

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
 Data File : VU043053.D
 Acq On : 13 Apr 2021 15:50
 Operator : SY/MD
 Sample : M1983-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 31019

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\82U041221W.M
 Title : SW846 8260

Signal : TIC: VU043053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.690	99	109	140	rBV	538618	743810	15.88%	1.722%
2	2.407	292	332	367	rBV2	668386	4518084	96.45%	10.459%
3	2.549	367	376	392	rVV	182698	334067	7.13%	0.773%
4	2.639	393	404	440	rVB	236143	498807	10.65%	1.155%
5	4.452	952	968	993	rBV3	60390	155624	3.32%	0.360%
6	4.716	1035	1050	1073	rBV	61466	148135	3.16%	0.343%
7	5.298	1214	1231	1244	rBV	126753	266716	5.69%	0.617%
8	5.382	1244	1257	1282	rVB	198145	417525	8.91%	0.967%
9	5.710	1343	1359	1375	rBV	140661	288933	6.17%	0.669%
10	5.973	1428	1441	1458	rBV5	22729	48678	1.04%	0.113%
11	6.256	1515	1529	1549	rVB	297363	558023	11.91%	1.292%
12	6.565	1609	1625	1656	rBV7	21066	97845	2.09%	0.227%
13	6.777	1680	1691	1709	rVB	68521	132591	2.83%	0.307%
14	6.886	1712	1725	1735	rBV	124523	243273	5.19%	0.563%
15	7.906	2022	2042	2057	rBV	470649	811082	17.32%	1.878%
16	8.243	2135	2147	2167	rBV6	17736	48170	1.03%	0.112%
17	8.459	2199	2214	2237	rBV	51878	120580	2.57%	0.279%
18	8.793	2305	2318	2346	rBV	844712	1429147	30.51%	3.308%
19	9.423	2501	2514	2530	rBV	432191	699474	14.93%	1.619%
20	10.005	2682	2695	2719	rBV	520966	987212	21.08%	2.285%
21	10.240	2759	2768	2780	rBV	51276	77062	1.65%	0.178%
22	10.353	2793	2803	2828	rVB3	29308	56939	1.22%	0.132%
23	10.639	2881	2892	2908	rVB	375663	583490	12.46%	1.351%
24	11.819	3245	3259	3272	rBV	471147	760707	16.24%	1.761%
25	11.915	3283	3289	3299	rVB3	34788	52424	1.12%	0.121%
26	12.066	3326	3336	3352	rBV	104808	216877	4.63%	0.502%
