

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
 Data File : VU044869.D
 Acq On : 26 Sep 2021 04:41
 Operator : SY/MD
 Sample : M3888-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 20896

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\82U092421W.M
 Title : SW846 8260

Signal : TIC: VU044869.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	74	79	80	rBV2	36705567	28431292	65.73%	15.669%
2	2.327	279	307	362	rBV	8203490	25800465	59.65%	14.219%
3	5.289	1208	1228	1241	rBV3	307774	685281	1.58%	0.378%
4	5.372	1241	1254	1275	rVB	413901	862100	1.99%	0.475%
5	5.584	1302	1320	1343	rBV	3320374	6842291	15.82%	3.771%
6	5.700	1343	1356	1365	rVV	276538	570252	1.32%	0.314%
7	5.771	1365	1378	1408	rVB	1188592	2554782	5.91%	1.408%
8	6.154	1480	1497	1512	rBV	4783894	13328455	30.81%	7.346%
9	7.472	1893	1907	1930	rBV	313133	535224	1.24%	0.295%
10	7.899	2027	2040	2050	rBV	1001650	1685094	3.90%	0.929%
11	7.970	2050	2062	2077	rVB	2867492	4863217	11.24%	2.680%
12	8.729	2285	2298	2308	rBV2	1479415	2493672	5.77%	1.374%
13	8.796	2308	2319	2339	rVB	2134350	3733007	8.63%	2.057%
14	9.420	2501	2513	2519	rBV	865919	1389541	3.21%	0.766%
15	9.465	2519	2527	2546	rVV	1488416	2573288	5.95%	1.418%
16	9.571	2546	2560	2576	rVB	377990	677378	1.57%	0.373%
17	9.690	2578	2597	2624	rBV2	26477430	43254998	100.00%	23.839%
18	9.832	2629	2641	2650	rBV2	455694	822237	1.90%	0.453%
19	10.022	2686	2700	2715	rBV2	463541	986624	2.28%	0.544%
20	10.105	2715	2726	2738	rBV4	2096750	3628095	8.39%	2.000%
21	10.169	2738	2746	2758	rBV2	330950	714226	1.65%	0.394%
22	10.369	2790	2808	2821	rBV4	1000441	2340679	5.41%	1.290%
23	10.436	2821	2829	2842	rVB2	383366	738163	1.71%	0.407%
24	10.629	2874	2889	2903	rBV3	1275821	2650705	6.13%	1.461%
25	10.973	2988	2996	3003	rBV	357184	517966	1.20%	0.285%
26	11.375	3112	3121	3128	rBV	1818442	2847516	6.58%	1.569%
27	11.414	3128	3133	3142	rVB3	1041723	1592224	3.68%	0.878%
28	11.468	3142	3150	3161	rVB	794117	1216981	2.81%	0.671%
29	11.536	3161	3171	3180	rBV3	291394	509103	1.18%	0.281%
30	11.658	3199	3209	3218	rBV	592108	932888	2.16%	0.514%
31	11.716	3219	3227	3240	rVV2	304544	590492	1.37%	0.325%
32	11.816	3244	3258	3268	rVB	770450	1334817	3.09%	0.736%
33	12.044	3317	3329	3342	rBV4	1043880	2449308	5.66%	1.350%
34	12.314	3398	3413	3427	rVB	1028433	1755386	4.06%	0.967%
35	12.542	3470	3484	3503	rVB8	195135	609849	1.41%	0.336%
36	12.767	3544	3554	3561	rBV	453020	718793	1.66%	0.396%

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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\82U092421W.M
Title : SW846 8260

37	12.812	3562	3568	3578	rVB	391854	618220	1.43%	0.341%
38	12.928	3595	3604	3615	rVB	575029	890300	2.06%	0.491%
39	14.092	3952	3966	3981	rBV2	5444524	9806578	22.67%	5.405%
40	15.015	4240	4253	4282	rVB2	309008	826703	1.91%	0.456%
41	15.224	4306	4318	4344	rVB2	683328	1293764	2.99%	0.713%
42	15.414	4365	4377	4396	rBV	436459	774421	1.79%	0.427%

