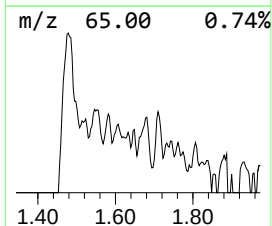
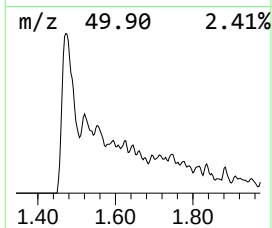
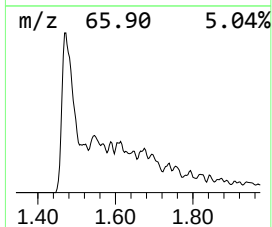
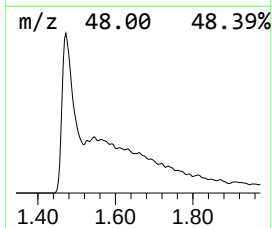
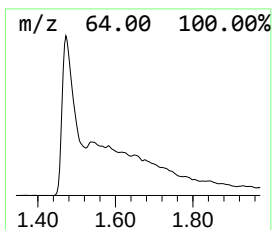
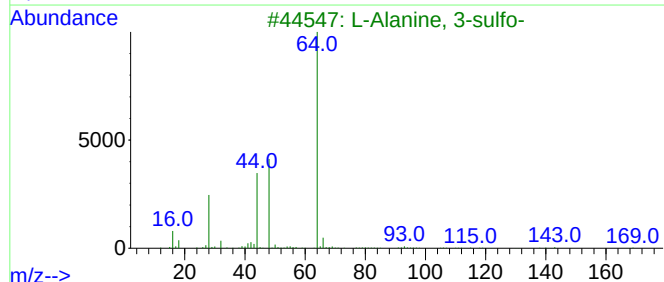
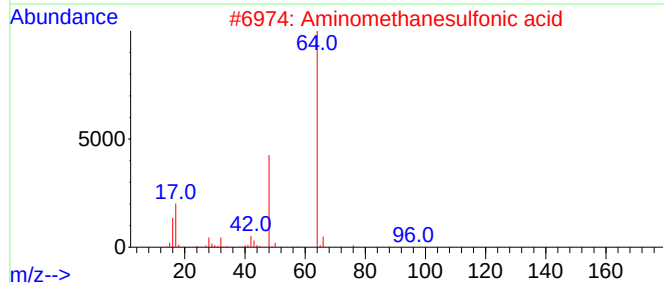
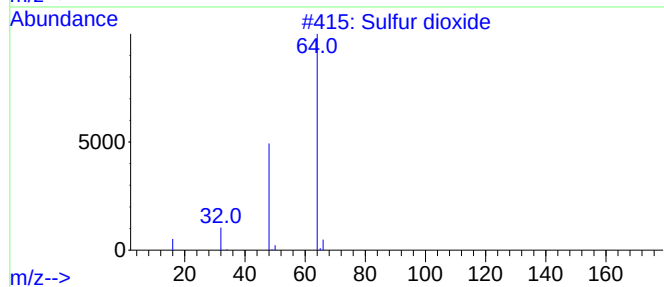
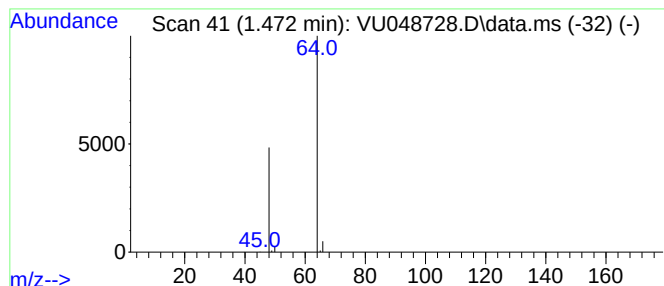
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.472	30.95 ug/l	403358	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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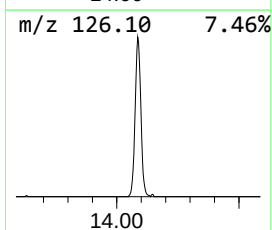
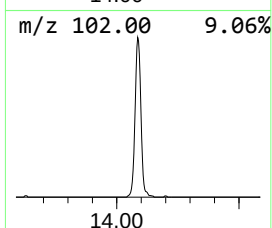
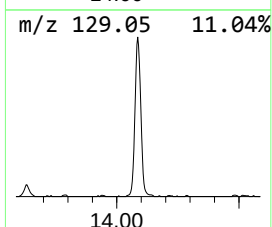
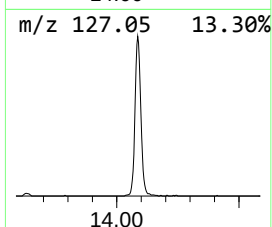
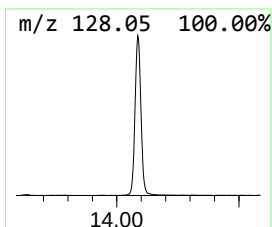
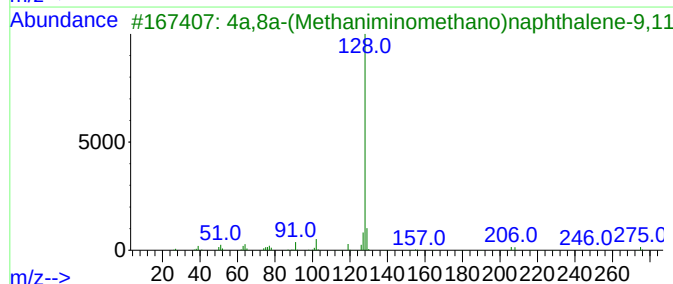
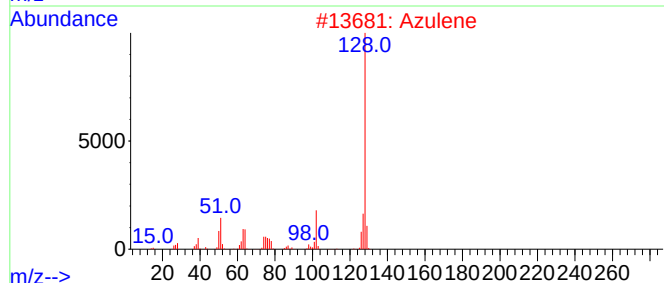
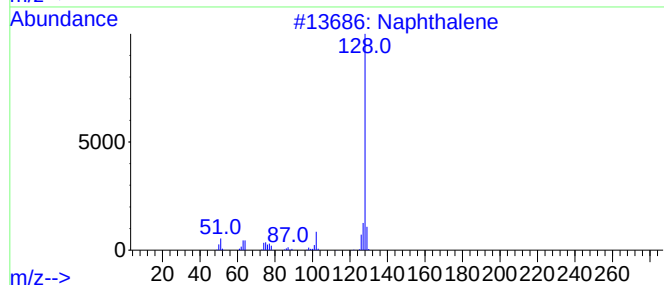
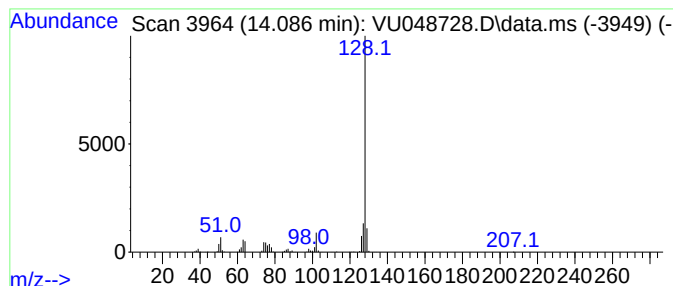