27	12.333	3409	3419	3430	rBV	620100	862144	18.41%	1.996%
28	12.388	3430	3436	3450	rVB8	27368	62567	1.34%	0.145%
29	12.497	3452	3470	3475	rBV9	42276	113470	2.42%	0.263%
30	12.549	3476	3486	3500	rVV5	111338	241455	5.15%	0.559%
31	12.613	3501	3506	3515	rVB3	41384	59382	1.27%	0.137%
32	12.671	3515	3524	3533	rBV2	103723	168647	3.60%	0.390%
33	12.963	3595	3615	3624	rBV7	225810	683053	14.58%	1.581%
34	13.015	3624	3631	3636	rVV	201506	307830	6.57%	0.713%
35	13.053	3637	3643	3652	rVB2	349678	515287	11.00%	1.193%
36	13.140	3663	3670	3678	rVB	280501	363644	7.76%	0.842%

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37	13.295	3712	3718	3729	rVB4	131277	225109	4.81%	0.521%
38	13.362	3731	3739	3747	rBV2	153669	253967	5.42%	0.588%
39	13.439	3753	3763	3785	rBV	2785505	4675970	99.82%	10.825%
40	13.594	3804	3811	3818	rBV	652742	960016	20.49%	2.222%
41	13.735	3848	3855	3863	rBV3	193391	314453	6.71%	0.728%