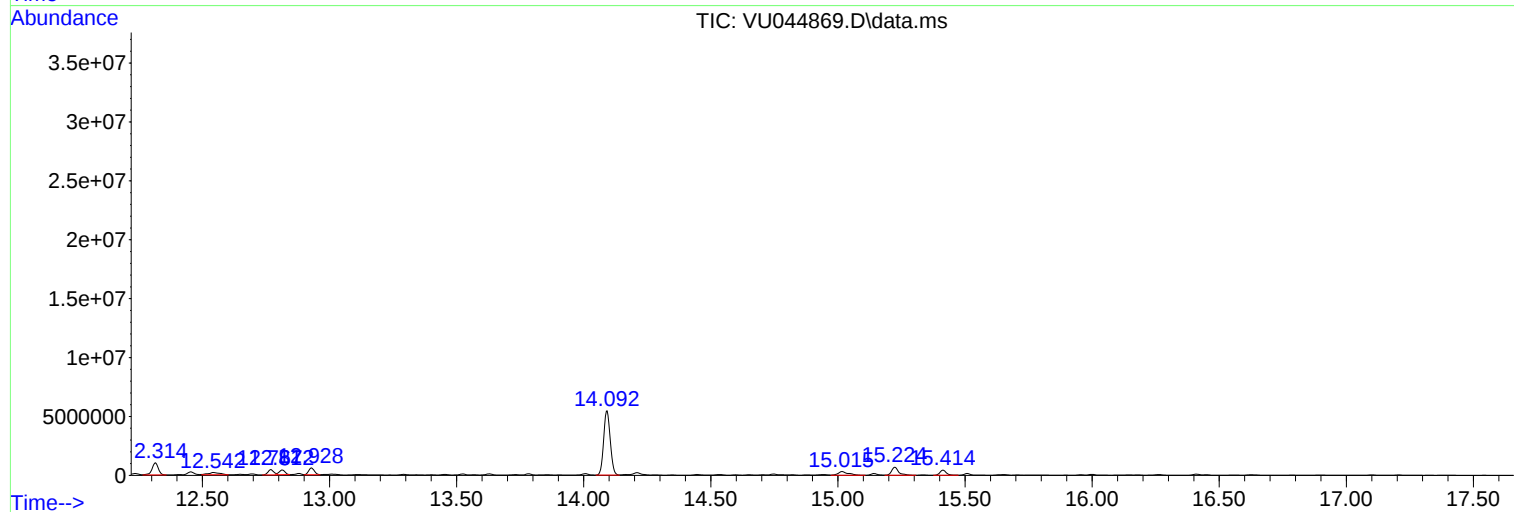
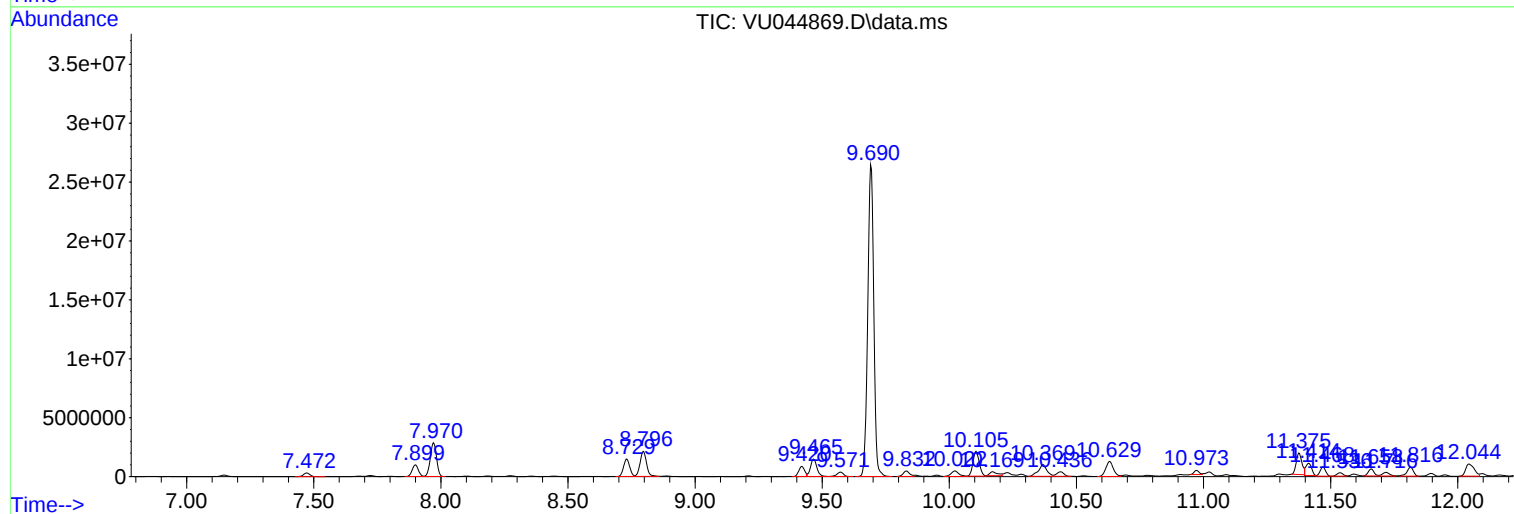
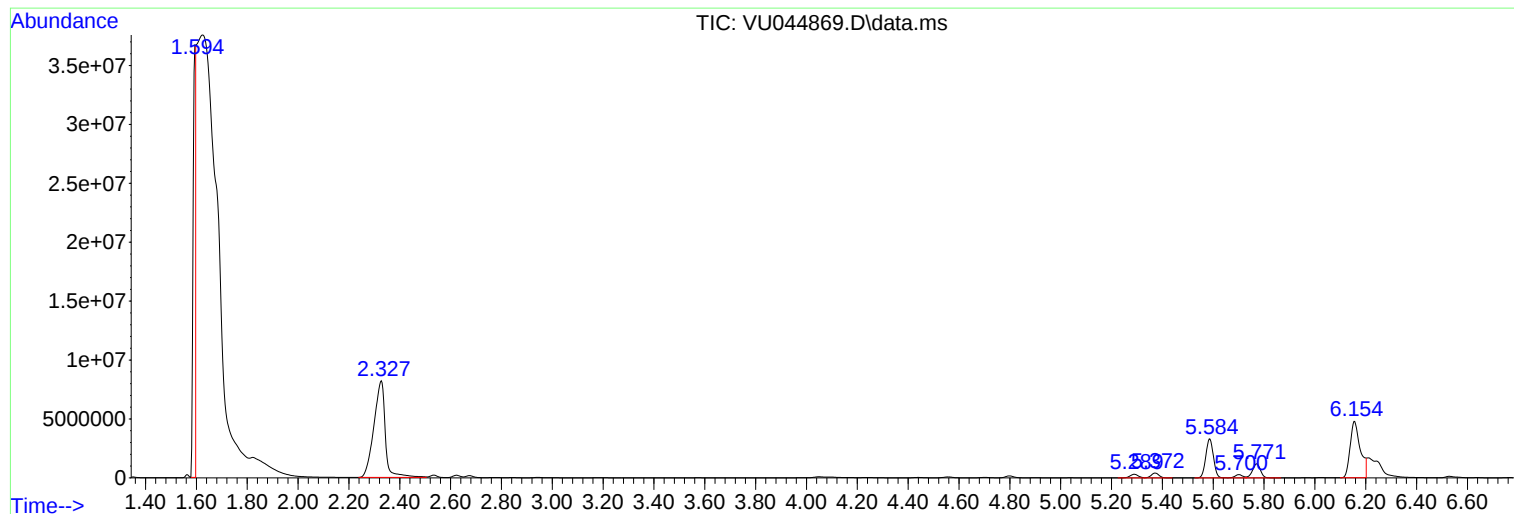
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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



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Operator : SY/MD
Sample : M3888-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
20896