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 2 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	26.38 ug/l	688449	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
4			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	53
5			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	50



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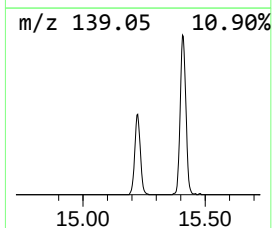
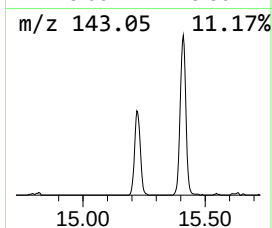
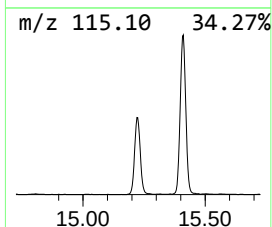
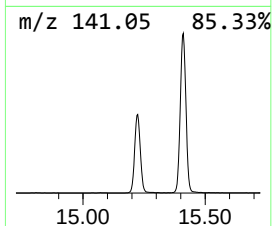
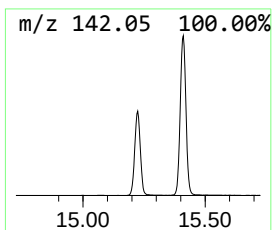
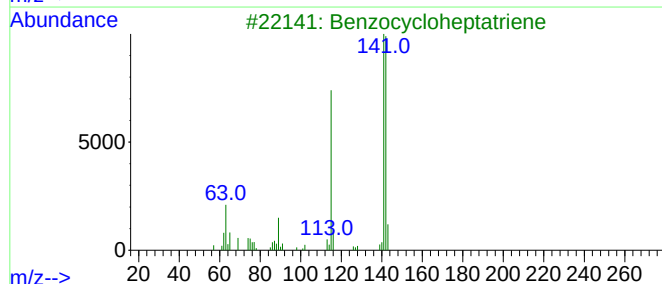
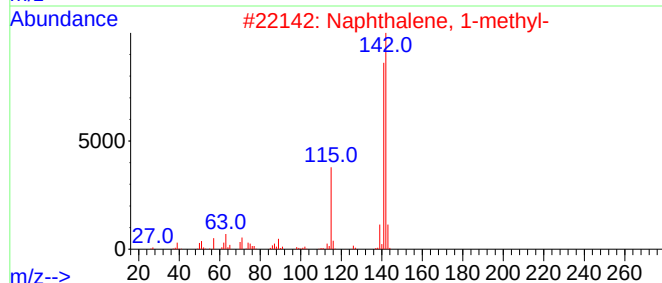
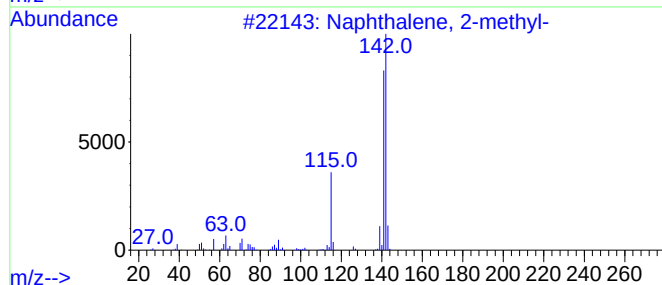
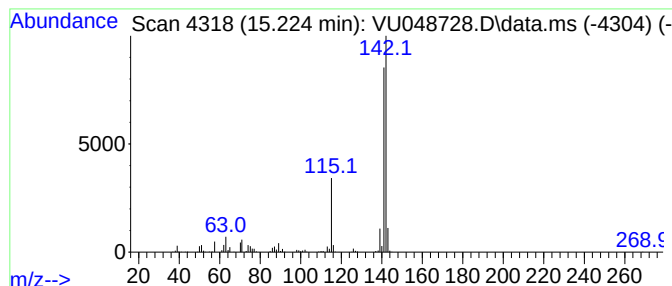
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Quant Title : SW846 8260

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

