

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
 Data File : VU048692.D
 Acq On : 27 May 2022 14:41
 Operator : SY/MD
 Sample : N3056-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 MW-13D

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: VU048692.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	37	46	60	rBV	34797	96929	7.88%	0.882%
2	2.774	433	446	468	rBV2	17157	42169	3.43%	0.384%
3	5.292	1212	1229	1242	rBV3	215872	463295	37.67%	4.215%
4	5.375	1242	1255	1273	rVB	292069	606222	49.29%	5.516%
5	5.703	1342	1357	1380	rBV	215067	443647	36.07%	4.037%
6	6.250	1511	1527	1545	rBV	439956	831913	67.64%	7.569%
7	7.899	2024	2040	2058	rBV	637062	1106362	89.95%	10.067%
8	8.552	2233	2243	2255	rBV3	16940	26599	2.16%	0.242%
9	9.417	2496	2512	2542	rBV	645617	1088048	88.46%	9.900%
10	9.571	2550	2560	2573	rVB	28972	46615	3.79%	0.424%
11	10.484	2834	2844	2852	rBV	9367	13296	1.08%	0.121%
12	10.632	2875	2890	2912	rBV	581020	936826	76.17%	8.524%
13	10.906	2965	2975	2988	rBV	10424	16465	1.34%	0.150%
14	11.295	3085	3096	3105	rBV2	11920	17925	1.46%	0.163%
15	11.468	3140	3150	3166	rBV	31319	47749	3.88%	0.434%
16	11.812	3244	3257	3275	rBV	773538	1229980	100.00%	11.191%
17	11.896	3275	3283	3295	rVB2	13342	21642	1.76%	0.197%