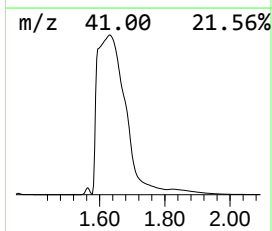
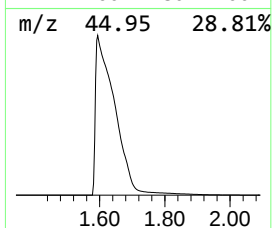
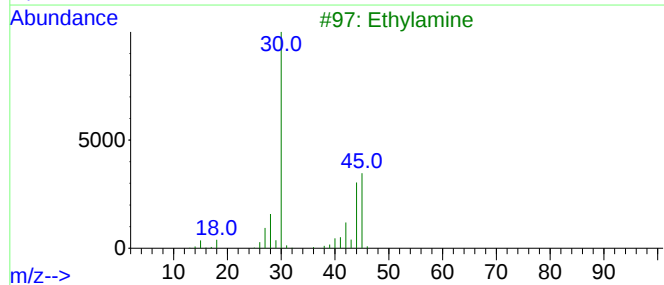
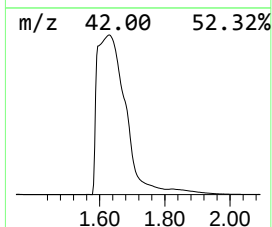
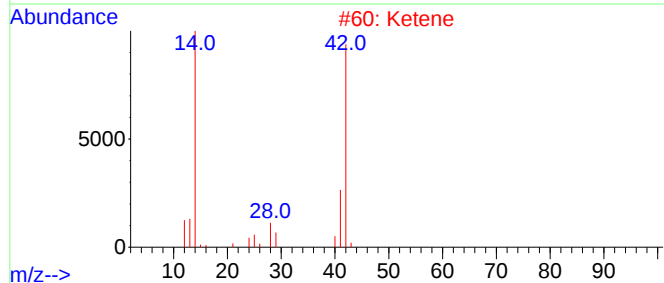
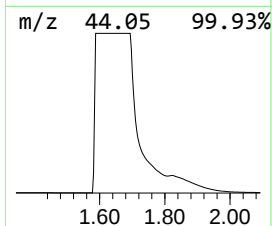
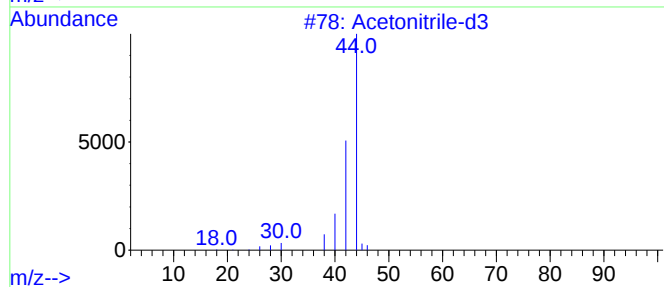
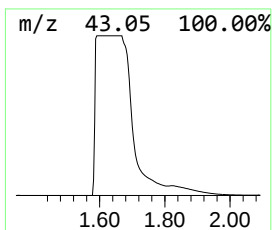
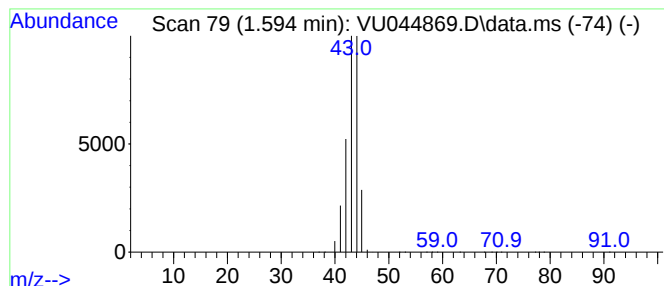
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.594 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.594	1648.96 ug/l	28431300	Pentafluorobenzene	5.372

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile-d3	44	C2D3N	002206-26-0	4
2			Ketene	42	C2H2O	000463-51-4	4
3			Ethylamine	45	C2H7N	000075-04-7	4
4			Ethylene oxide	44	C2H4O	000075-21-8	3
5			Dimethylamine	45	C2H7N	000124-40-3	3



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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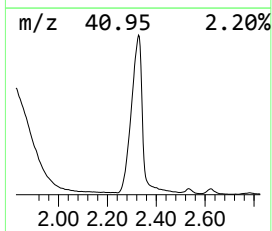
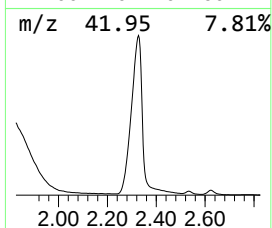
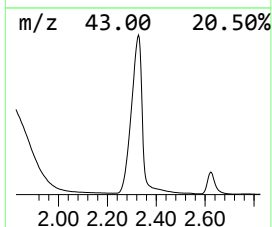
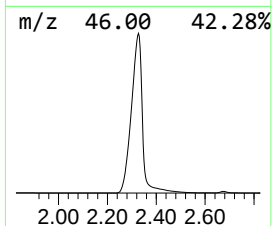
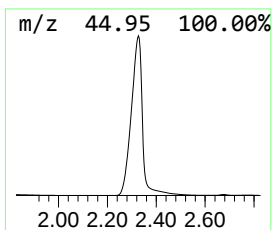
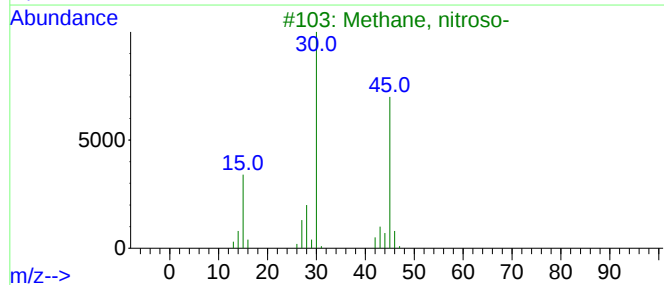
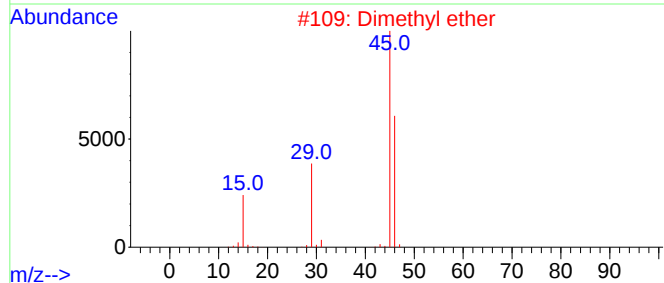
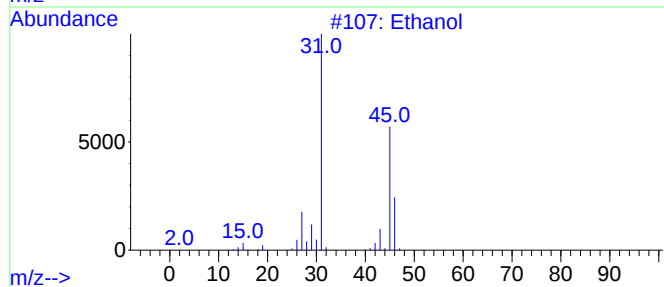
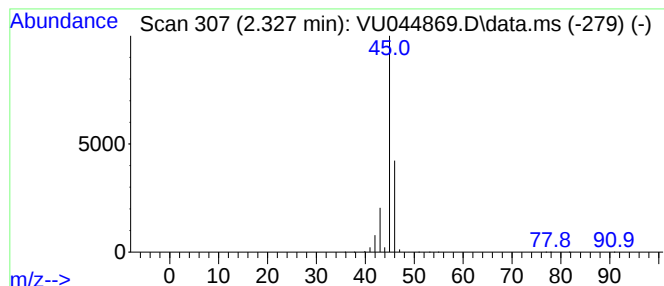
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.327	1496.37 ug/l	25800500	Pentafluorobenzene	5.372