42	13.986	3918	3933	3935	rBV4	338506	671205	14.33%	1.554%
43	14.102	3963	3969	3975	rBV2	434471	564492	12.05%	1.307%
44	14.198	3987	3999	4014	rVB4	1232202	2635397	56.26%	6.101%
45	14.288	4019	4027	4035	rBV4	306822	620728	13.25%	1.437%
46	14.458	4072	4080	4088	rBV	3488344	4684181	100.00%	10.844%
47	14.819	4186	4192	4198	rBV4	215524	297603	6.35%	0.689%
48	15.028	4249	4257	4265	rBV3	942673	1560994	33.32%	3.614%
49	15.214	4305	4315	4329	rBV4	1250357	3070046	65.54%	7.107%
50	15.282	4330	4336	4350	rVB4	525038	900060	19.21%	2.084%
51	15.410	4368	4376	4389	rBV2	987703	1611357	34.40%	3.730%
52	15.513	4404	4408	4418	rVB7	372370	571297	12.20%	1.323%
53	15.937	4531	4540	4559	rVB4	406277	950870	20.30%	2.201%
54	16.159	4602	4609	4617	rBV3	149347	225090	4.81%	0.521%
55	16.272	4638	4644	4648	rBV3	152864	214494	4.58%	0.497%
56	16.417	4681	4689	4696	rBV3	165074	250092	5.34%	0.579%
57	16.892	4830	4837	4850	rBV9	33581	77408	1.65%	0.179%