Peak Number 3 Benzocycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.224	19.67 ug/l	513381	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



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-2

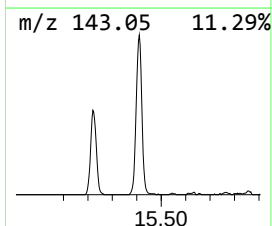
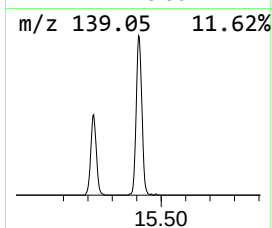
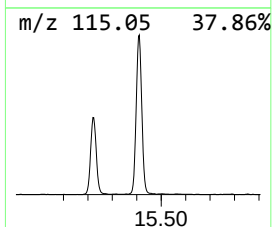
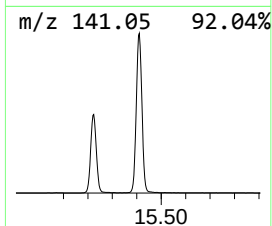
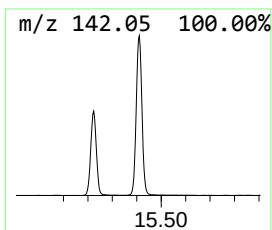
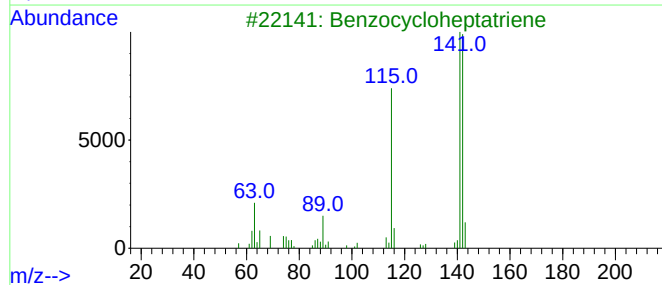
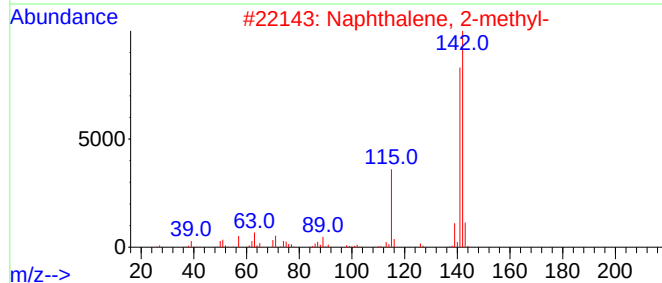
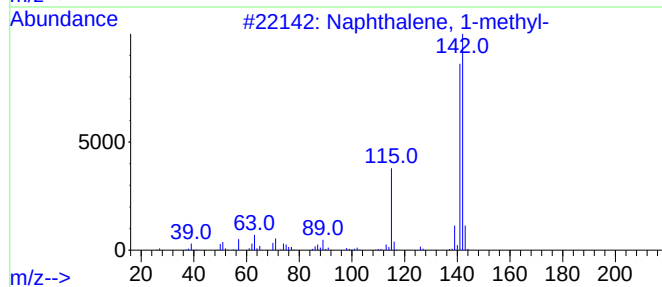
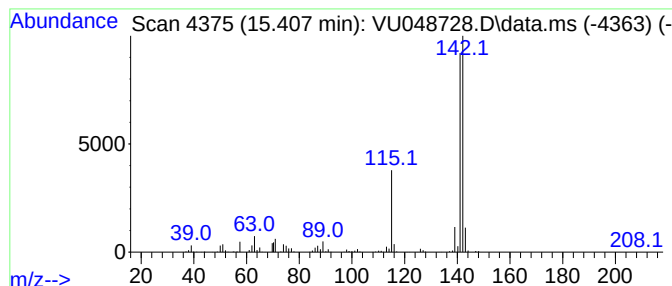
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.407	39.71 ug/l	1036220	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	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	72



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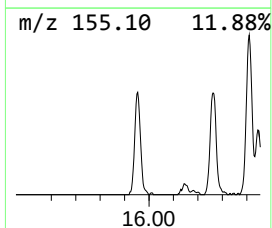
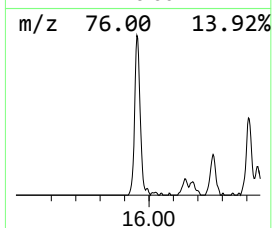
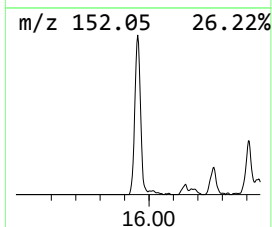
