

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062922\
 Data File : VU049518.D
 Acq On : 29 Jun 2022 17:31
 Operator : SY/MD
 Sample : N3499-04 50X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 31052-WATER

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\82U062722W.M
 Title : SW846 8260

Signal : TIC: VU049518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.983	188	200	222	rVB	1129885	1560245	1.19%	0.433%
2	2.195	257	266	282	rVB2	937131	1547062	1.18%	0.429%
3	2.424	282	337	344	rBV2	21317784	131343407	100.00%	36.413%
4	3.073	531	539	550	rVV	1224240	2446217	1.86%	0.678%
5	3.359	607	628	654	rVB3	1407142	3392182	2.58%	0.940%
6	3.690	712	731	753	rBV	1133275	2502964	1.91%	0.694%
7	4.112	838	862	898	rVB5	386339	1603493	1.22%	0.445%
8	4.526	975	991	1007	rVB	1020699	2465898	1.88%	0.684%
9	5.372	1239	1254	1270	rVV5	1758512	4465421	3.40%	1.238%
10	5.459	1270	1281	1304	rVB	667489	1589786	1.21%	0.441%
11	5.587	1304	1321	1345	rBV	1236829	2775641	2.11%	0.770%
12	5.774	1364	1379	1392	rVV	6539175	13363572	10.17%	3.705%
13	5.899	1406	1418	1435	rVV	3399949	8014945	6.10%	2.222%
14	6.131	1475	1490	1503	rBV	1300888	2483858	1.89%	0.689%
15	6.761	1663	1686	1695	rBV2	1479936	3571878	2.72%	0.990%
16	7.256	1824	1840	1855	rVB	1597387	3192510	2.43%	0.885%
17	7.382	1856	1879	1888	rBV3	1528359	3445620	2.62%	0.955%
18	7.841	2009	2022	2031	rBV3	767687	1816395	1.38%	0.504%
19	7.899	2031	2040	2050	rVV2	1901919	3296039	2.51%	0.914%
20	7.976	2050	2064	2077	rVV2	31814862	56450713	42.98%	15.650%
21	8.131	2103	2112	2131	rVB2	752408	1433674	1.09%	0.397%
22	9.417	2501	2512	2528	rBV	775370	1367189	1.04%	0.379%
23	9.571	2548	2560	2573	rBV	5545689	8780892	6.69%	2.434%
24	9.697	2585	2599	2610	rBV	17866894	29457383	22.43%	8.167%
25	10.102	2712	2725	2742	rVB	8683857	13597694	10.35%	3.770%
26	10.517	2832	2854	2875	rBV	3730590	7616114	5.80%	2.111%
27	10.632	2881	2890	2919	rVB3	691881	1572888	1.20%	0.436%
28	10.906	2965	2975	2991	rVB	1144312	1772344	1.35%	0.491%
29	10.999	2992	3004	3021	rVV	4537338	9522696	7.25%	2.640%
30	11.089	3021	3032	3057	rVB	1964754	3448148	2.63%	0.956%
31	11.291	3084	3095	3113	rVB	1748531	2763292	2.10%	0.766%
32	11.468	3138	3150	3167	rVB	7607293	11620734	8.85%	3.222%
33	11.812	3244	3257	3269	rBV	840343	1395722	1.06%	0.387%
34	11.893	3269	3282	3293	rBV	1949721	3121247	2.38%	0.865%
35	12.095	3326	3345	3351	rBV2	1607614	2765538	2.11%	0.767%
36	12.188	3363	3374	3391	rVB4	1215098	2449717	1.87%	0.679%

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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
31052-WATER

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\82U062722W.M
Title : SW846 8260

37	12.571	3482	3493	3501	rBV	1124302	1708142	1.30%	0.474%
38	13.024	3625	3634	3649	rVB	871552	1400147	1.07%	0.388%
39	13.452	3758	3767	3781	rVB3	1058521	1821623	1.39%	0.505%
40	14.086	3952	3964	3982	rVB	1105252	1762071	1.34%	0.489%