18	12.095	3329	3345	3363	rVV2	47587	87387	7.10%	0.795%
19	12.684	3518	3528	3541	rBV2	17026	28453	2.31%	0.259%
20	13.294	3709	3718	3731	rVB5	15160	22913	1.86%	0.208%
21	13.449	3755	3766	3779	rBV4	16788	27770	2.26%	0.253%
22	13.629	3813	3822	3833	rBV6	11073	18557	1.51%	0.169%
23	14.085	3950	3964	3988	rBV	399345	646496	52.56%	5.882%
24	14.221	3996	4006	4015	rVB8	7995	13498	1.10%	0.123%
25	15.224	4306	4318	4332	rBV	276227	436168	35.46%	3.969%
26	15.410	4363	4376	4392	rBV	585202	919144	74.73%	8.363%
27	15.954	4532	4545	4558	rBV	178531	292987	23.82%	2.666%
28	16.146	4594	4605	4611	rBV2	41939	66134	5.38%	0.602%
29	16.182	4612	4616	4628	rVB	23981	33453	2.72%	0.304%
30	16.262	4628	4641	4654	rBV	96199	175222	14.25%	1.594%
31	16.407	4671	4686	4693	rBV	176456	302918	24.63%	2.756%
32	16.445	4694	4698	4716	rVB2	64244	96077	7.81%	0.874%
33	16.638	4739	4758	4778	rBV2	67329	184494	15.00%	1.679%
34	16.786	4793	4804	4816	rBV	59632	98398	8.00%	0.895%
35	16.883	4824	4834	4844	rBV3	25728	41185	3.35%	0.375%
36	16.982	4859	4865	4875	rVB8	11927	18651	1.52%	0.170%

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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

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37	17.095	4888	4900	4919	rBV	244503	428779	34.86%	3.901%