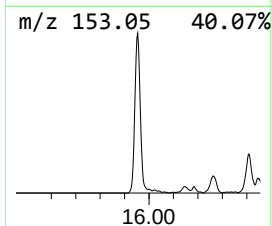
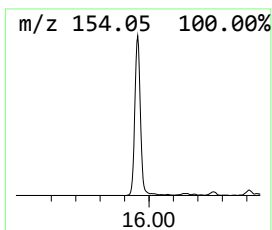
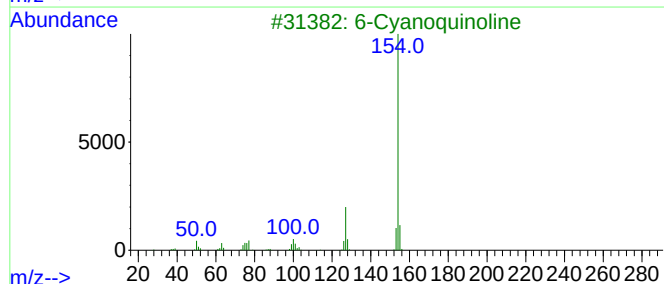
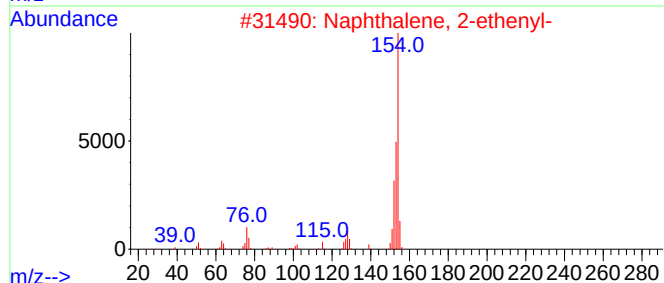
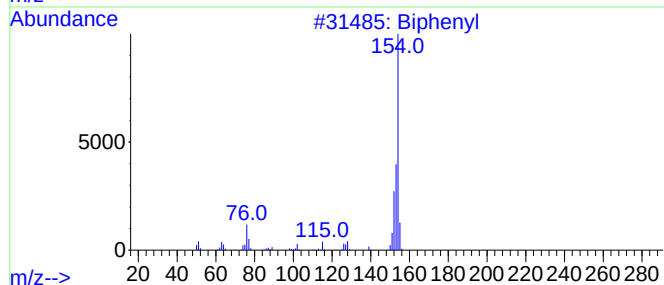
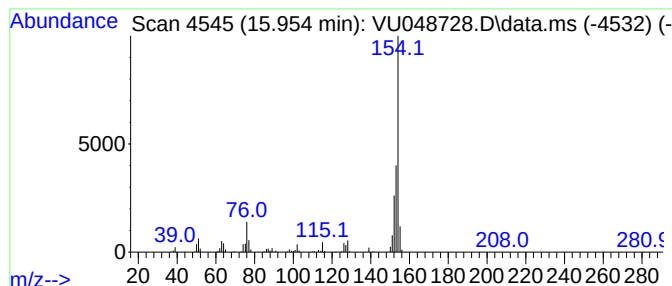
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Quant Title : SW846 8260

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

Peak Number 5 Biphenyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.954	12.80 ug/l	334090	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	95
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	87
3			6-Cyanoquinoline	154	C10H6N2	023395-72-4	49
4			1-Isoquinolinecarbonitrile	154	C10H6N2	001198-30-7	47
5			3-Quinolinecarbonitrile	154	C10H6N2	034846-64-5	47



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Operator : SY/MD
Sample : N3033-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-2