58	17.143	4907	4915	4925	rVB	127193	189883	4.05%	0.440%

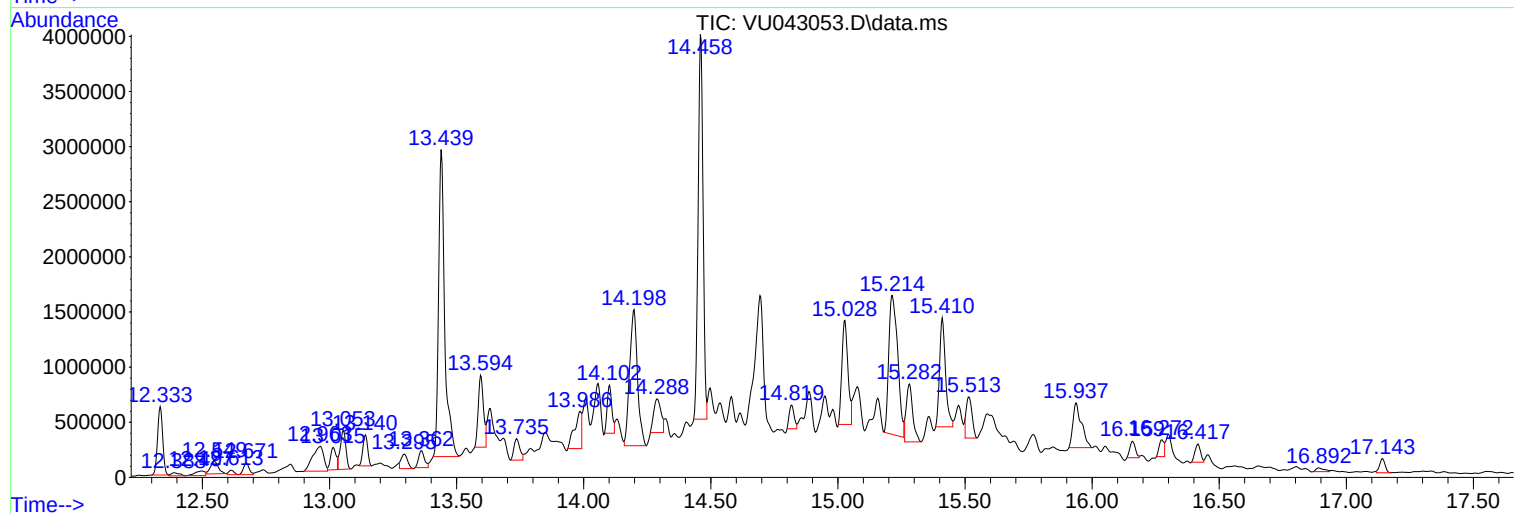
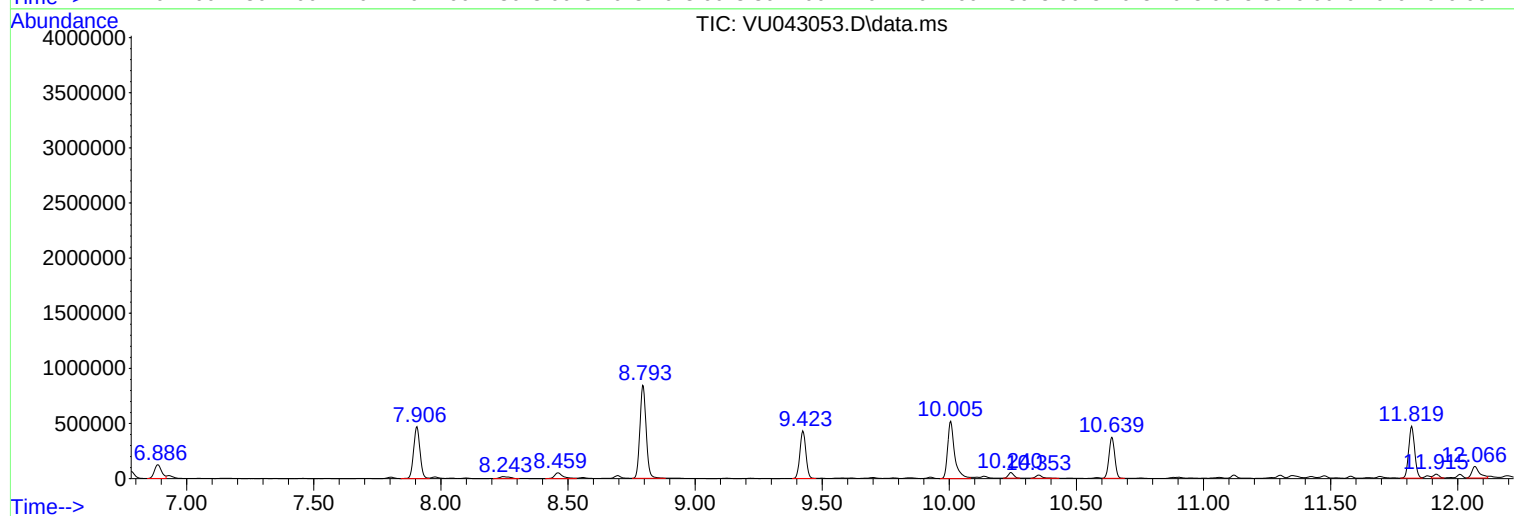
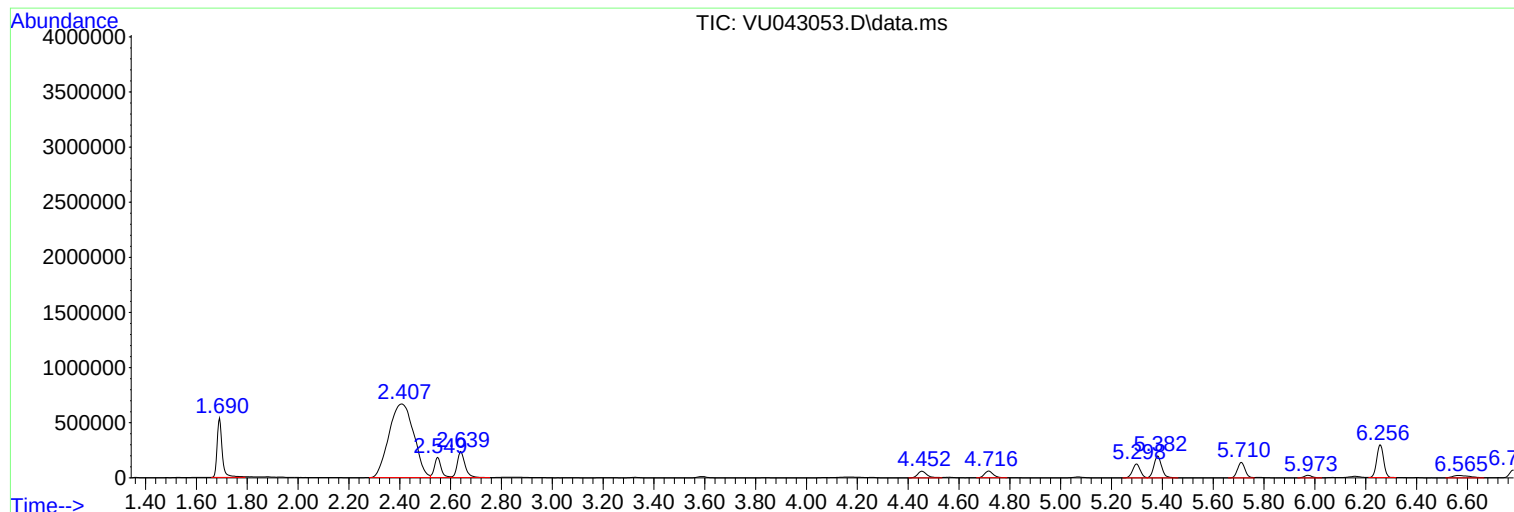
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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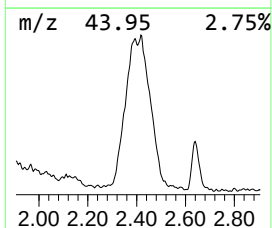
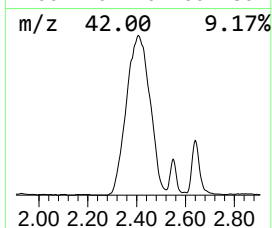
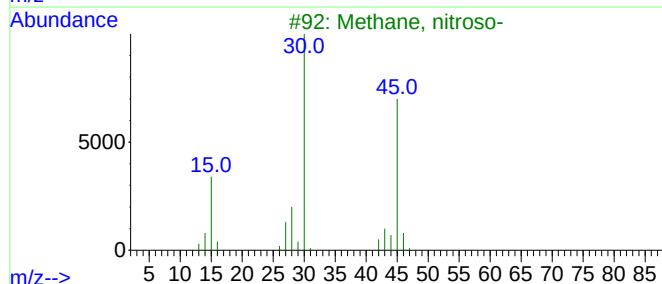
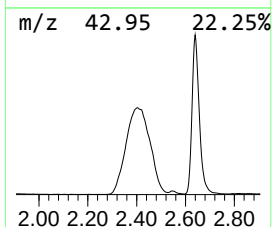
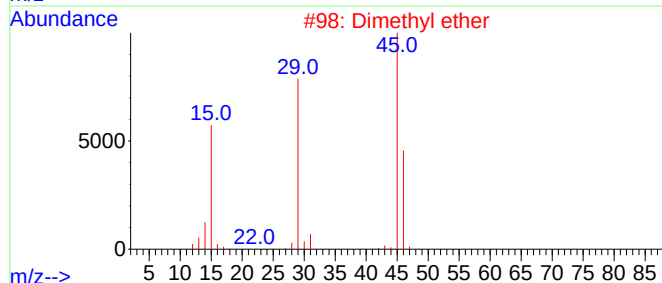
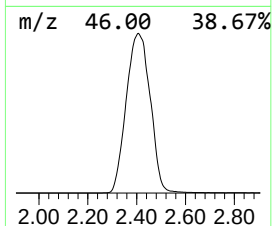
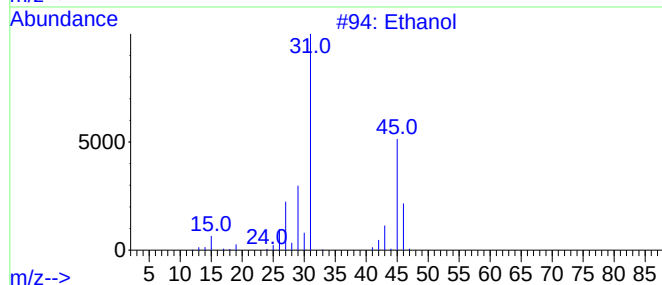
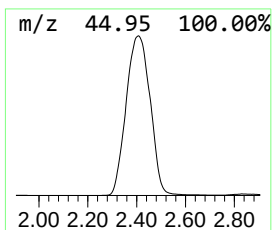
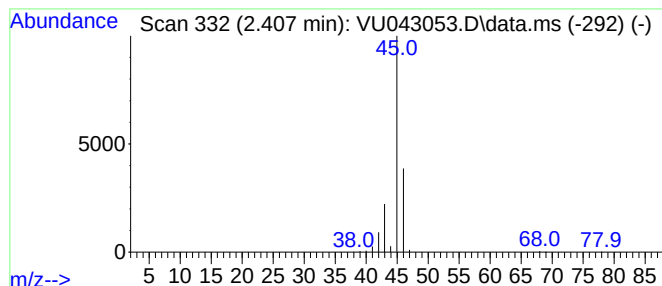
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.407	541.06 ug/l	4518080	Pentafluorobenzene	5.382

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
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			L-Lactic acid	90	C3H6O3	000079-33-4	2