38	17.535	5033	5037	5048	rVB5	10151	16159	1.31%	0.147%

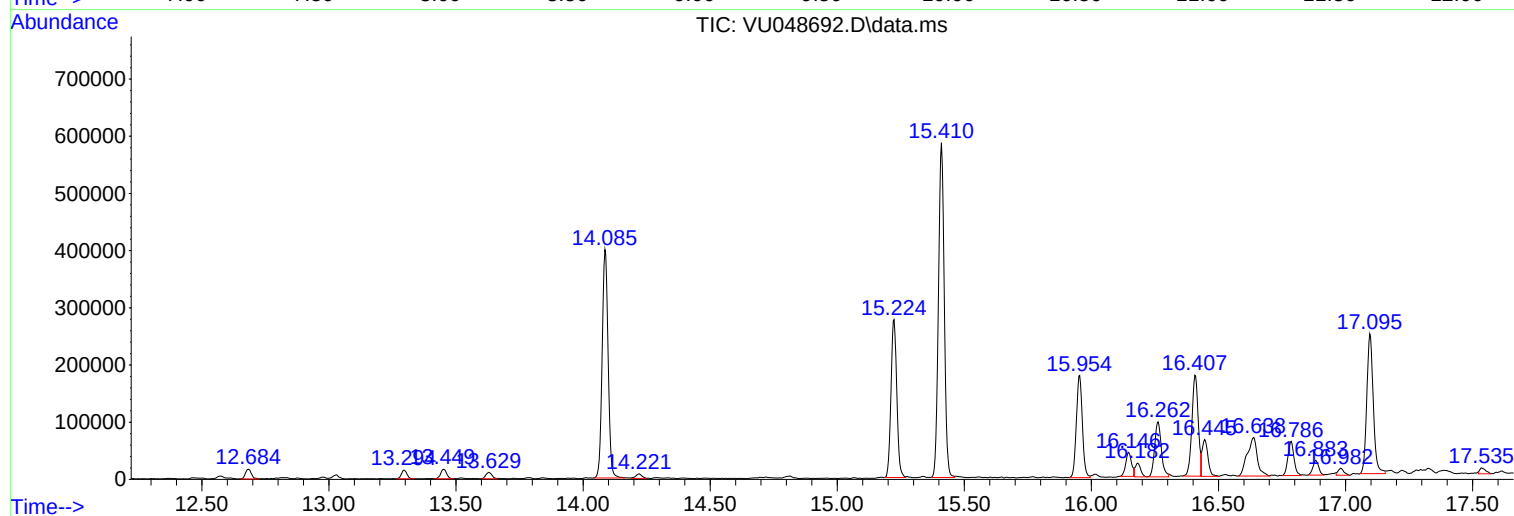
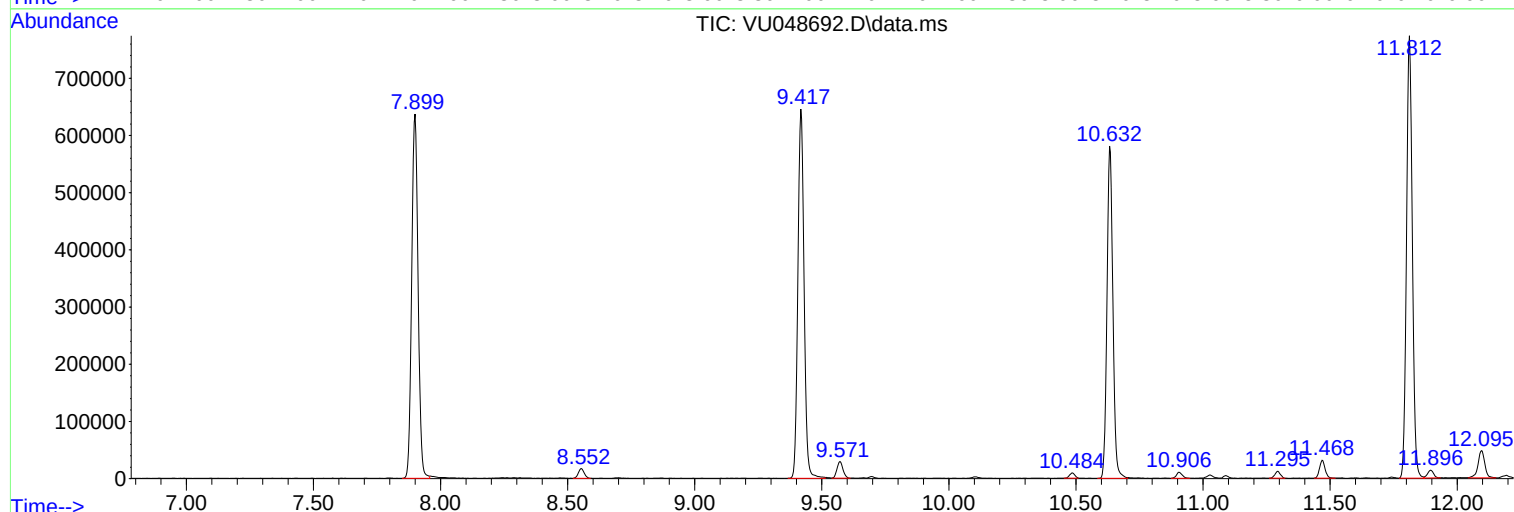
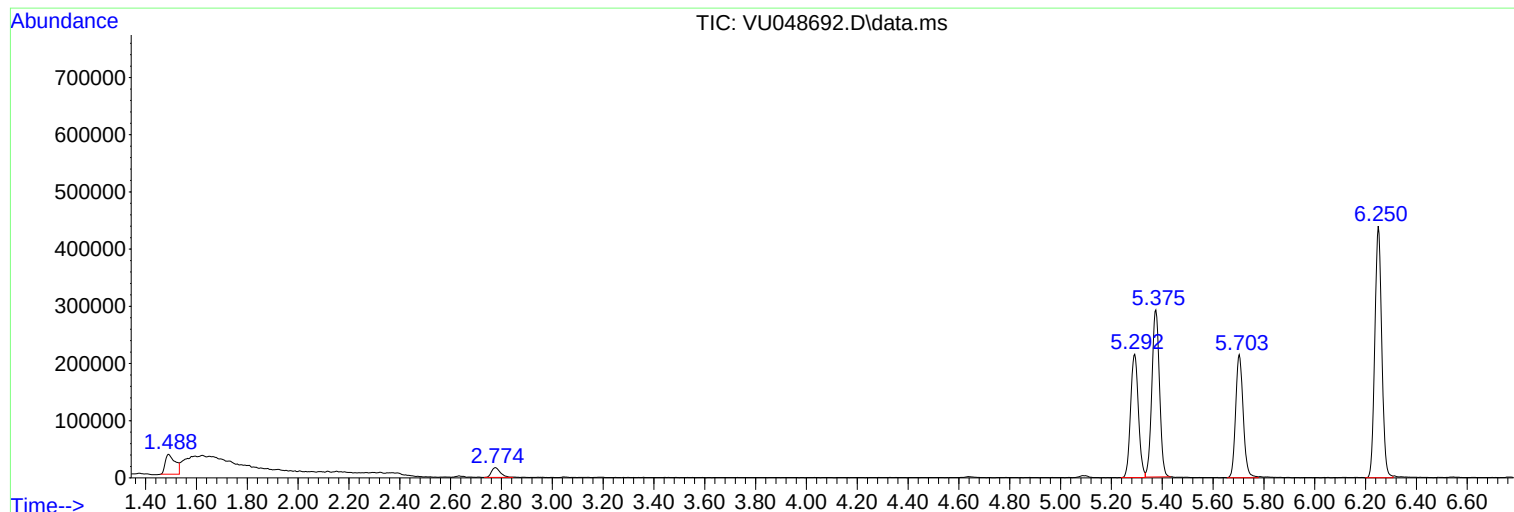
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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



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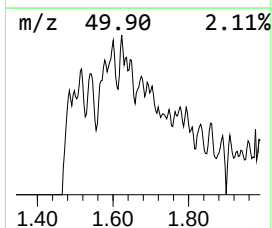
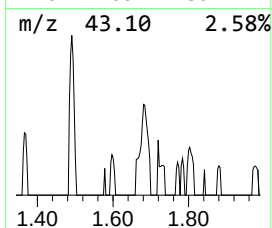
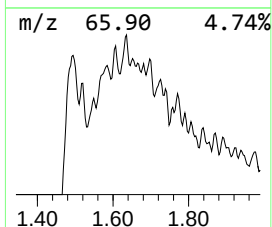
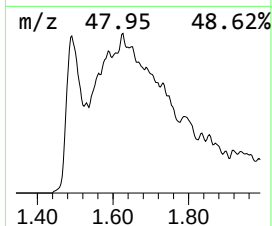
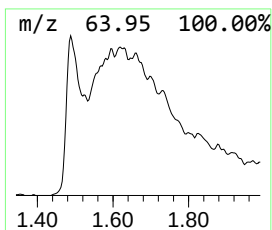
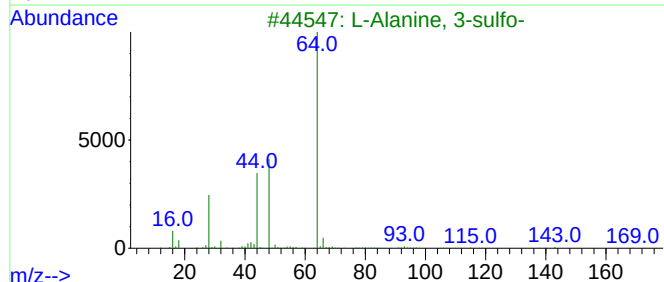
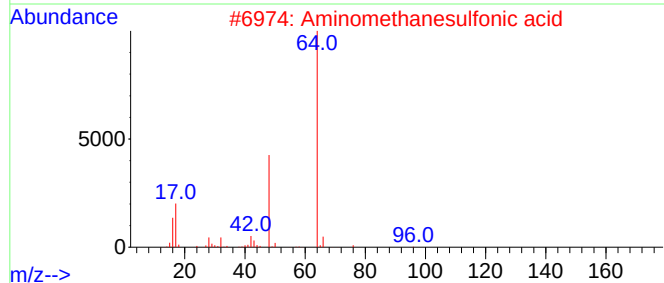
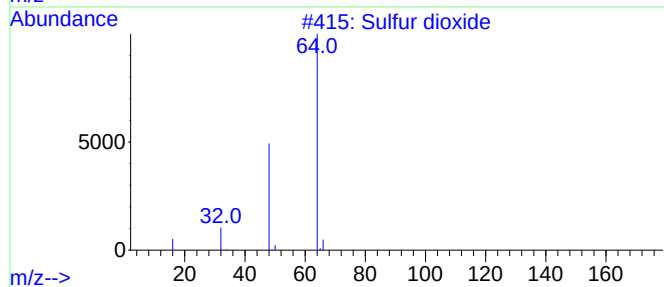
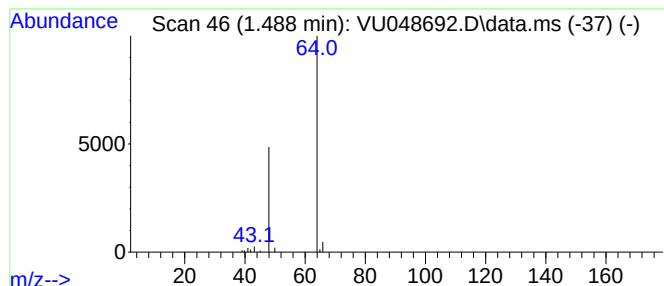
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.488	7.99 ug/l	96929	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	5
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4



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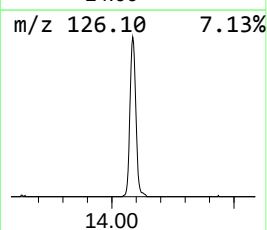
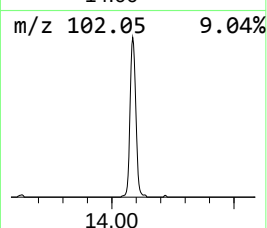
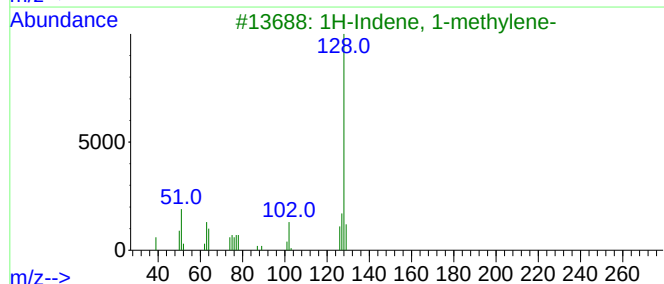
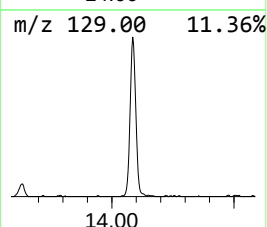
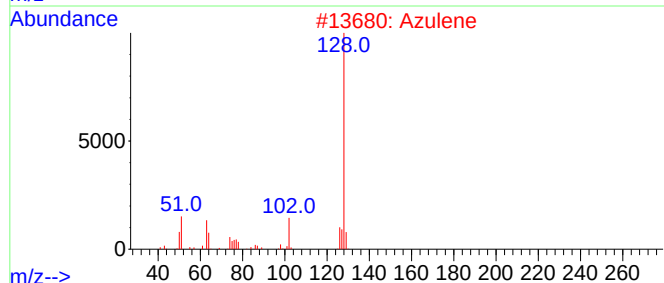
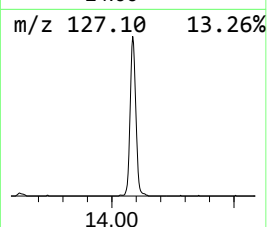
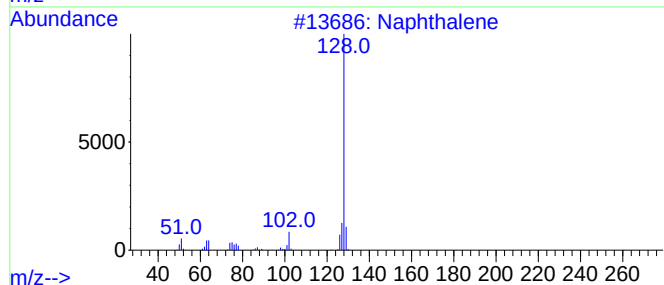
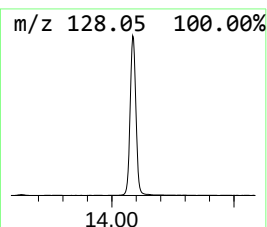