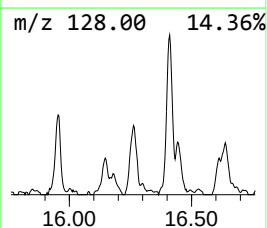
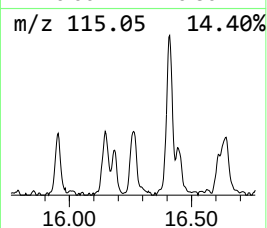
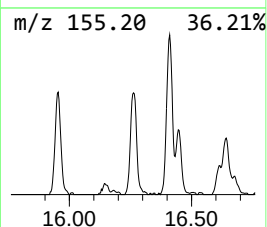
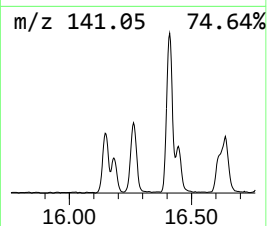
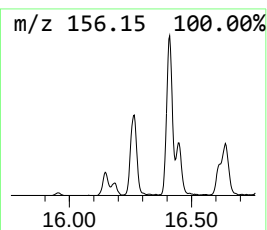
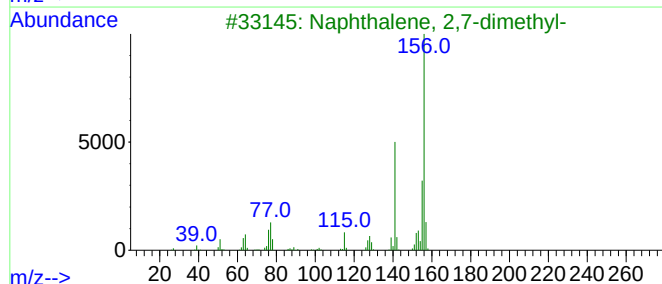
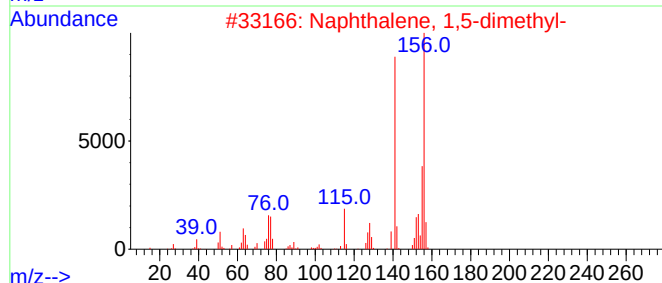
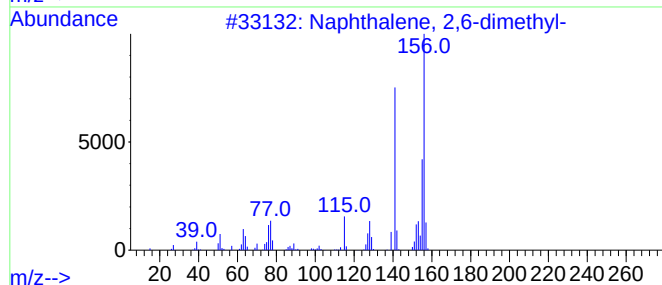
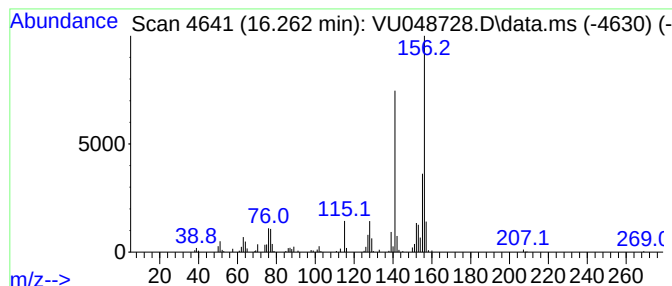
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	7.28 ug/l	189845	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	98
2			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048728.D
Acq On : 28 May 2022 05:55
Operator : SY/MD
Sample : N3033-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-2

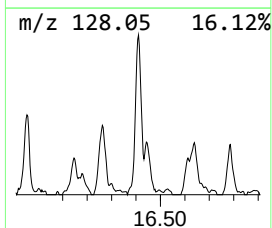
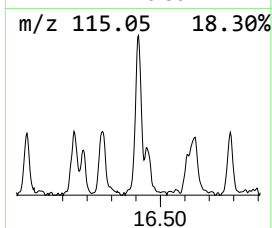
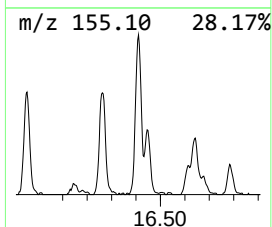
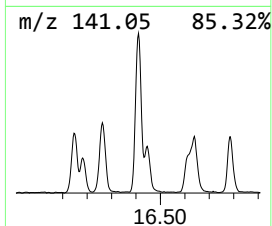
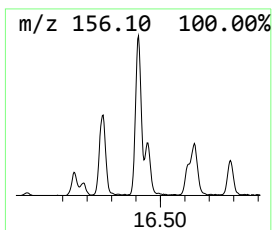