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

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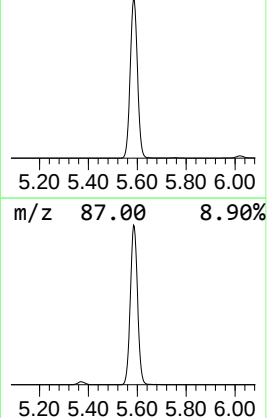
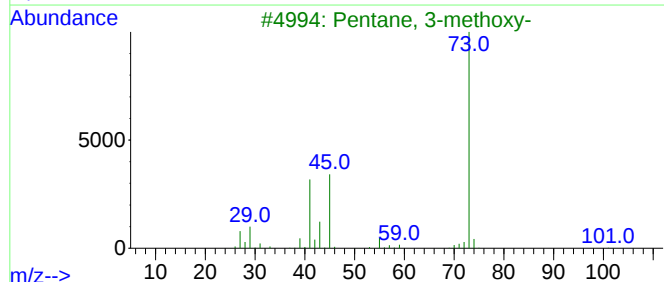
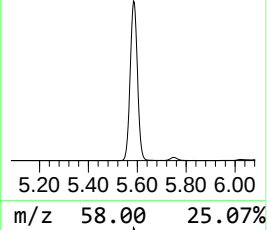
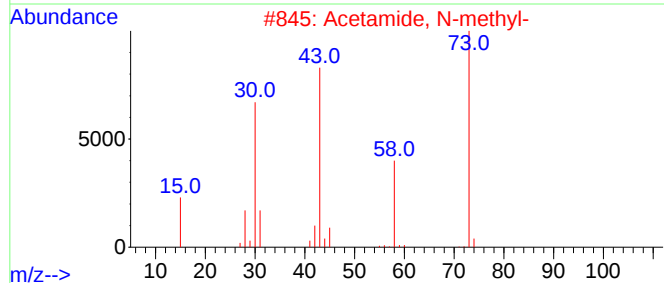
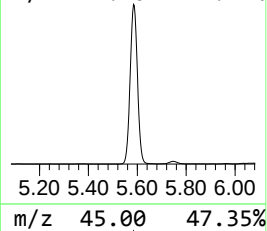
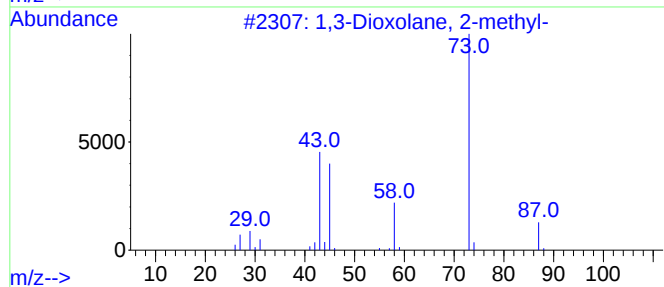
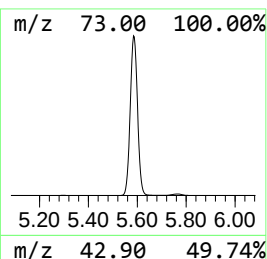
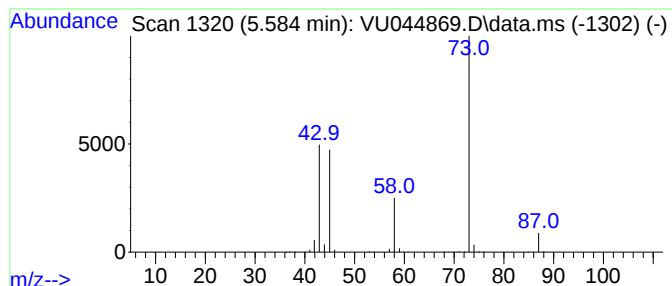
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 3 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.584	396.84 ug/l	6842290	Pentafluorobenzene	5.372

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	46
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
5			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9



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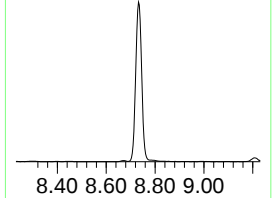
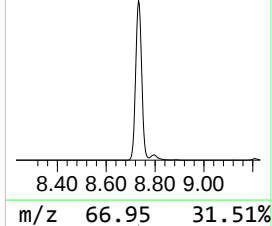
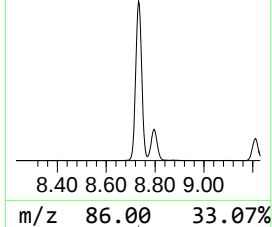
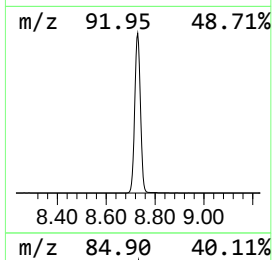
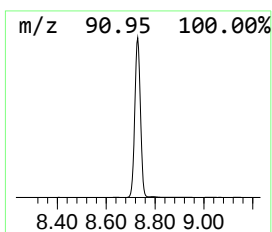
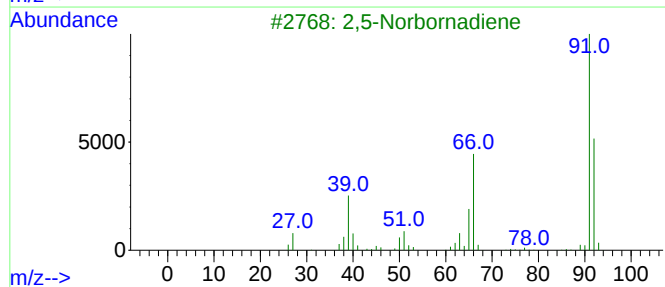
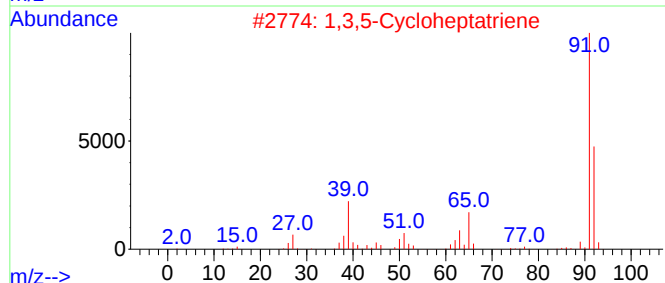
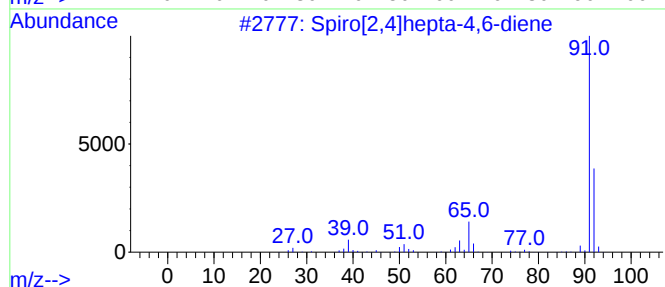
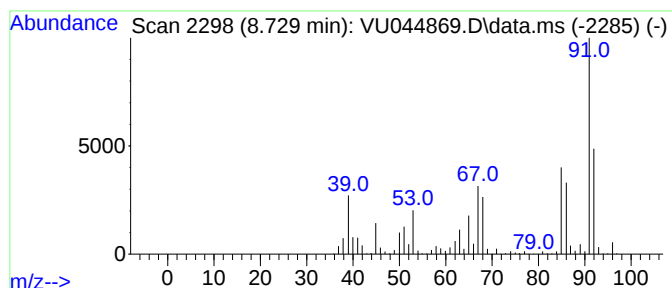
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Quant Title : SW846 8260