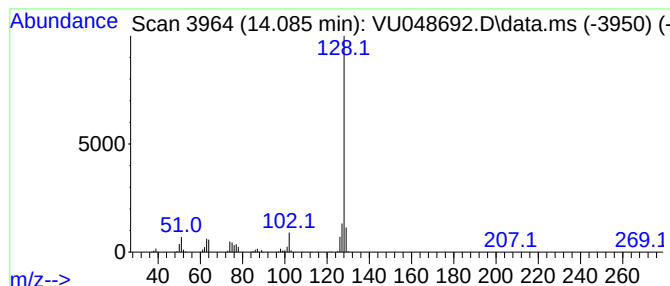
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	26.28 ug/l	646496	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			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	87
4			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
5			m-Fluorothiophenol	128	C6H5FS	002557-77-9	56



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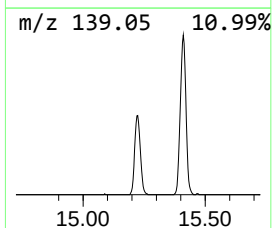
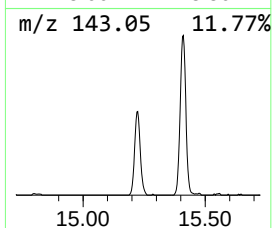
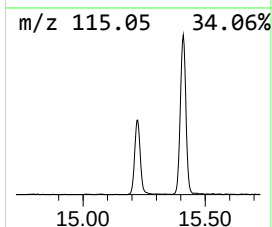
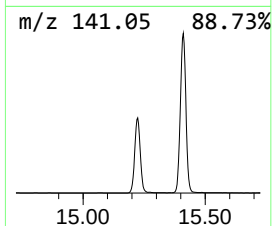
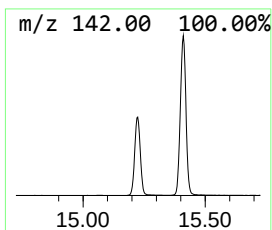
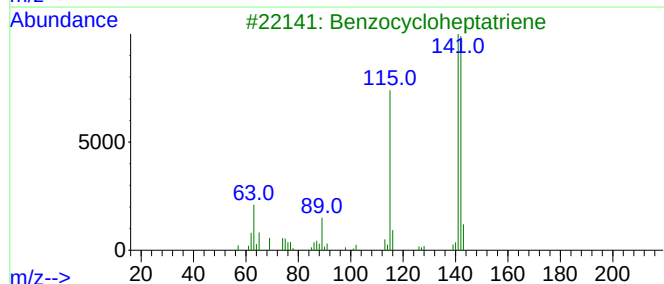
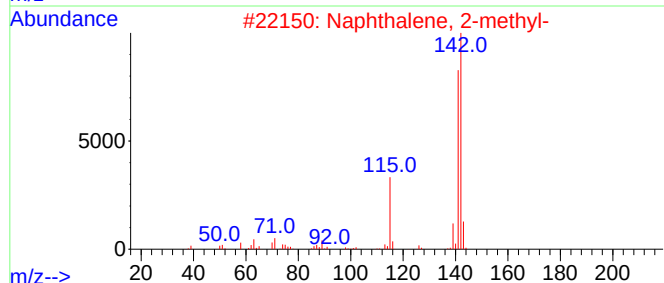
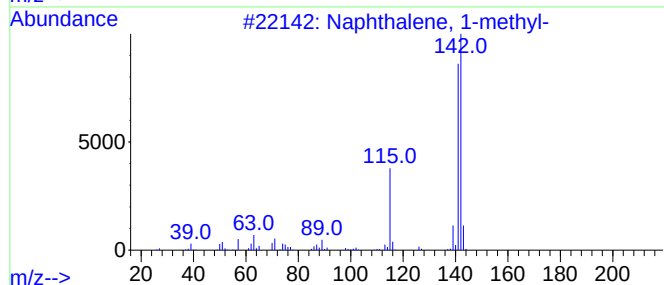
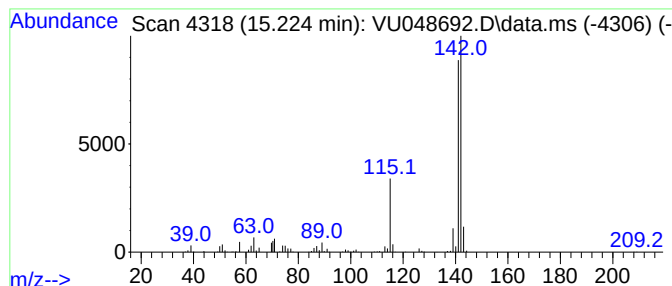
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.224	17.73 ug/l	436168	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	90
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5			1H-Indole-4-carbonitrile	142	C9H6N2	016136-52-0	46



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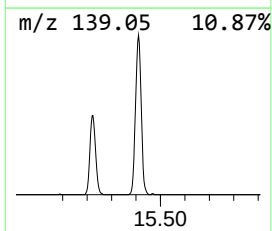
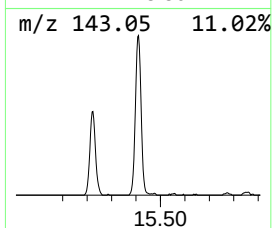
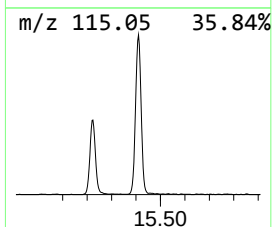
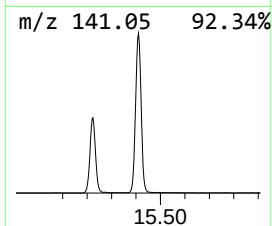
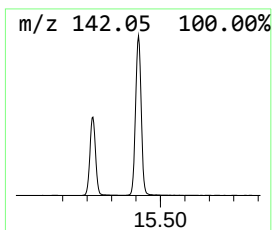