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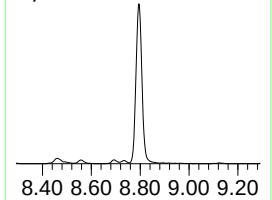
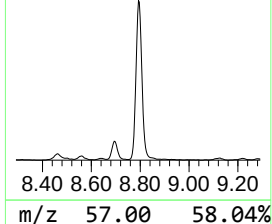
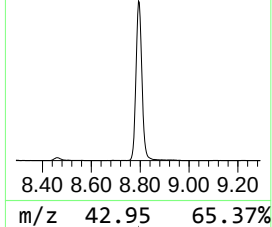
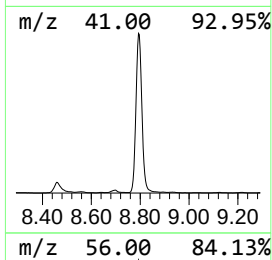
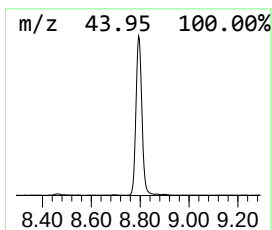
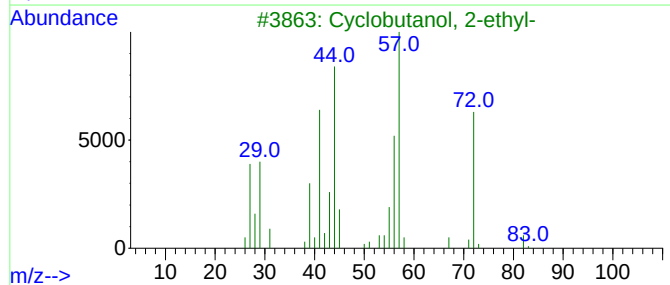
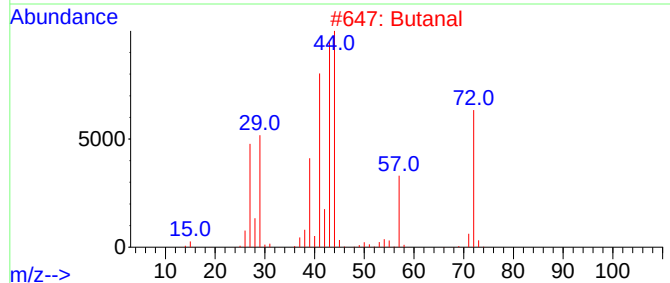
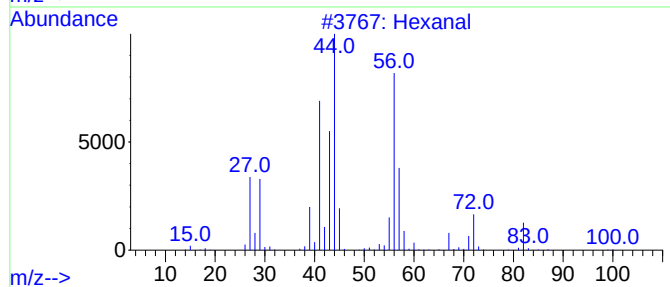
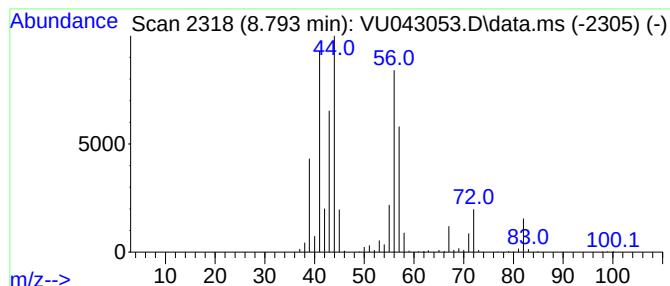
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.793	102.16 ug/l	1429150	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	76
2			Butanal	72	C4H8O	000123-72-8	47
3			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	42
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	25
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	25



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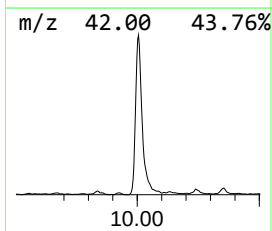