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

Peak Number 4 Spiro[2,4]hepta-4,6-diene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	89.73 ug/l	2493670	Chlorobenzene-d5	9.420

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	64
2		1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	60
3		2,5-Norbornadiene	92	C7H8	000121-46-0	35
4		Toluene	92	C7H8	000108-88-3	35
5		Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	18



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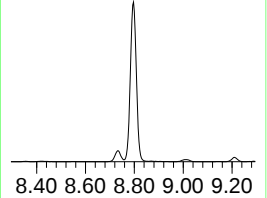
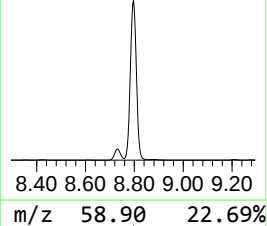
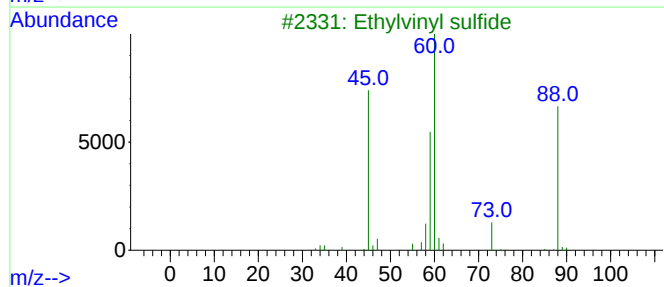
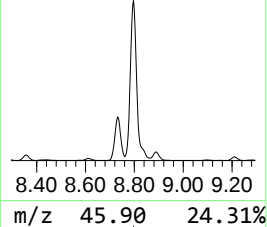
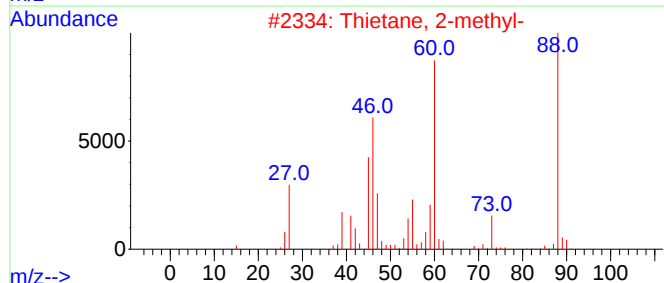
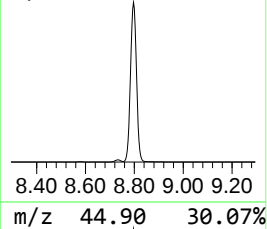
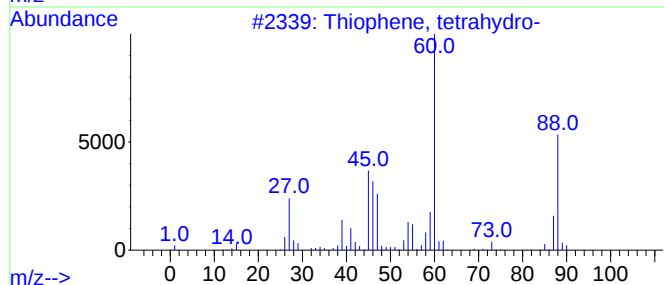
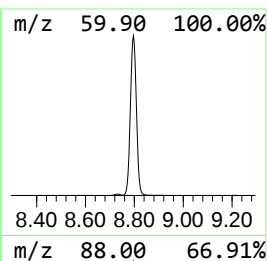
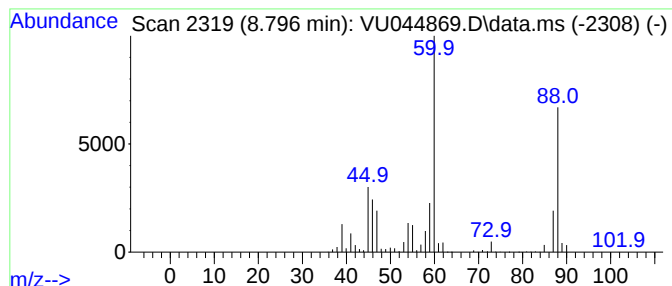
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Quant Title : SW846 8260

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

Peak Number 5 Thiophene, tetrahydro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.796	134.32 ug/l	3733010	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	38
4			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044869.D
Acq On : 26 Sep 2021 04:41
Operator : SY/MD
Sample : M3888-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
20896

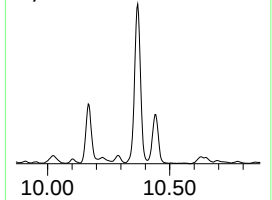
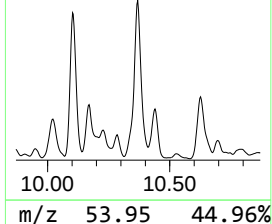
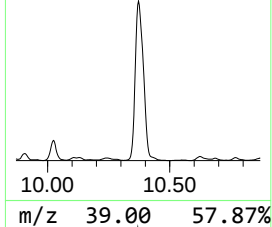
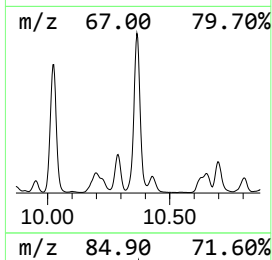
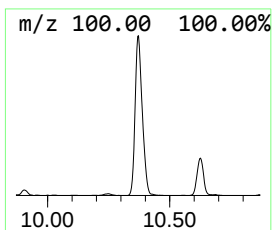
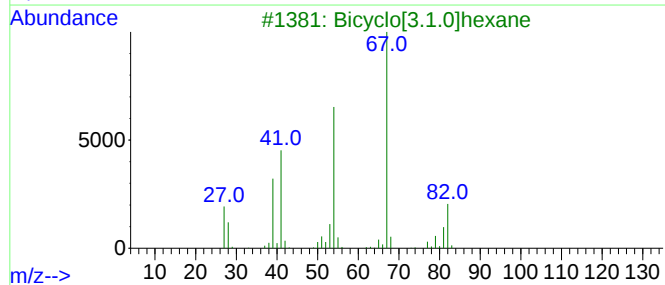
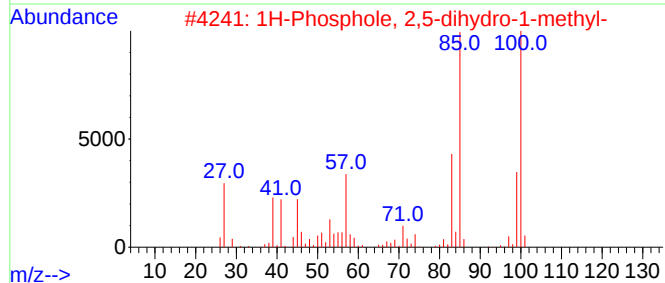
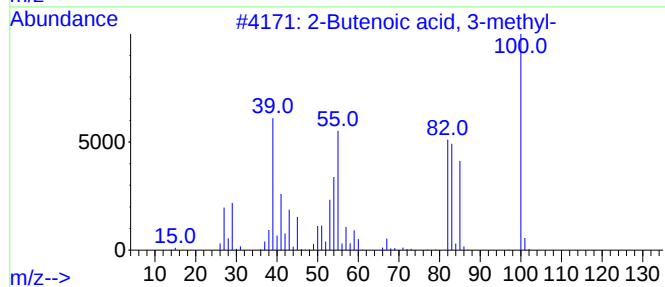
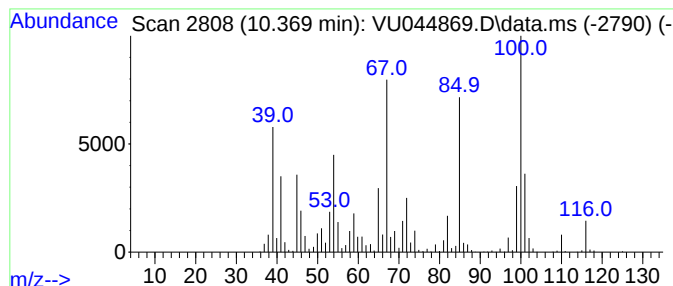
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Quant Title : SW846 8260