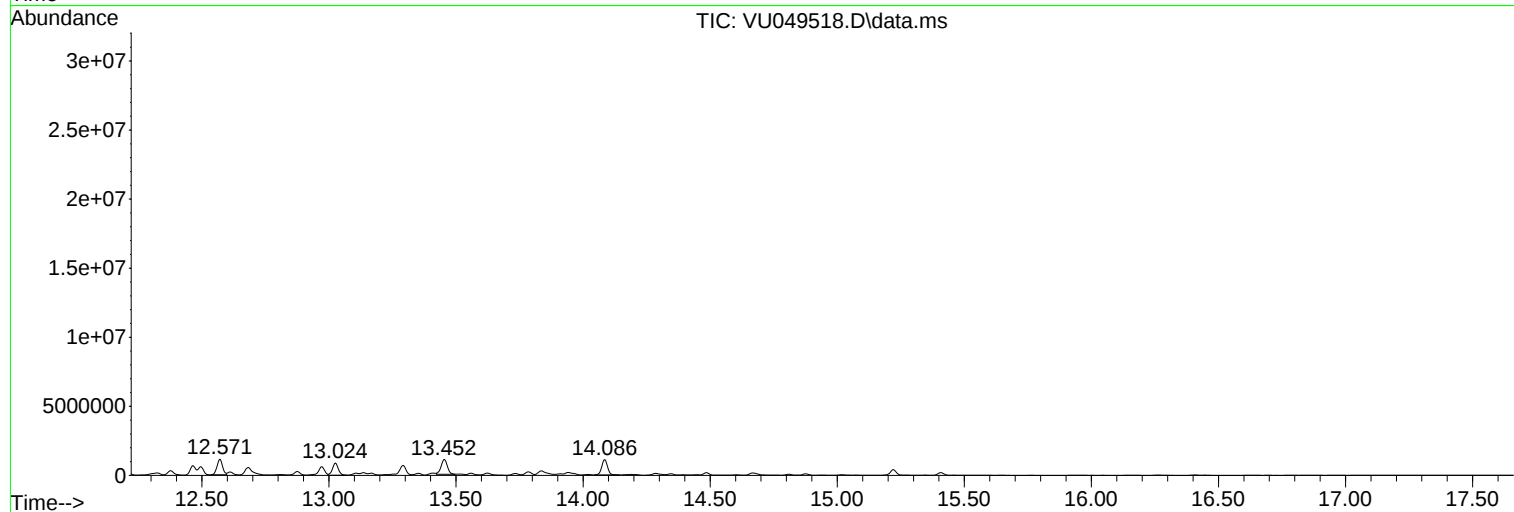
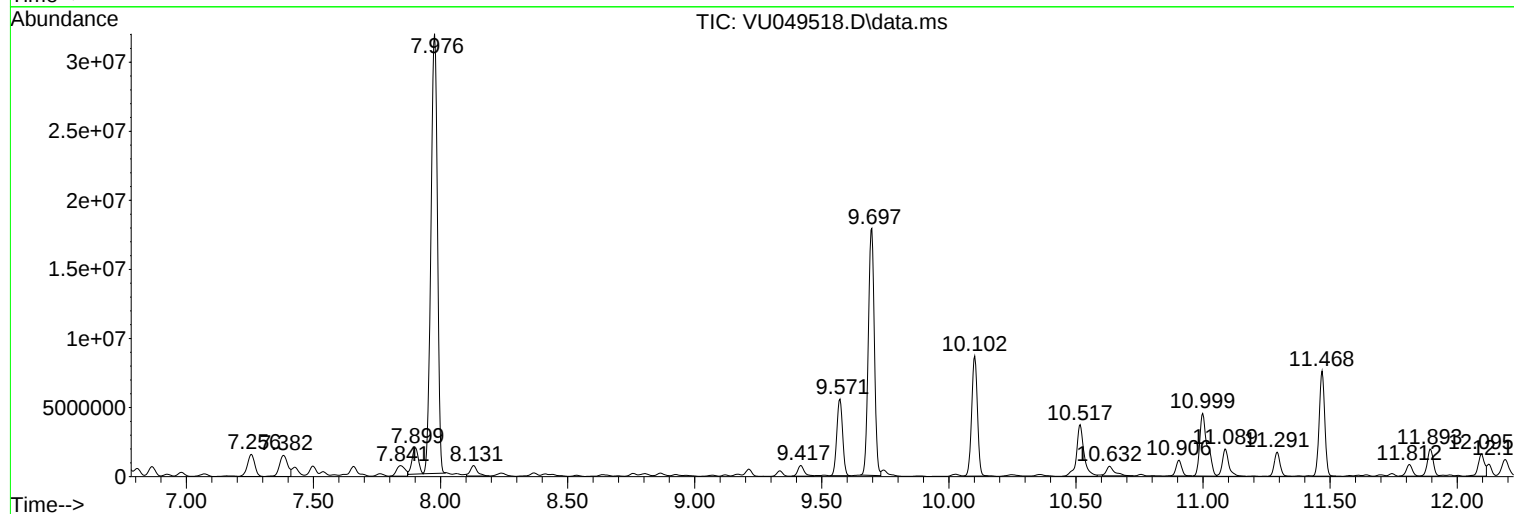
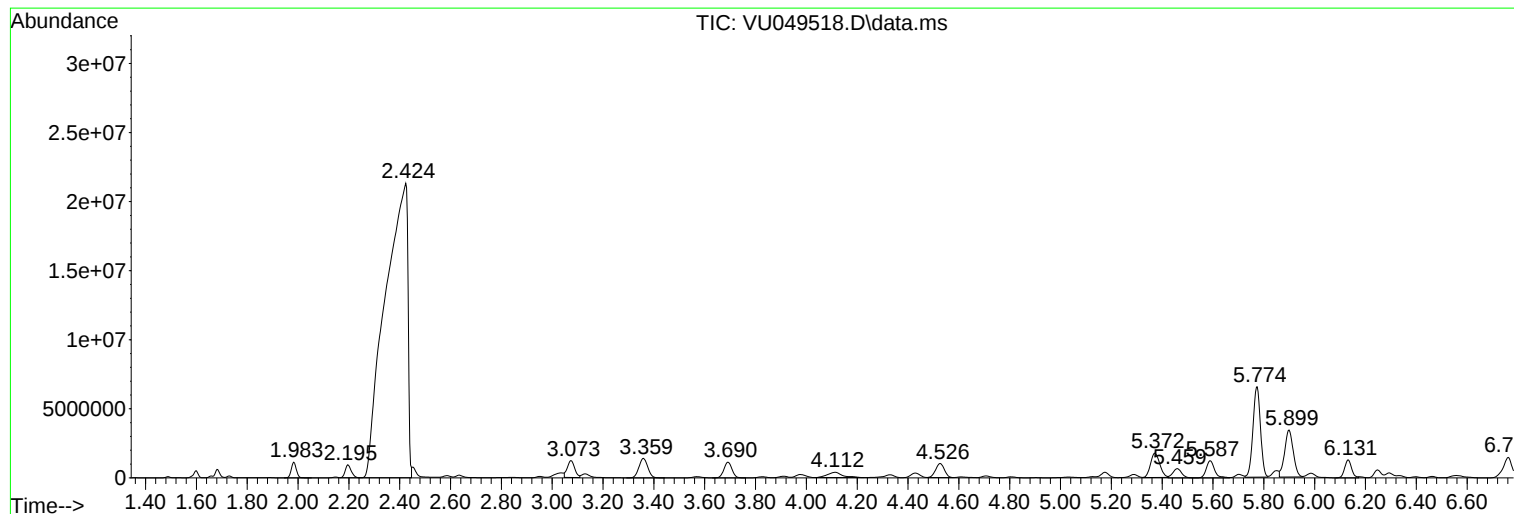
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ClientSampleId :
31052-WATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U062722W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_U/WATER
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Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