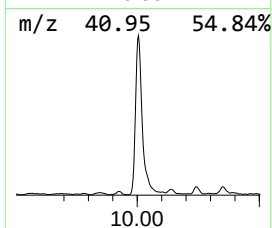
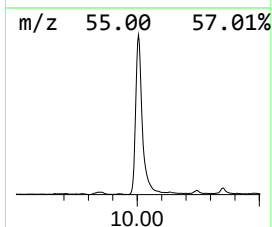
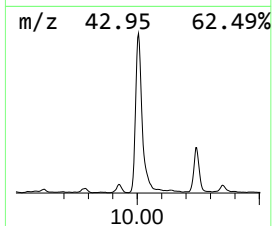
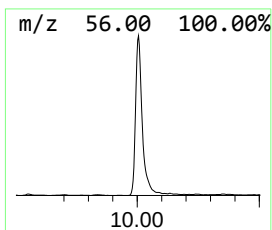
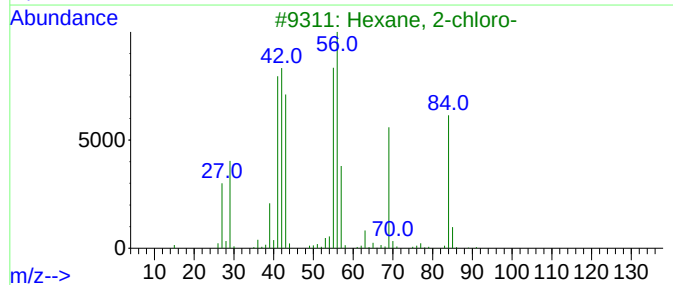
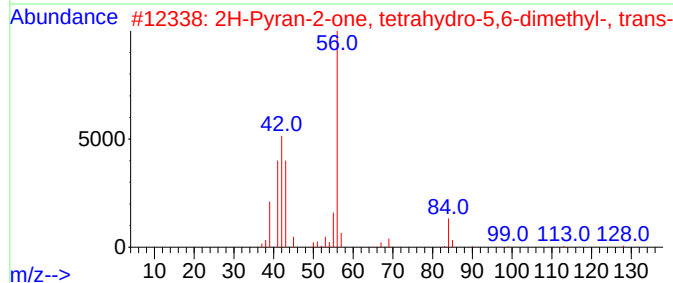
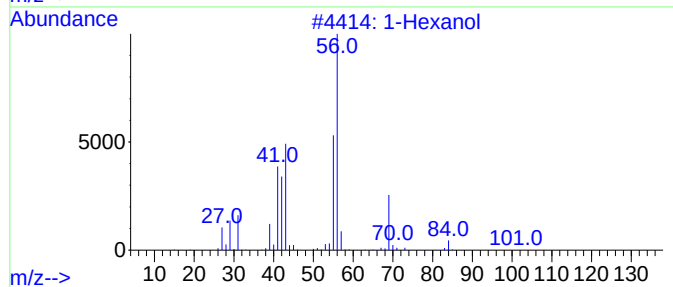
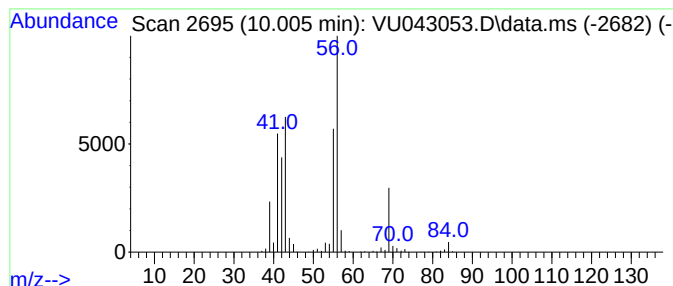
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.005	70.57 ug/l	987212	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol	102	C6H14O	000111-27-3	83
2			2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	78
3			Hexane, 2-chloro-	120	C6H13Cl	000638-28-8	72
4			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	64
5			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	64



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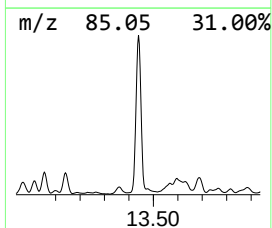
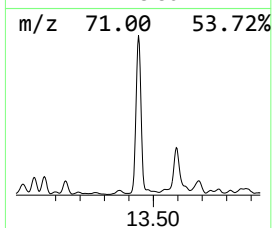
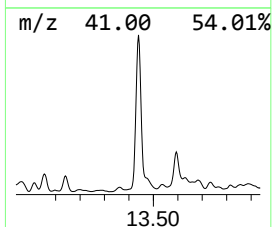