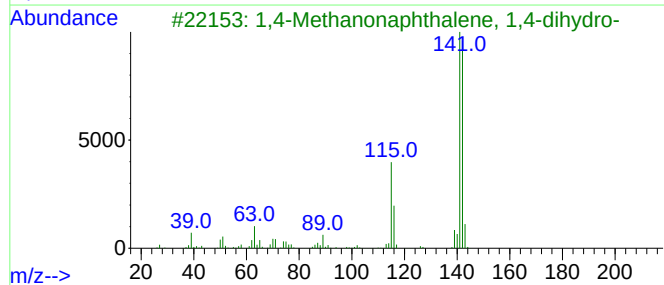
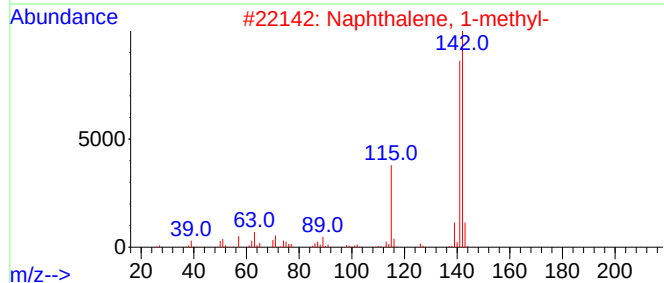
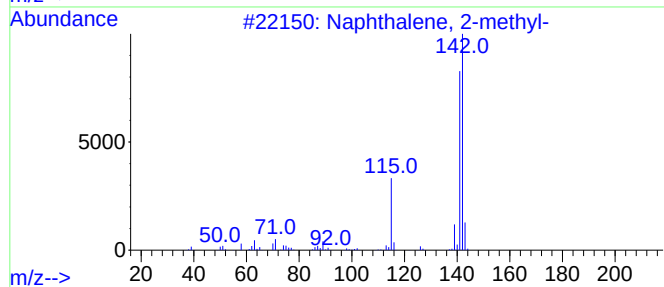
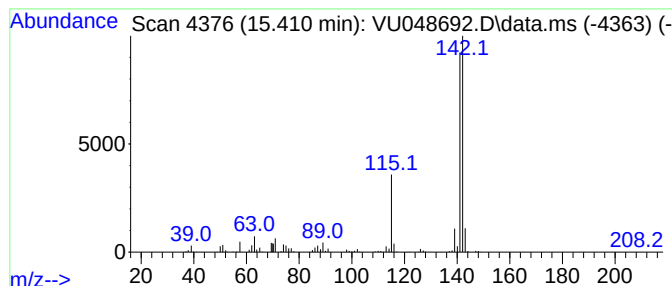
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	37.36 ug/l	919144	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	94
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	86



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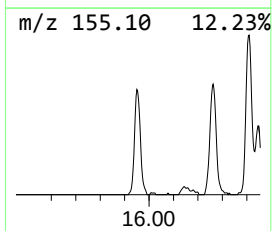
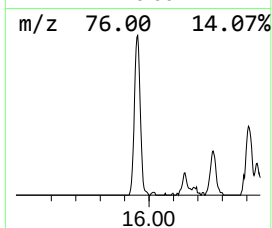
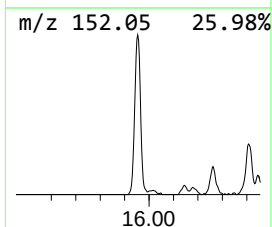
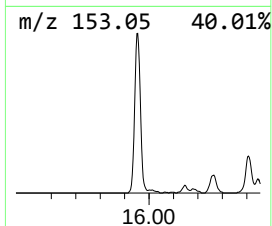
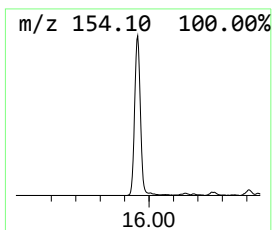
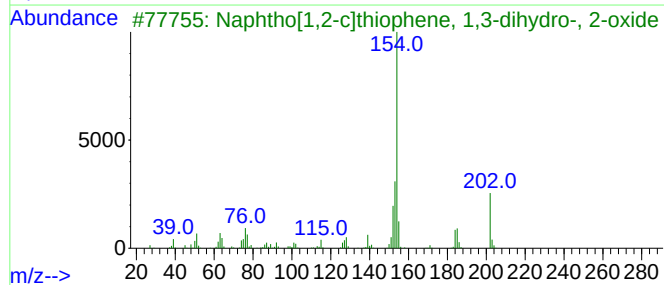
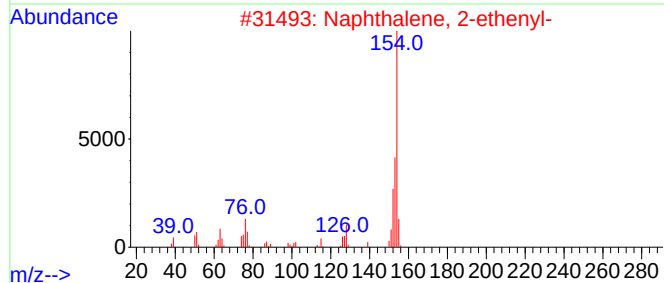
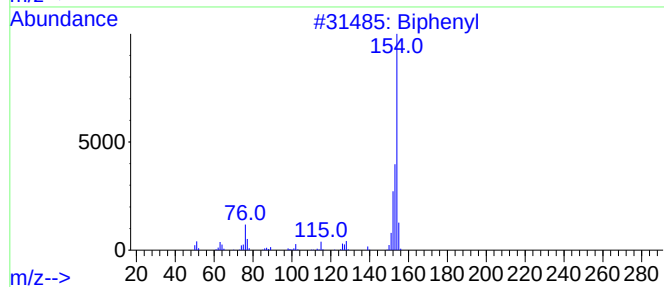
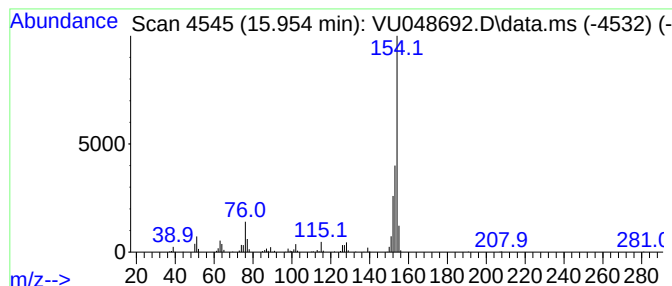
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 5 Biphenyl Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.954	11.91 ug/l	292987	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			Naphtho[1,2-c]thiophene, 1,3-dih...	202	C12H100S	031739-49-8	64
4			1,3-Cyclohexadien-5-ol, 1-phenyl-	172	C12H12O	1000159-61-9	50
5			Acenaphthene	154	C12H10	000083-32-9	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048692.D
Acq On : 27 May 2022 14:41
Operator : SY/MD