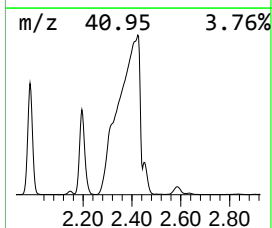
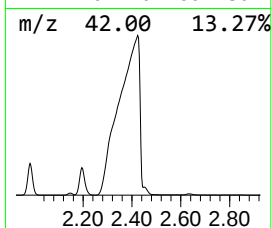
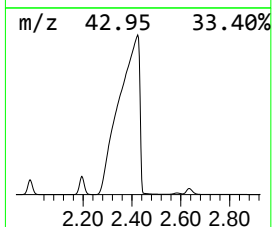
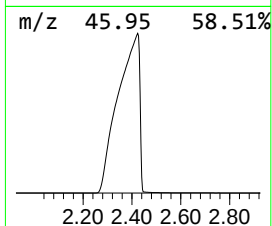
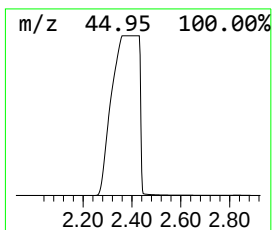
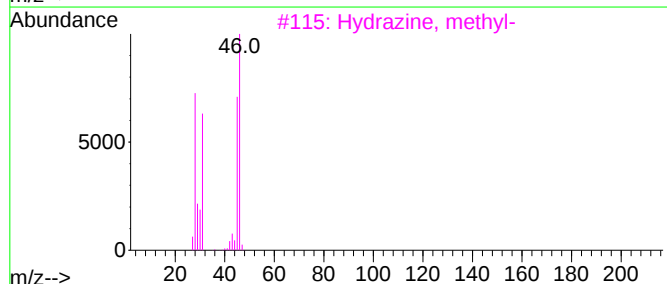
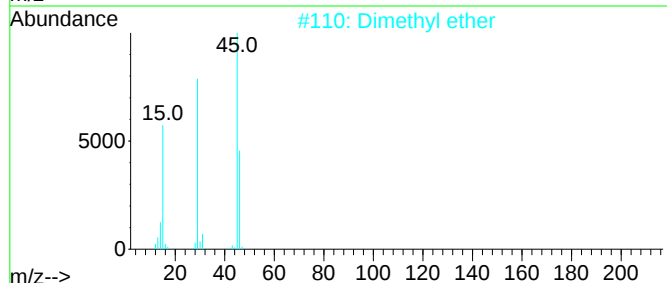
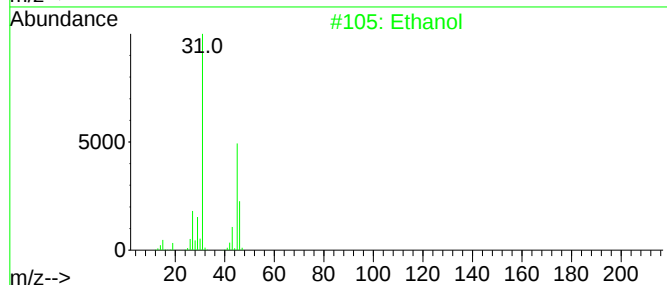
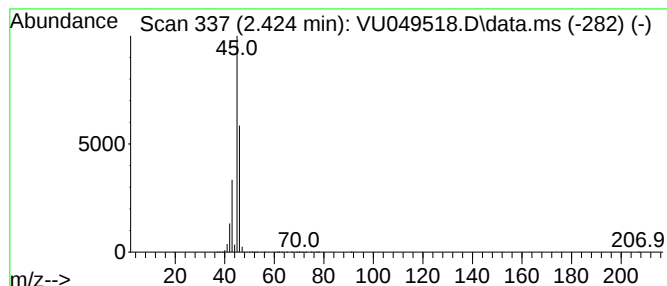
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U062722W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.424	1470.67 ug/l	131343000	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			Hydrazine, methyl-	46	CH6N2	000060-34-4	9
4			Methane, nitroso-	45	CH3NO	000865-40-7	4
5			Ethene, fluoro-	46	C2H3F	000075-02-5	4



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

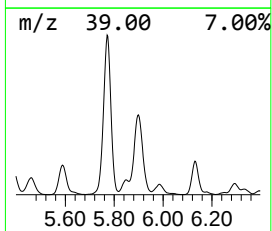
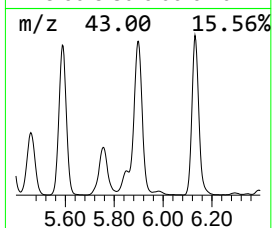
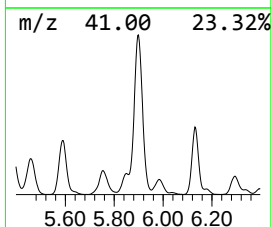
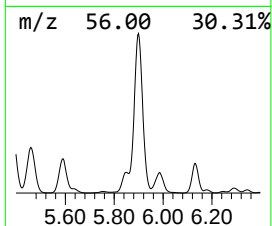
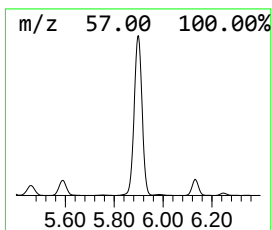
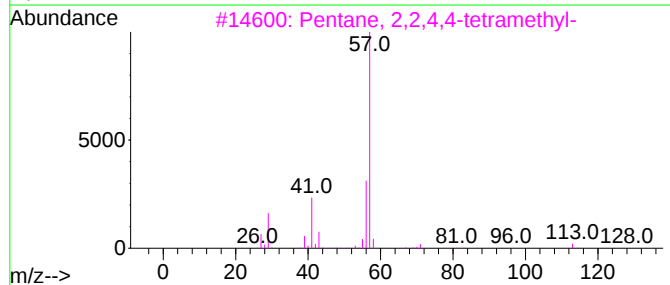
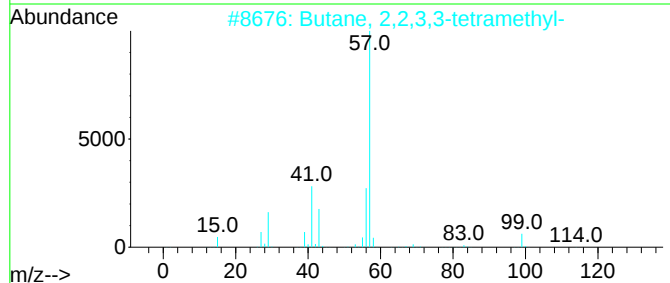
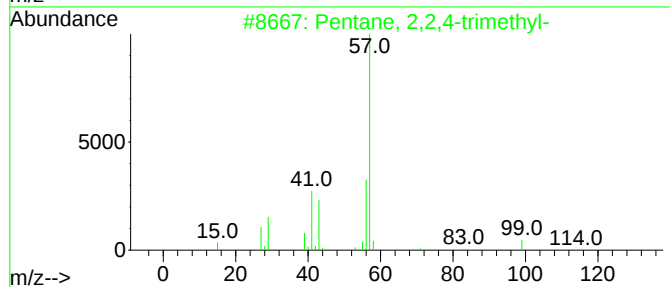
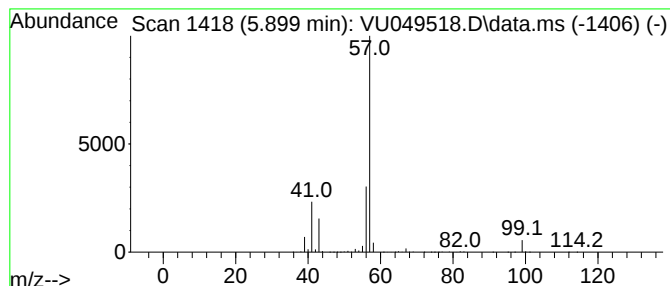
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U062722W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,2,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.899	161.34 ug/l	8014950	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
3			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
4			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	56