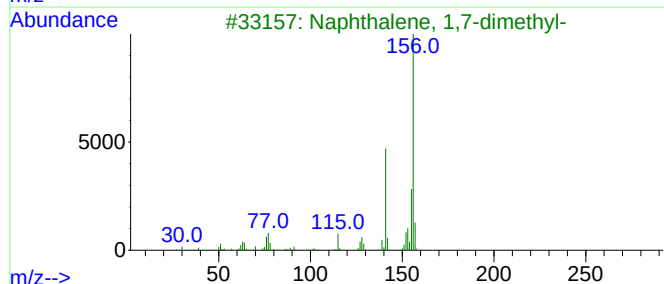
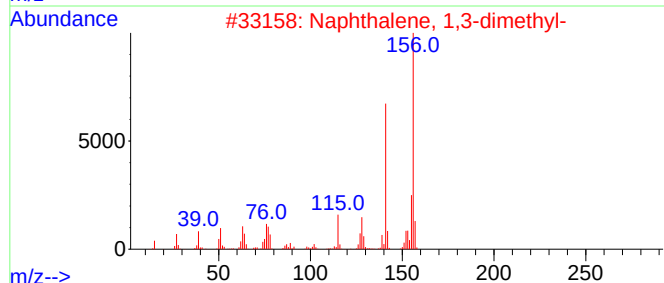
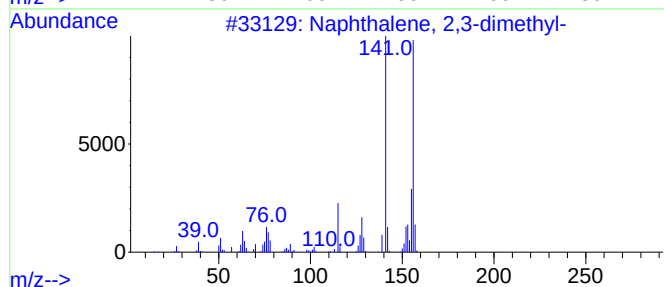
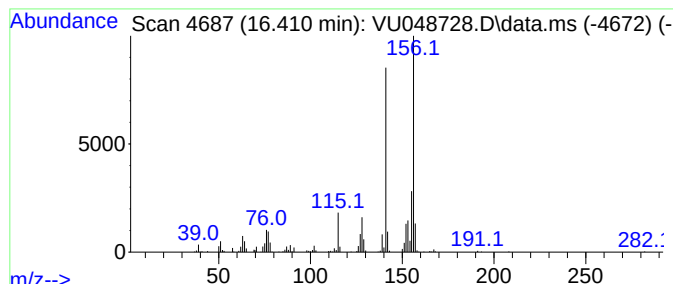
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.410	13.82 ug/l	360631	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048728.D
Acq On : 28 May 2022 05:55
Operator : SY/MD
Sample : N3033-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-2

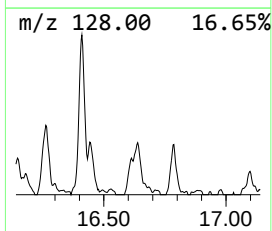
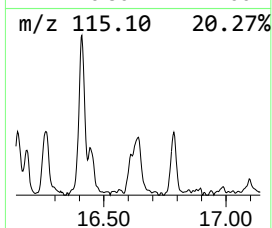
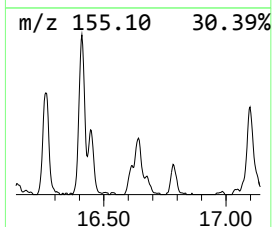
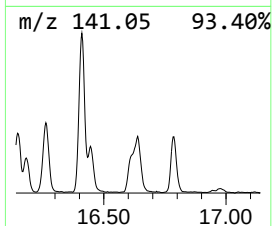
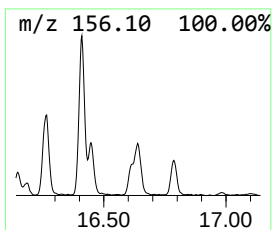
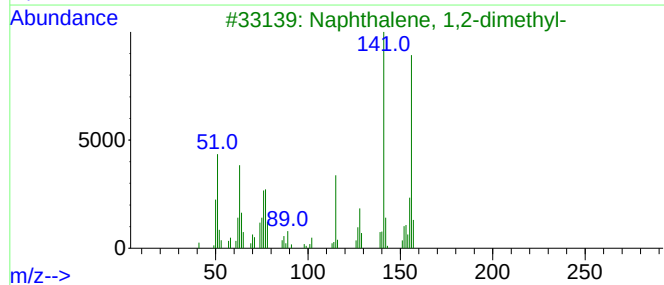
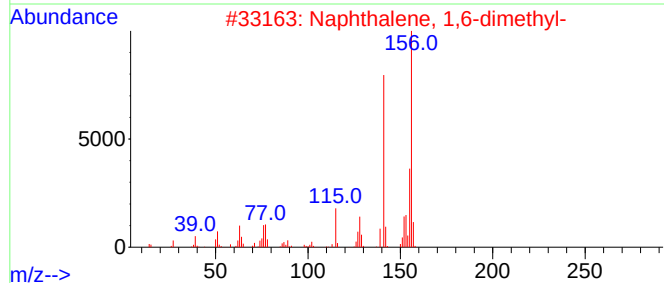
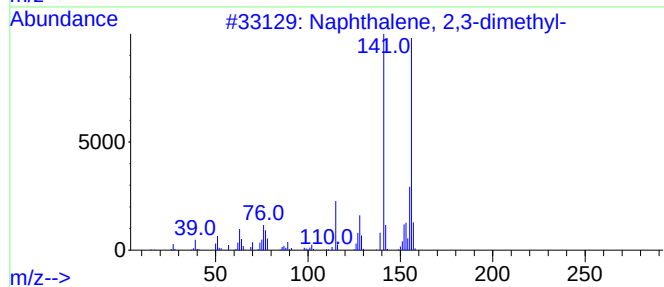
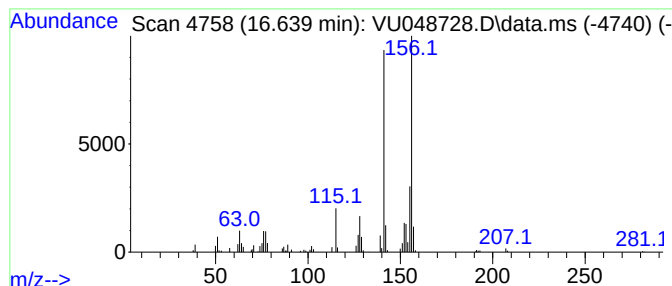
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.639	7.57 ug/l	197447	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