Sample : N3056-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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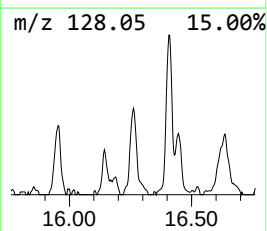
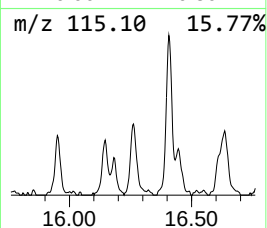
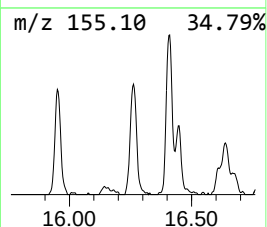
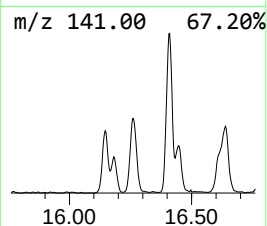
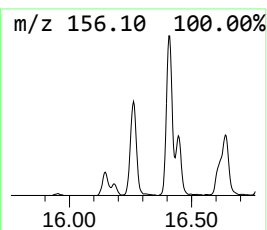
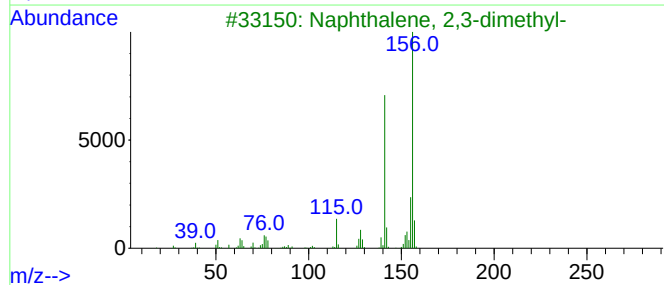
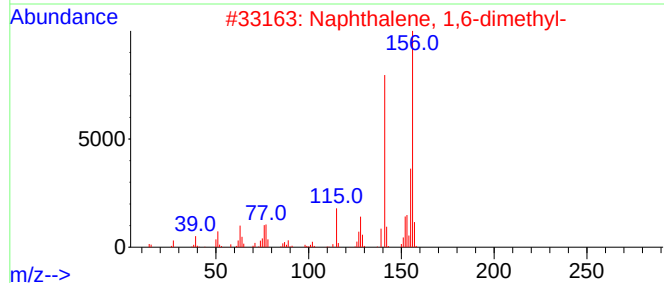
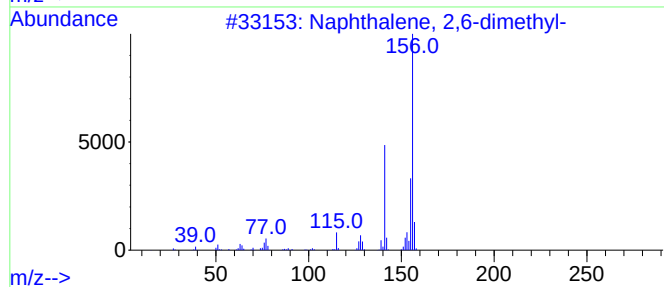
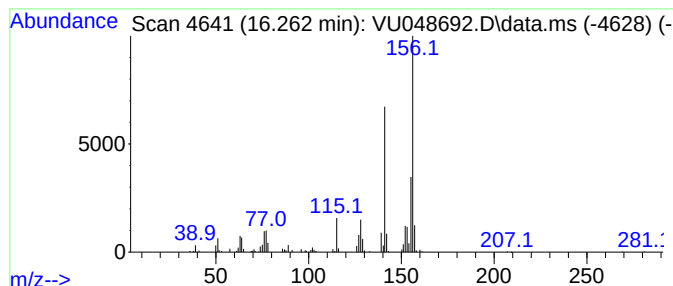
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	7.12 ug/l	175222	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	97
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048692.D
Acq On : 27 May 2022 14:41
Operator : SY/MD
Sample : N3056-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-13D

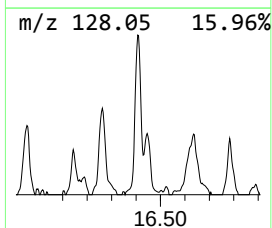
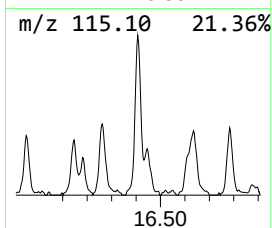
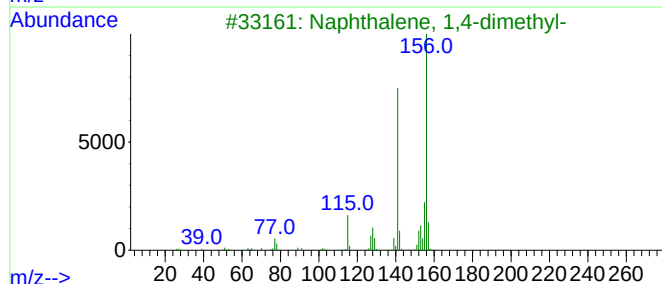
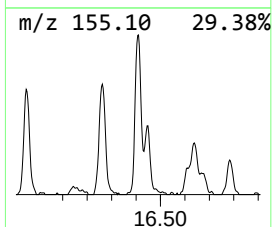
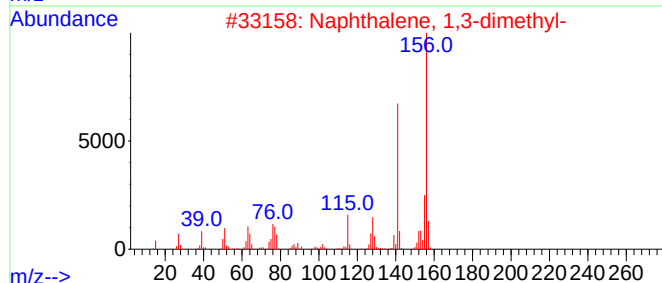
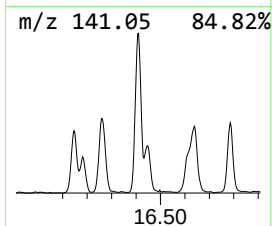
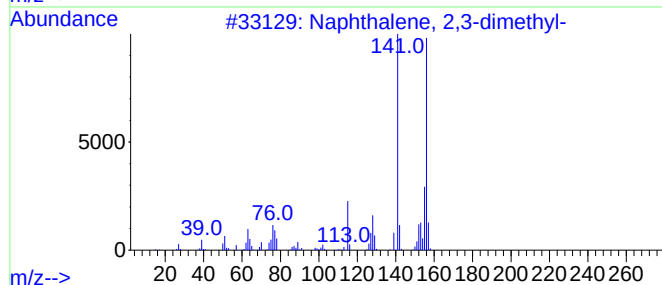
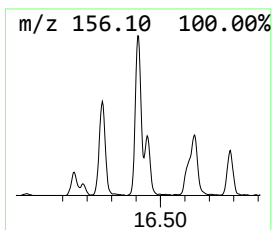
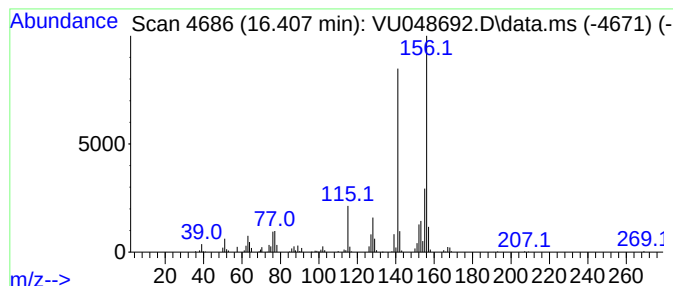
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.407	12.31 ug/l	302918	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, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048692.D