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

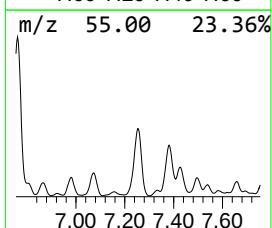
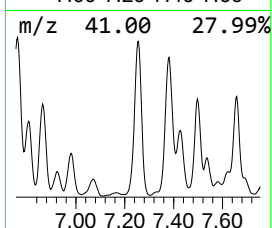
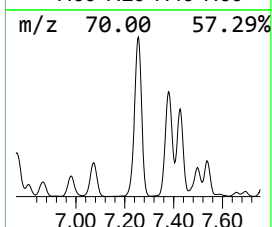
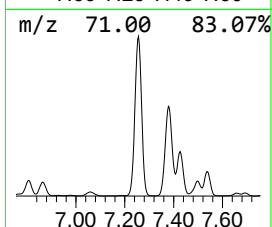
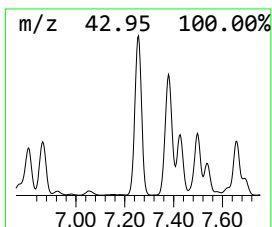
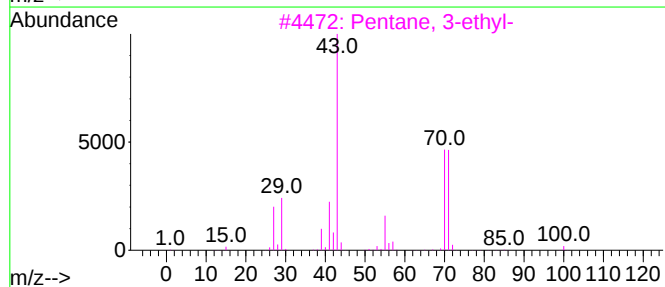
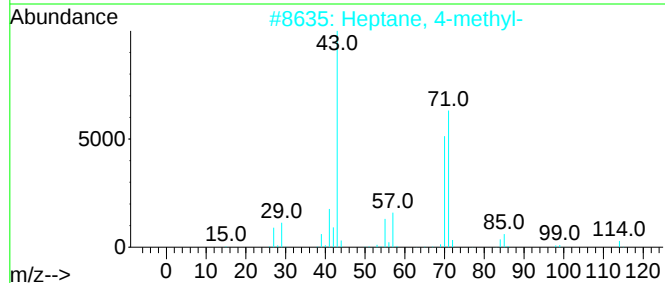
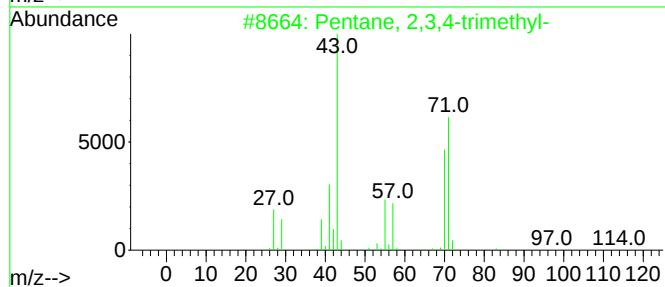
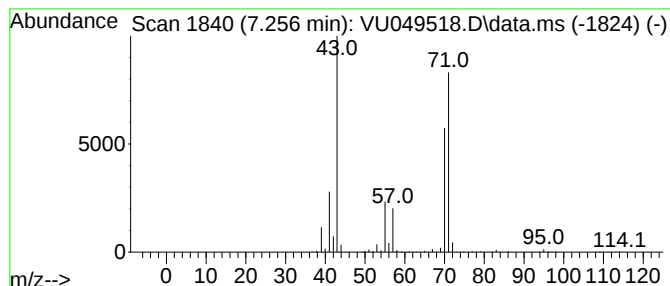
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U062722W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.256	64.27 ug/l	3192510	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	72
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	72



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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

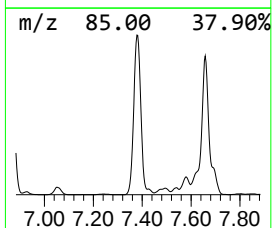
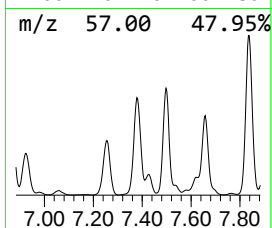
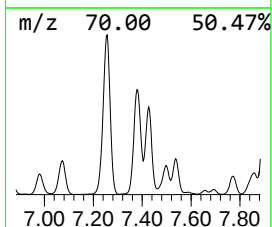
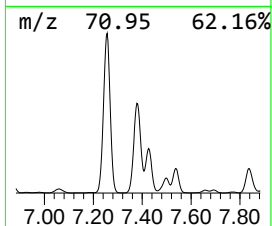
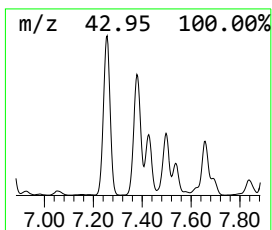
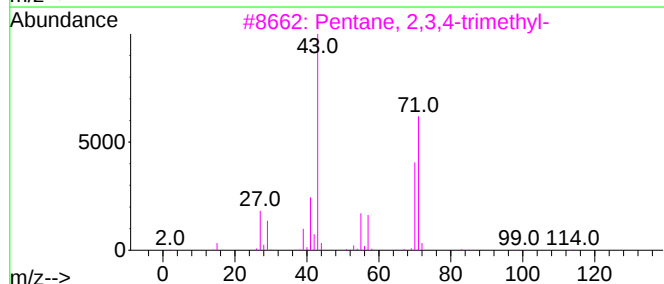
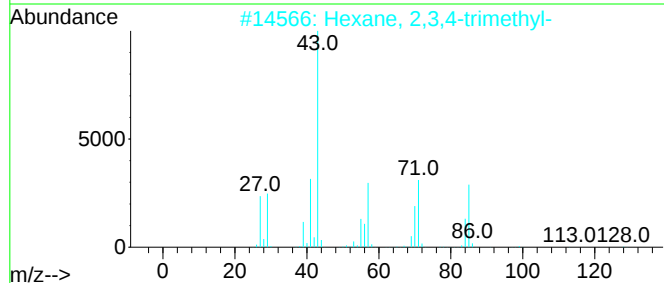
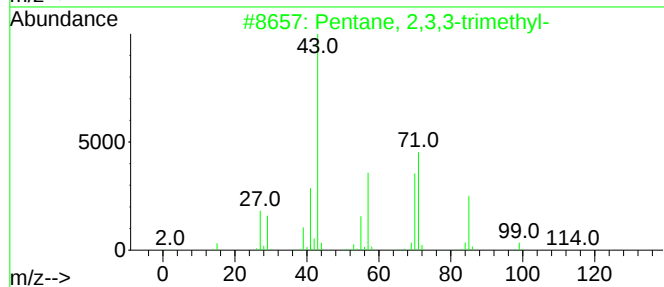
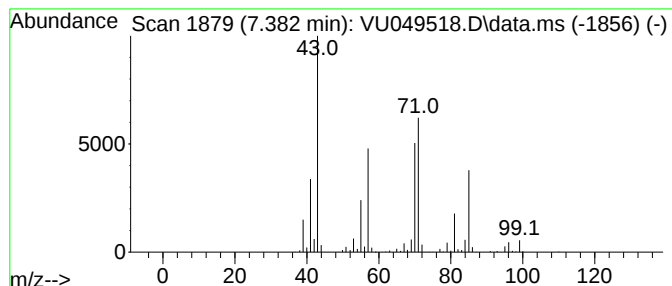
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.382	69.36 ug/l	3445620	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	86
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
5			Octane, 4-methyl-	128	C9H20	002216-34-4	50