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

Peak Number 6 unknown10.369 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.369	84.22 ug/l	2340680	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenoic acid, 3-methyl-	100	C5H8O2	000541-47-9	35
2			1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	27
3			Bicyclo[3.1.0]hexane	82	C6H10	000285-58-5	25
4			Cyclohexene	82	C6H10	000110-83-8	22
5			2-Butenoic acid, 2-methyl-, (Z)-	100	C5H8O2	000565-63-9	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044869.D
Acq On : 26 Sep 2021 04:41
Operator : SY/MD
Sample : M3888-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

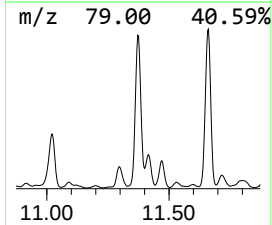
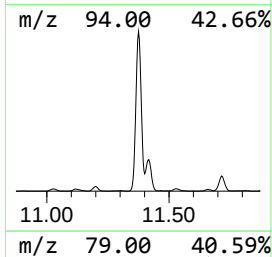
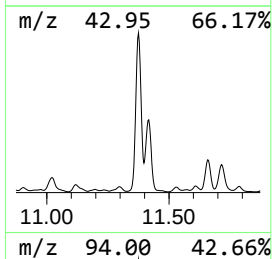
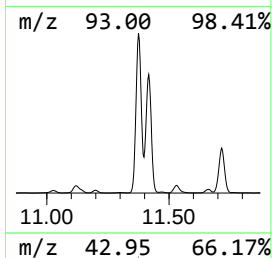
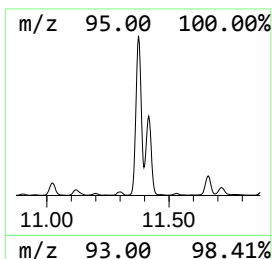
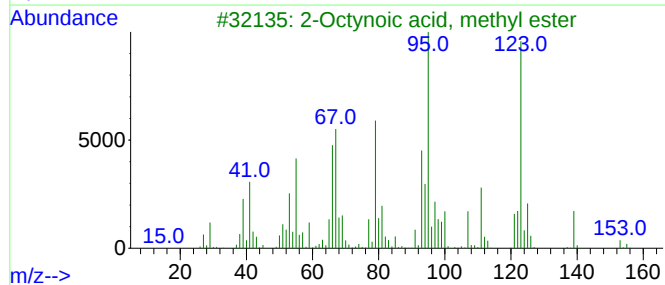
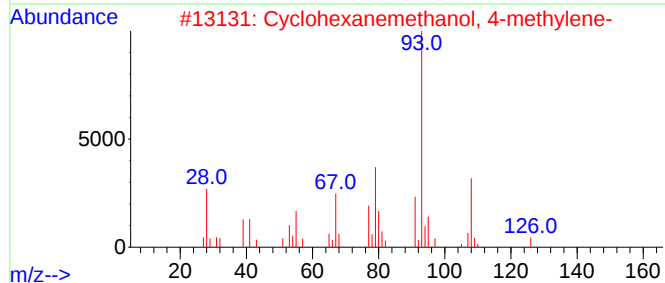
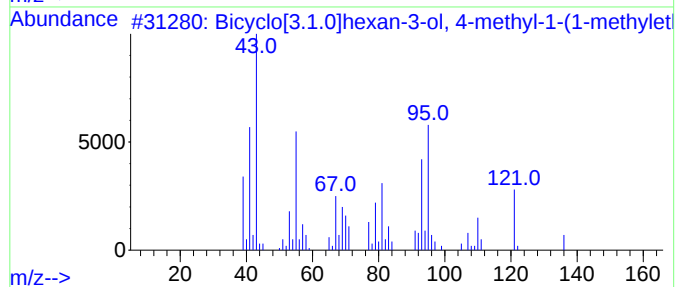
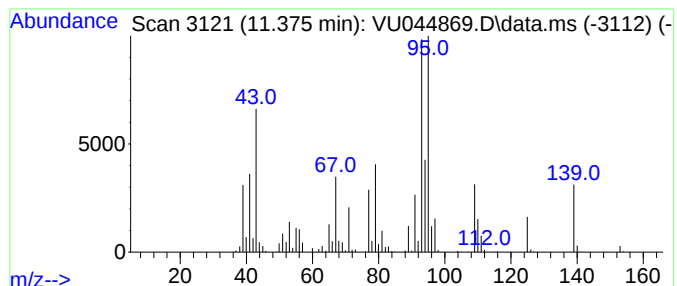
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 7 Bicyclo[3.1.0]hexan-3-ol, 4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.375	106.66 ug/l	2847520	1,4-Dichlorobenzene-d4		11.816	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexan-3-ol, 4-meth...		154	C10H18O	000513-23-5	53
2	Cyclohexanemethanol, 4-methylene-		126	C8H14O	001004-24-6	27
3	2-Octynoic acid, methyl ester		154	C9H14O2	000111-12-6	27
4	Cyclopentene, 1,2,3-trimethyl-		110	C8H14	000473-91-6	25
5	N-(5-Methylfurfuryl)dimethylamine		139	C8H13NO	014496-35-6	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044869.D
Acq On : 26 Sep 2021 04:41
Operator : SY/MD
Sample : M3888-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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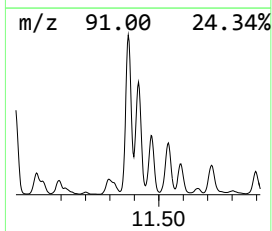
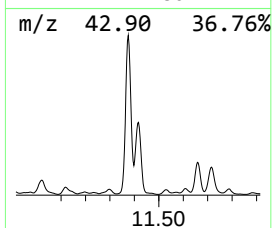
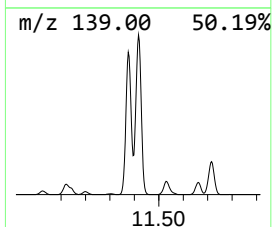
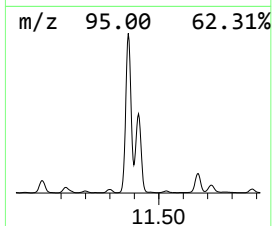
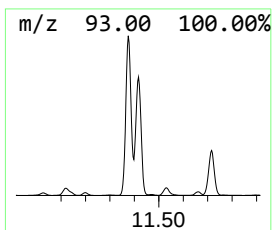
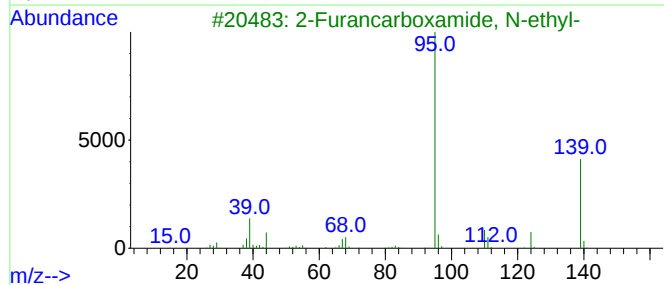
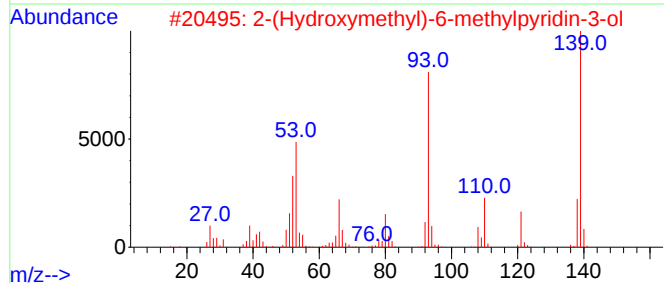
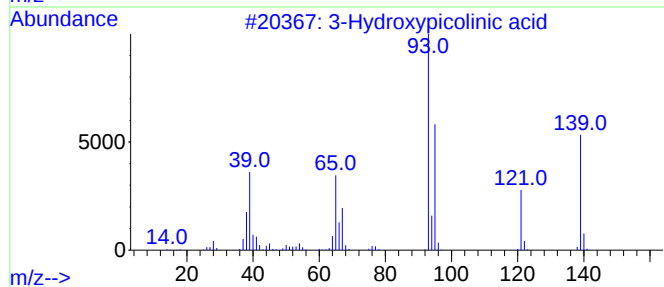
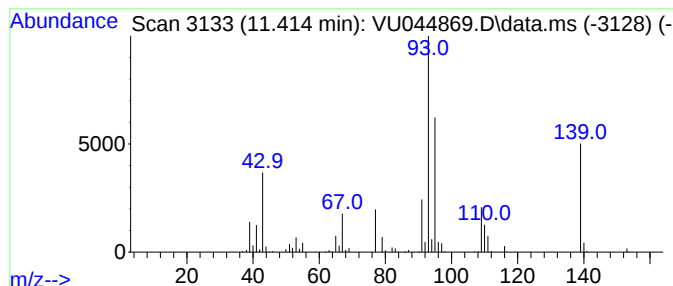
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Quant Title : SW846 8260