3			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	97
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048728.D
Acq On : 28 May 2022 05:55
Operator : SY/MD
Sample : N3033-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-2

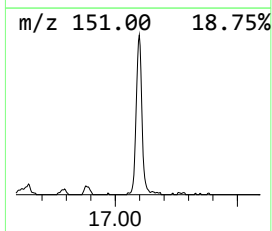
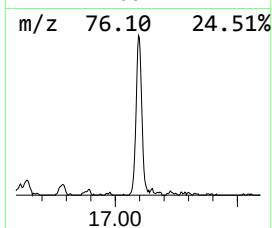
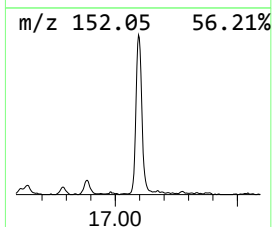
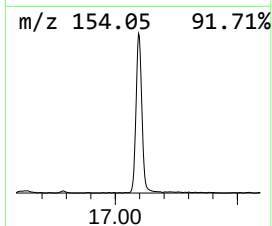
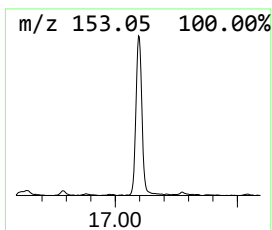
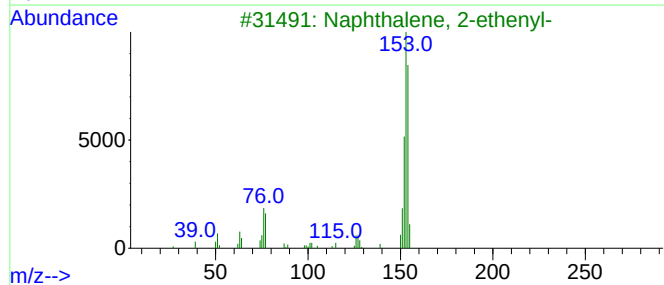
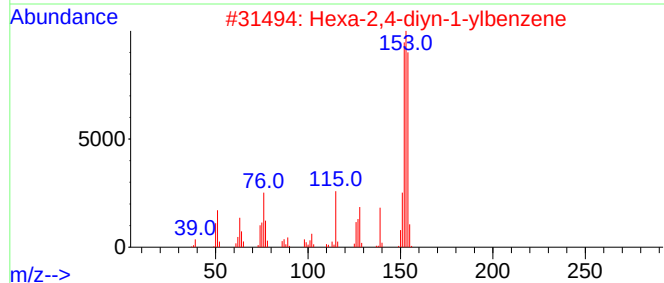
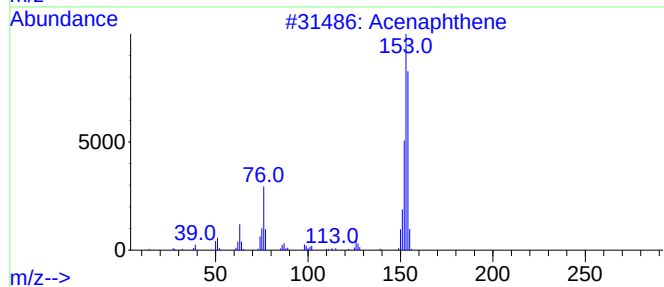
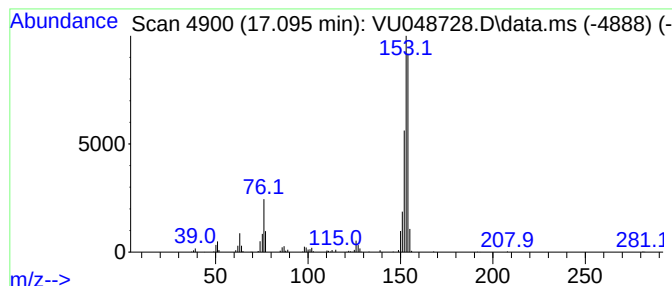
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 9 Acenaphthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.095	16.87 ug/l	440226	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	93
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	64
3			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	59
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	53
5			2,4,6-Trihydroxybenzaldehyde	154	C7H6O4	000487-70-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048728.D
Acq On : 28 May 2022 05:55
Operator : SY/MD
Sample : N3033-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
TW-2

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
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Azulene	14.086	26.4	ug/l	688449	4	11.812	1304740	50.0
Benzocyclohepta...	15.224	19.7	ug/l	513381	4	11.812	1304740	50.0
1,4-Methanonaph...	15.407	39.7	ug/l	1036220	4	11.812	1304740	50.0
Biphenyl	15.954	12.8	ug/l	334090	4	11.812	1304740	50.0
Naphthalene, 2,...	16.262	7.3	ug/l	189845	4	11.812	1304740	50.0
Naphthalene, 2,...	16.410	13.8	ug/l	360631	4	11.812	1304740	50.0
Naphthalene, 1,...	16.639	7.6	ug/l	197447	4	11.812	1304740	50.0
Acenaphthene	17.095	16.9	ug/l	440226	4	11.812	1304740	50.0