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

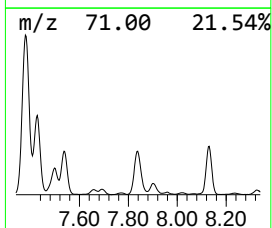
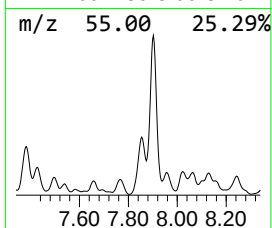
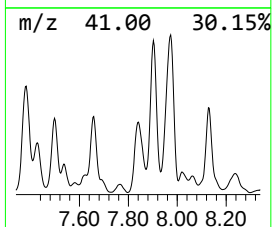
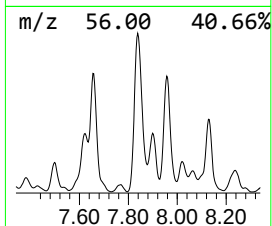
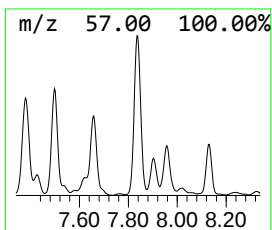
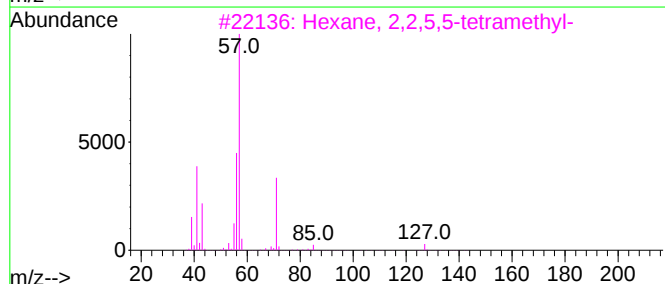
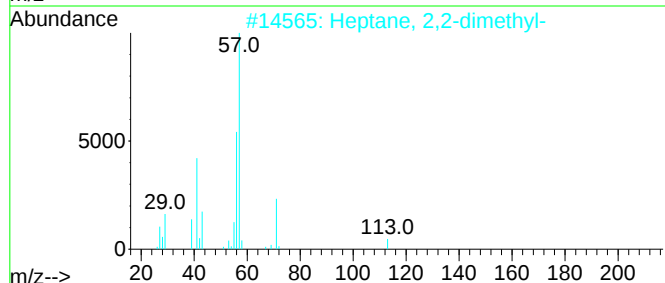
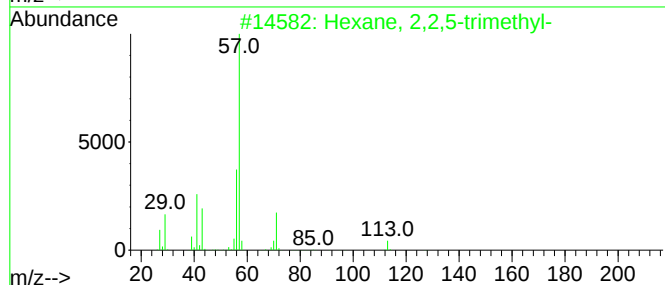
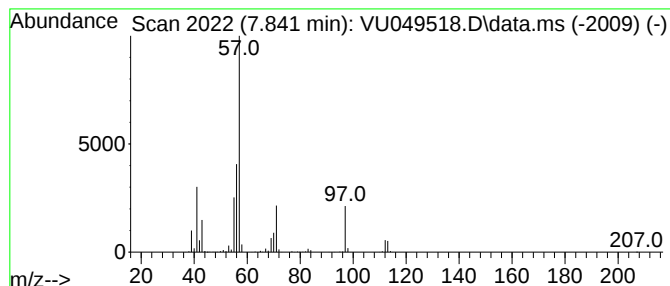
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Quant Title : SW846 8260

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

Peak Number 5 Hexane, 2,2,5-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.841	66.43 ug/l	1816400	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59
2			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	53
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	47
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45
5			2,4,4-Trimethyl-1-pentanol	130	C8H18O	016325-63-6	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062922\
Data File : VU049518.D
Acq On : 29 Jun 2022 17:31
Operator : SY/MD
Sample : N3499-04 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