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

Peak Number 8 unknown11.414 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.414	59.64 ug/l	1592220	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxypicolinic acid	139	C6H5NO3	000874-24-8	42
2			2-(Hydroxymethyl)-6-methylpyridi...	139	C7H9NO2	042097-42-7	37
3			2-Furancarboxamide, N-ethyl-	139	C7H9NO2	1000407-23-8	35
4			Bis[bicyclo[3.2.0]hept-2-en-4-yl...	202	C14H18O	1000153-89-5	35
5			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044869.D
Acq On : 26 Sep 2021 04:41
Operator : SY/MD
Sample : M3888-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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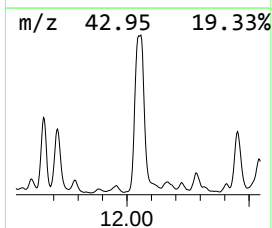
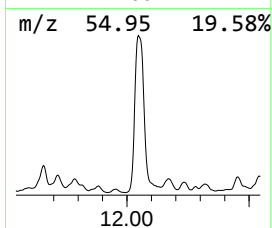
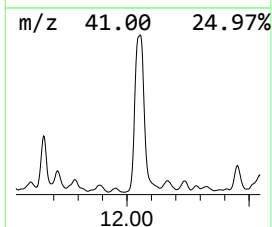
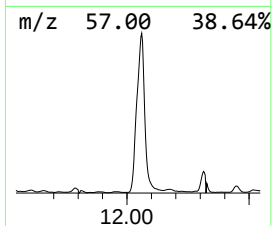
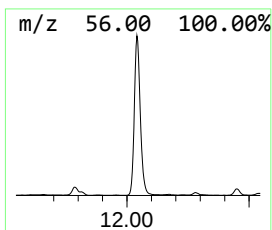
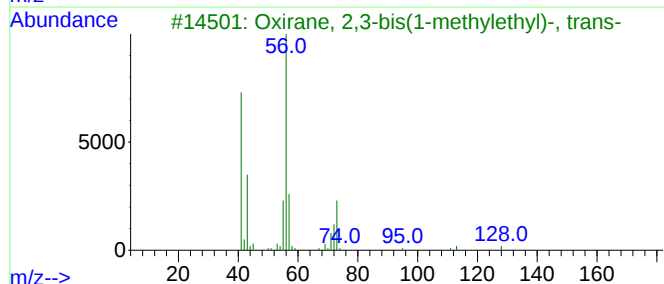
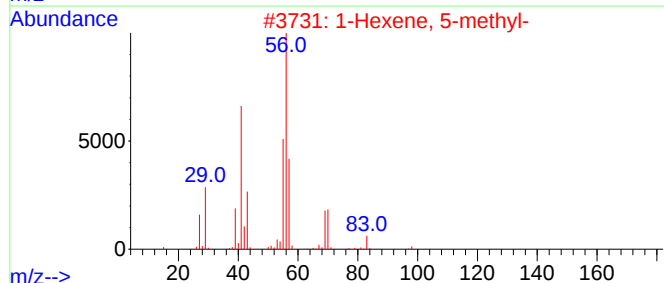
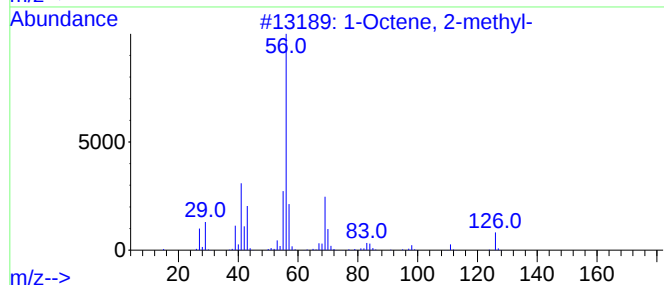
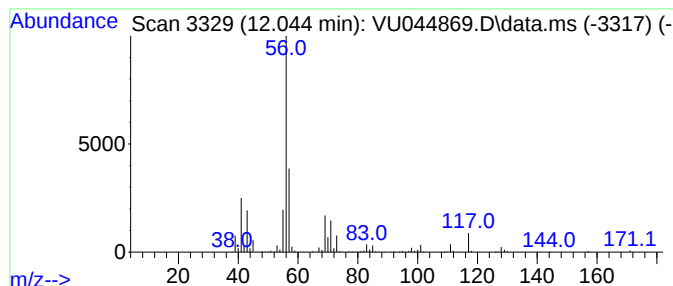
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Quant Title : SW846 8260