Acq On : 27 May 2022 14:41
Operator : SY/MD
Sample : N3056-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-13D

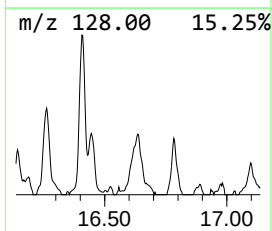
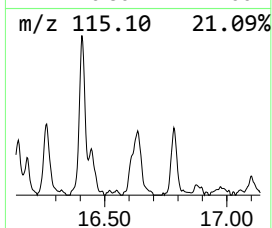
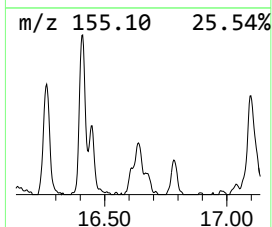
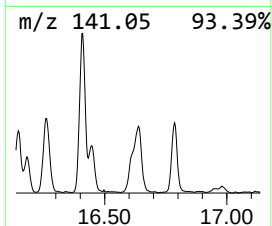
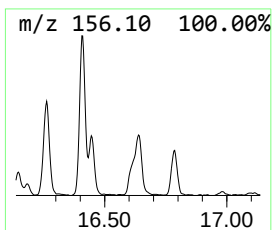
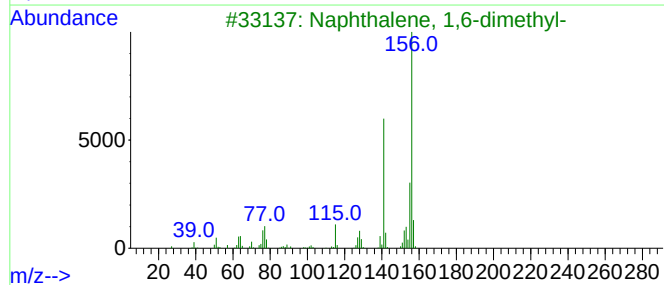
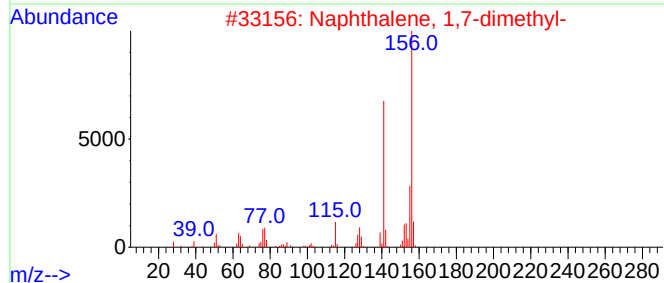
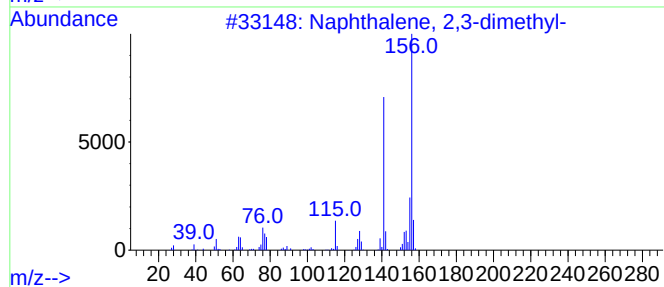
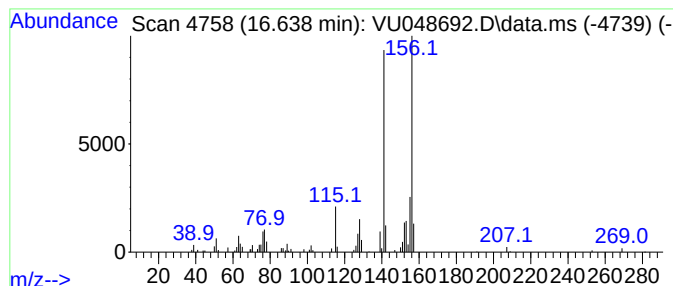
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,7-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.638	7.50 ug/l	184494	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	97
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048692.D
Acq On : 27 May 2022 14:41
Operator : SY/MD
Sample : N3056-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

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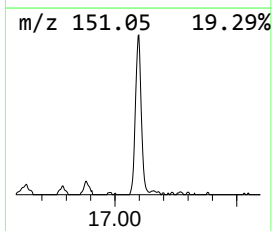
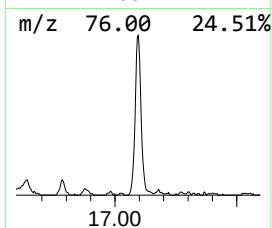
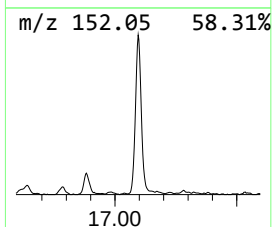
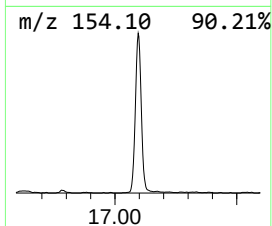
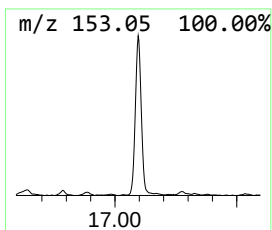
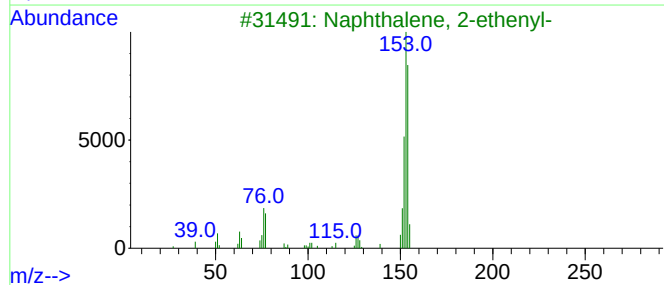
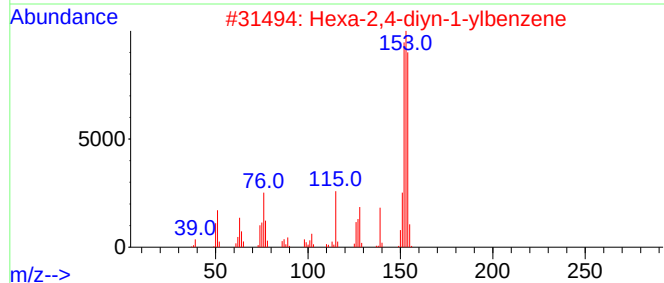