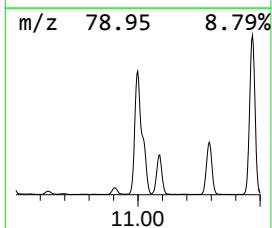
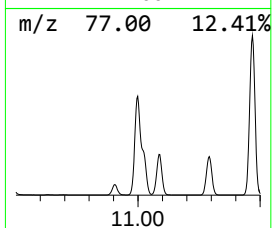
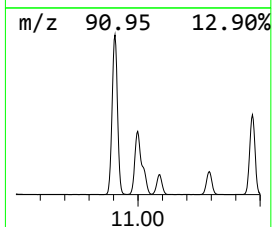
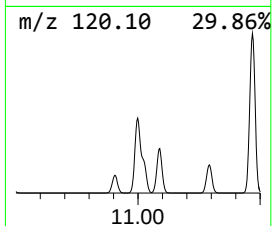
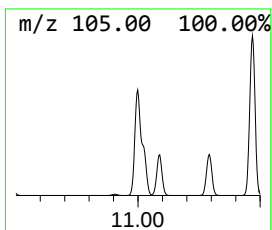
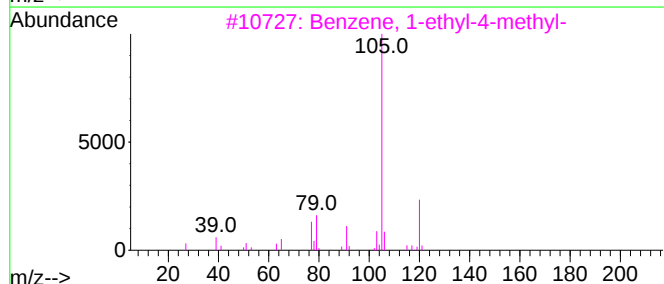
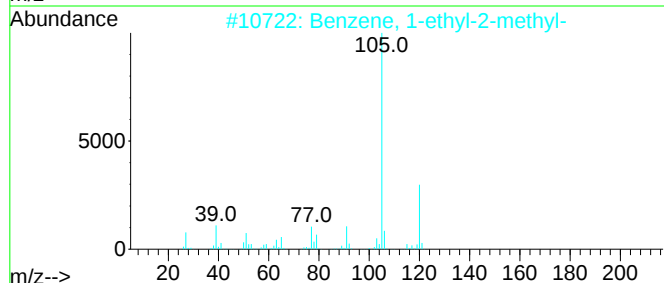
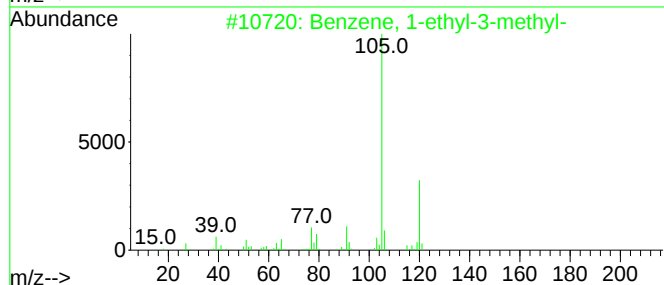
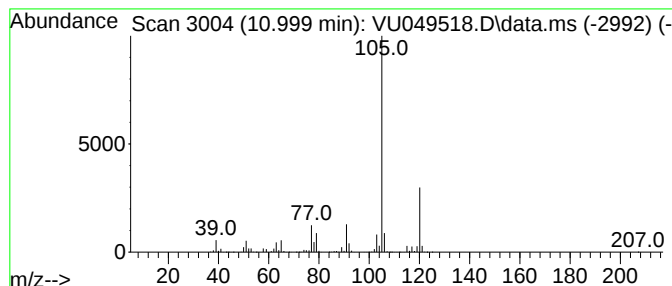
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.999	341.14 ug/l	9522700	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062922\
Data File : VU049518.D
Acq On : 29 Jun 2022 17:31
Operator : SY/MD
Sample : N3499-04 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

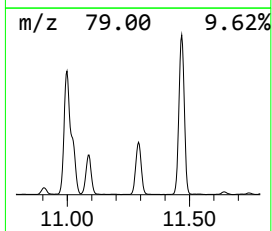
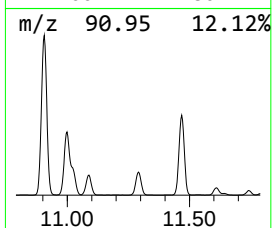
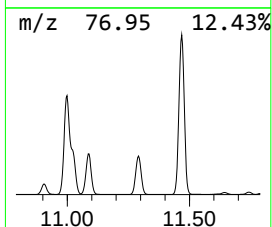
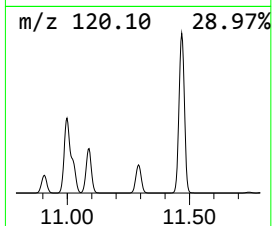
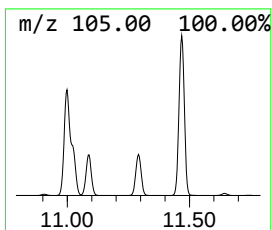
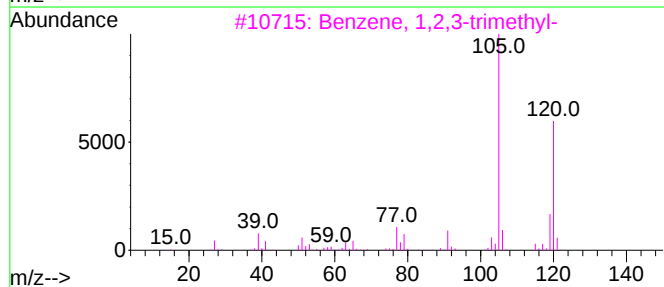
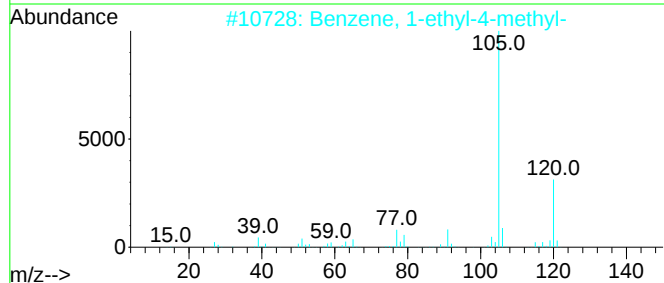
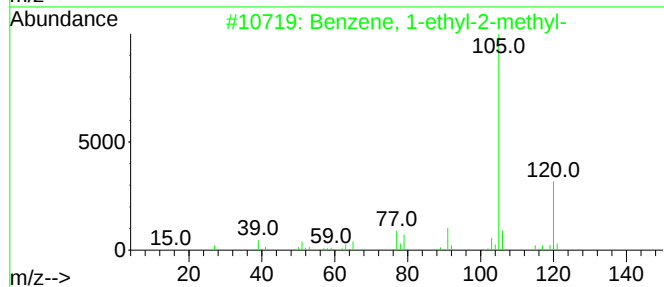
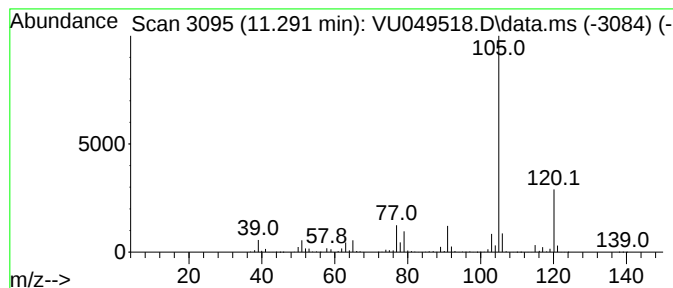
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.291	98.99 ug/l	2763290	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	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062922\
Data File : VU049518.D
Acq On : 29 Jun 2022 17:31
Operator : SY/MD
Sample : N3499-04 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