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

Peak Number 9 1-Octene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.044	91.75 ug/l	2449310	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octene, 2-methyl-	126	C9H18	004588-18-5	64
2			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	59
3			Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	59
4			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	45
5			Nonane, 5-methylene-	140	C10H20	006795-79-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044869.D
Acq On : 26 Sep 2021 04:41
Operator : SY/MD
Sample : M3888-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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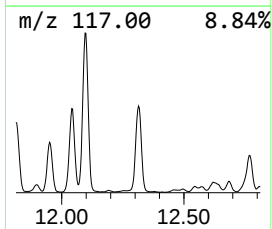
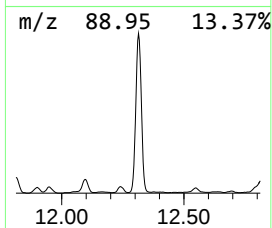
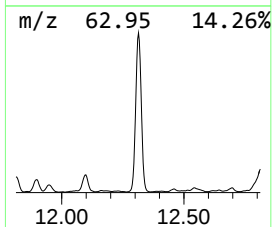
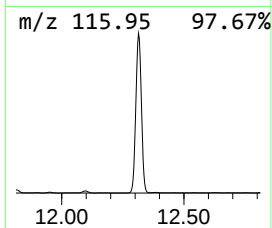
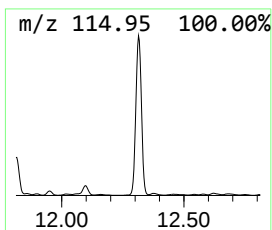
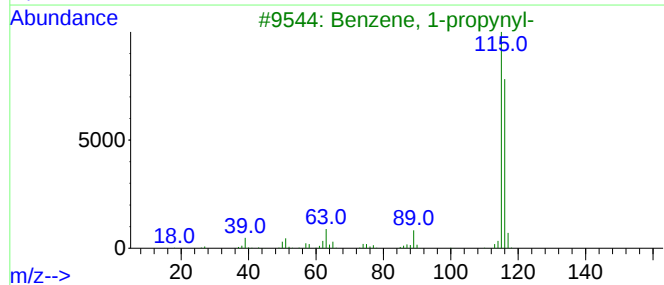
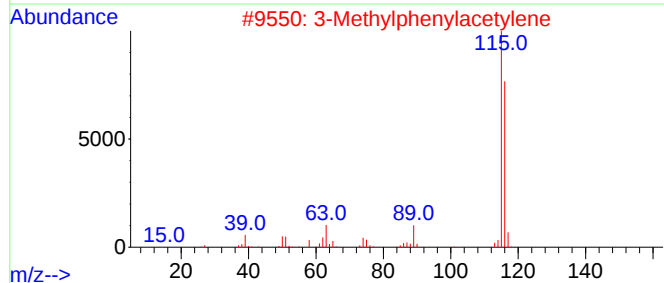
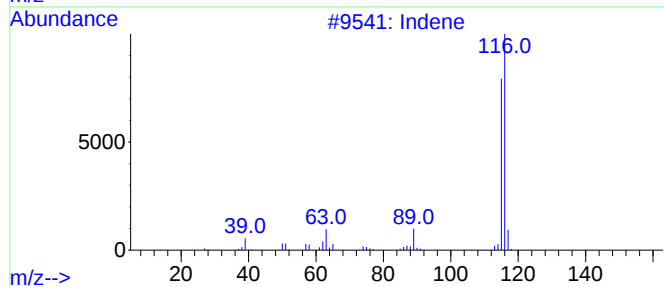
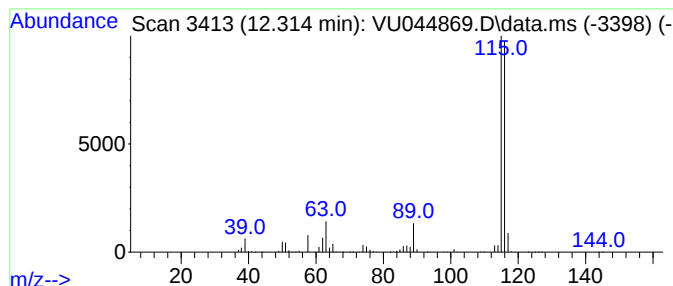
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Quant Title : SW846 8260

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

Peak Number 10 Indene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.314	65.75 ug/l	1755390	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	95
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5			2-Methylphenylacetylene	116	C9H8	000766-47-2	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044869.D
Acq On : 26 Sep 2021 04:41
Operator : SY/MD
Sample : M3888-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.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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Ethanol	2.327	1496.4	ug/l	25800500	1	5.372	862100	50.0
1,3-Dioxolane, ...	5.584	396.8	ug/l	6842290	1	5.372	862100	50.0
Spiro[2,4]hepta...	8.729	89.7	ug/l	2493670	3	9.420	1389540	50.0
Thiophene, tetr...	8.796	134.3	ug/l	3733010	3	9.420	1389540	50.0
unknown10.369	10.369	84.2	ug/l	2340680	3	9.420	1389540	50.0
Bicyclo[3.1.0]h...	11.375	106.7	ug/l	2847520	4	11.816	1334820	50.0
unknown11.414	11.414	59.6	ug/l	1592220	4	11.816	1334820	50.0
1-Octene, 2-met...	12.044	91.8	ug/l	2449310	4	11.816	1334820	50.0
Indene	12.314	65.8	ug/l	1755390	4	11.816	1334820	50.0