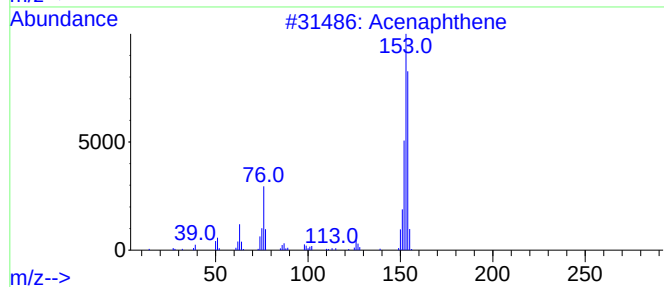
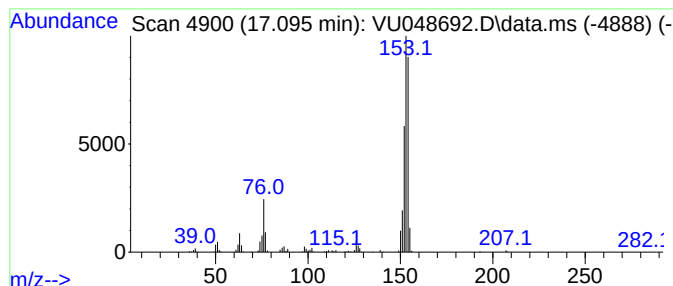
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 9 Acenaphthene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.095	17.43 ug/l	428779	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	89
2			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	58
3			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	58
4			3-Fluoro-para-anisaldehyde	154	C8H7FO2	000351-54-2	50
5			.beta.-(1-Naphthyl)acrylic acid	198	C13H10O2	013026-12-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052722\
Data File : VU048692.D
Acq On : 27 May 2022 14:41
Operator : SY/MD
Sample : N3056-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
MW-13D

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	26.3	ug/l	646496	4	11.812	1229980	50.0
Naphthalene, 1-...	15.224	17.7	ug/l	436168	4	11.812	1229980	50.0
Naphthalene, 2-...	15.410	37.4	ug/l	919144	4	11.812	1229980	50.0
Biphenyl	15.954	11.9	ug/l	292987	4	11.812	1229980	50.0
Naphthalene, 2,...	16.262	7.1	ug/l	175222	4	11.812	1229980	50.0
Naphthalene, 2,...	16.407	12.3	ug/l	302918	4	11.812	1229980	50.0
Naphthalene, 1,...	16.638	7.5	ug/l	184494	4	11.812	1229980	50.0
Acenaphthene	17.095	17.4	ug/l	428779	4	11.812	1229980	50.0