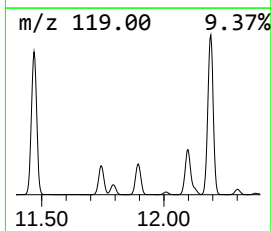
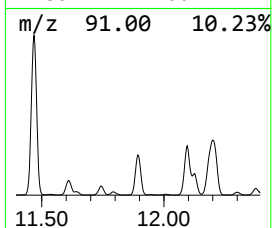
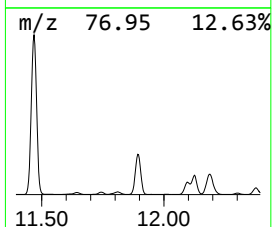
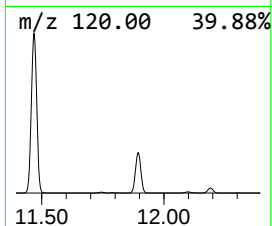
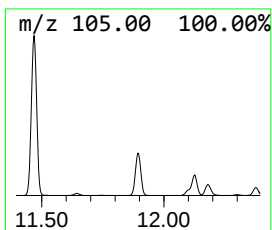
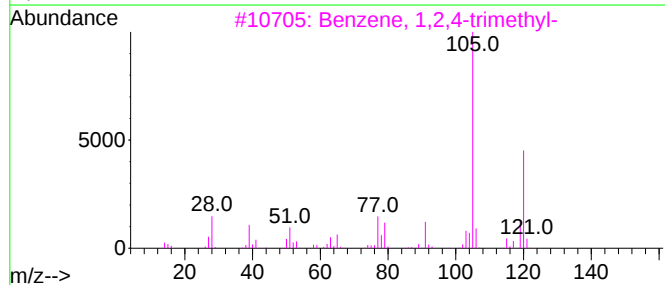
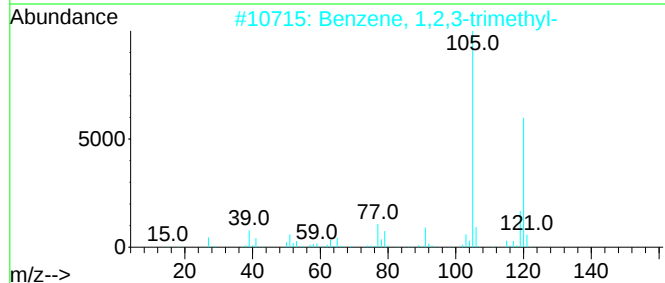
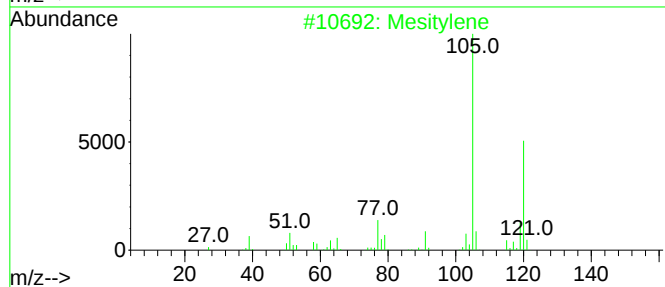
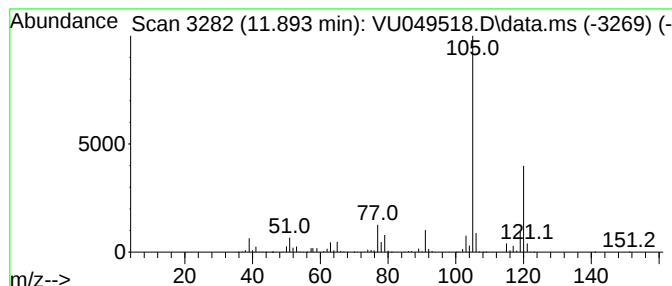
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.893	111.82 ug/l	3121250	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	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062922\
Data File : VU049518.D
Acq On : 29 Jun 2022 17:31
Operator : SY/MD
Sample : N3499-04 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

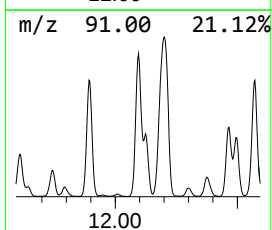
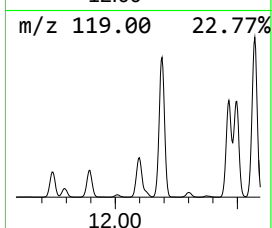
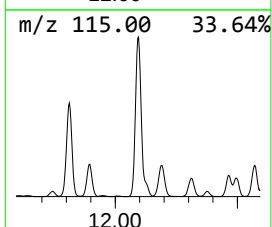
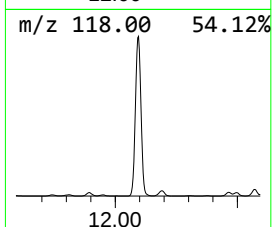
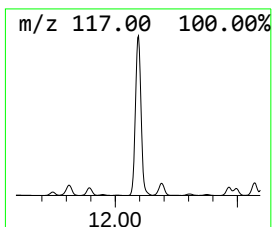
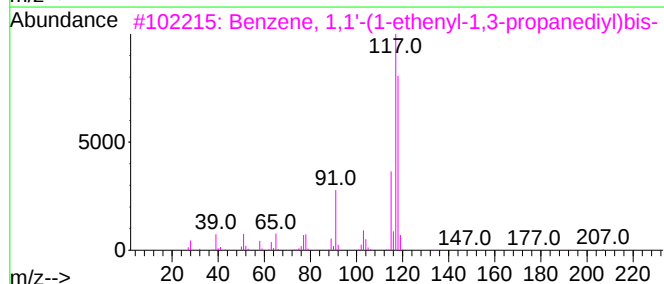
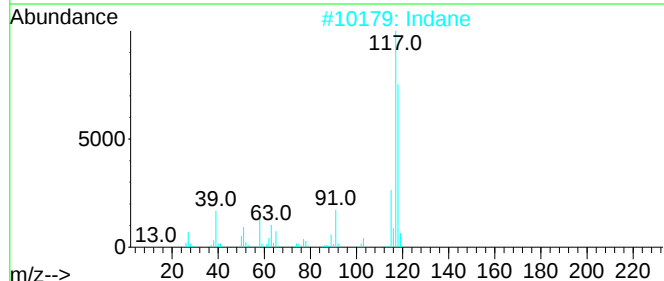
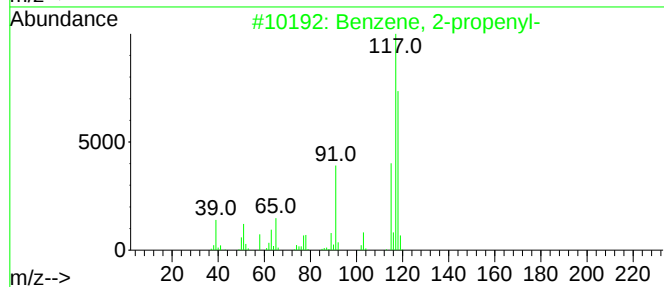
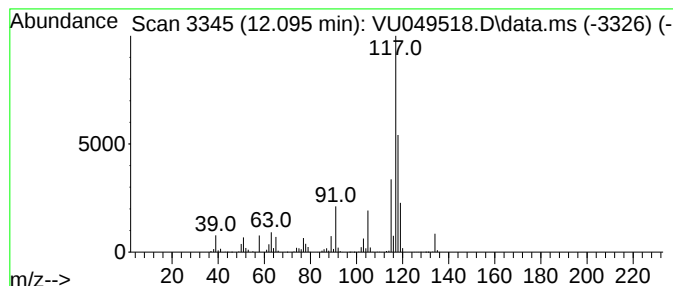
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.095	99.07 ug/l	2765540	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
2			Indane	118	C9H10	000496-11-7	70
3			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	64
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062922\
Data File : VU049518.D
Acq On : 29 Jun 2022 17:31
Operator : SY/MD
Sample : N3499-04 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

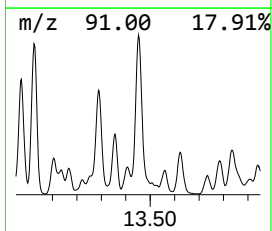
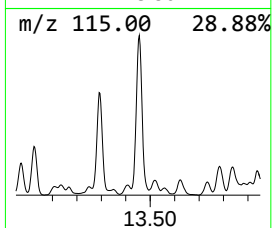
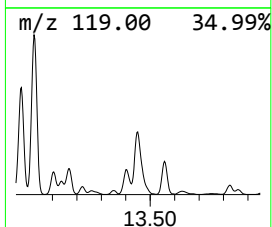
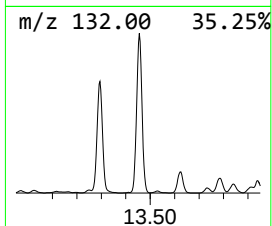
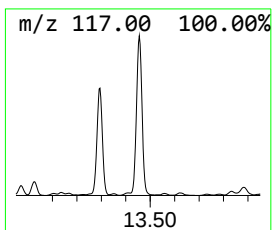
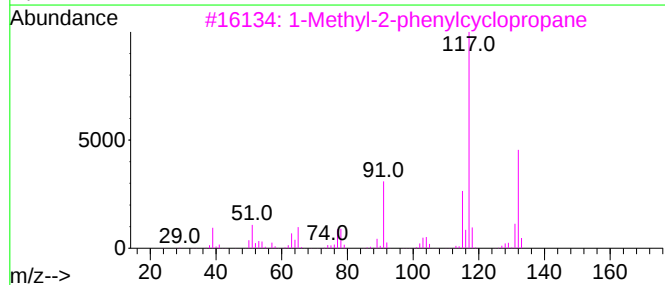
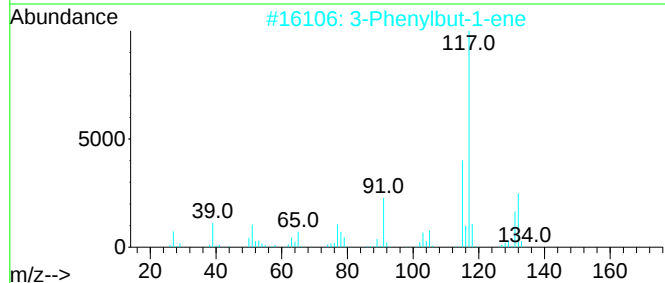
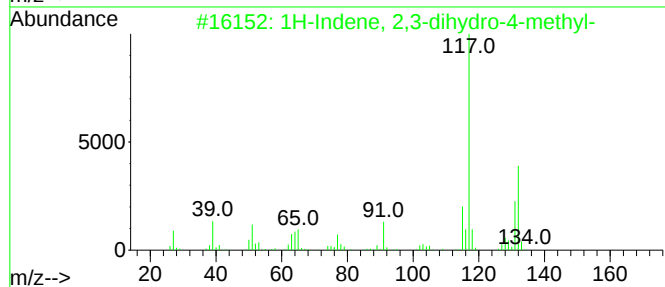
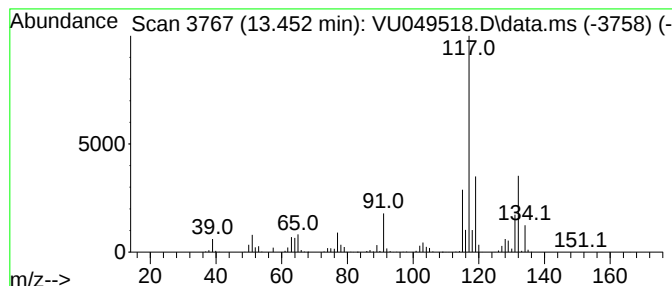
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.452	65.26 ug/l	1821620	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	89
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
3		1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81
4		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	81
5		Benzene, 2-butenyl-	132	C10H12	001560-06-1	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062922\
Data File : VU049518.D
Acq On : 29 Jun 2022 17:31
Operator : SY/MD
Sample : N3499-04 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31052-WATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U062722W.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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Pentane, 2,2,4-...	5.899	161.3	ug/l	8014950	2	6.247	2483860	50.0
Pentane, 2,3,4-...	7.256	64.3	ug/l	3192510	2	6.247	2483860	50.0
Pentane, 2,3,3-...	7.382	69.4	ug/l	3445620	2	6.247	2483860	50.0
Hexane, 2,2,5-t...	7.841	66.4	ug/l	1816400	3	9.417	1367190	50.0
Benzene, 1-ethy...	10.999	341.1	ug/l	9522700	4	11.812	1395720	50.0
Benzene, 1-ethy...	11.291	99.0	ug/l	2763290	4	11.812	1395720	50.0
Benzene, 1,2,3-...	11.893	111.8	ug/l	3121250	4	11.812	1395720	50.0
Benzene, 2-prop...	12.095	99.1	ug/l	2765540	4	11.812	1395720	50.0
1H-Indene, 2,3-...	13.452	65.3	ug/l	1821620	4	11.812	1395720	50.0