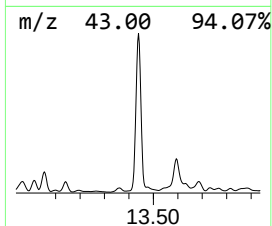
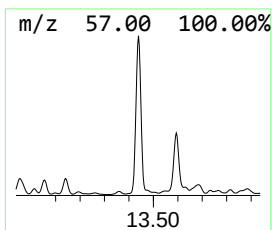
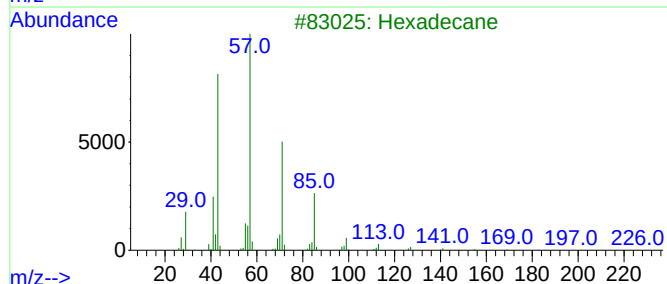
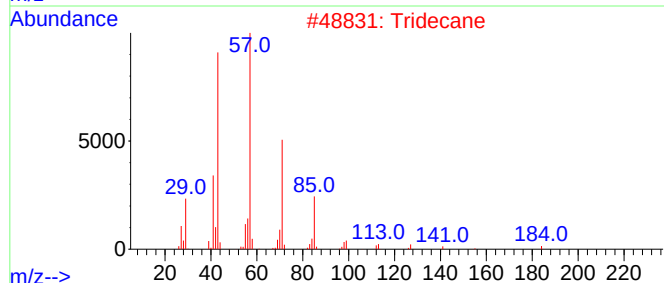
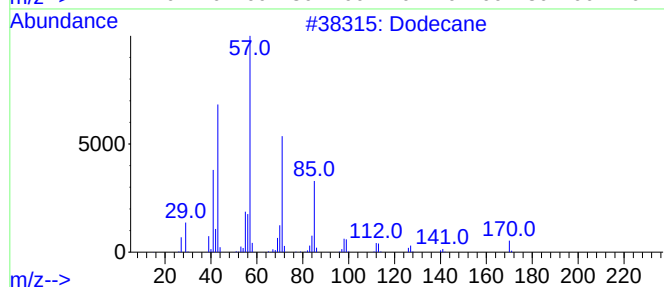
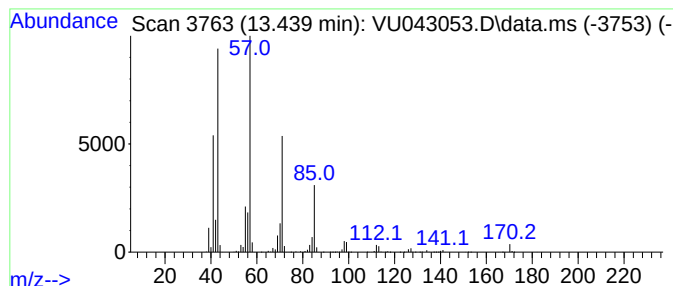
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.439	307.34 ug/l	4675970	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Tridecane	184	C13H28	000629-50-5	86
3			Hexadecane	226	C16H34	000544-76-3	78
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
5			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72



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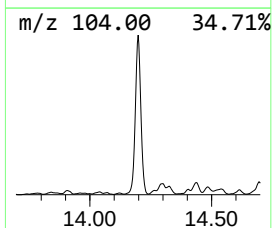
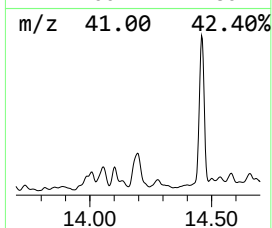
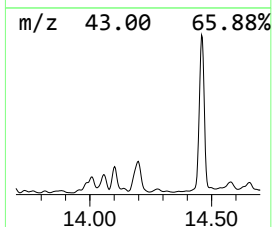
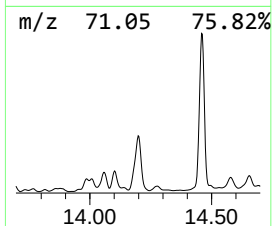
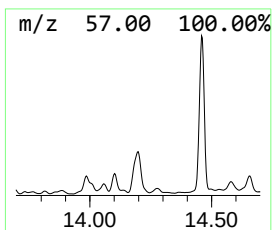
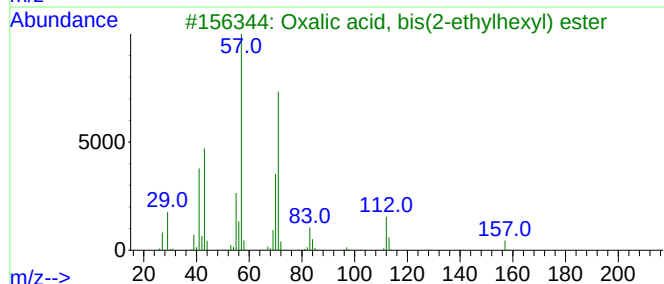
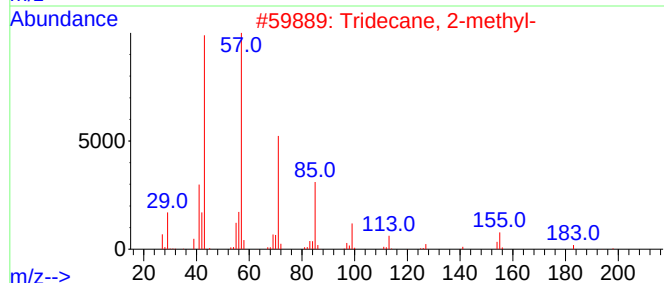
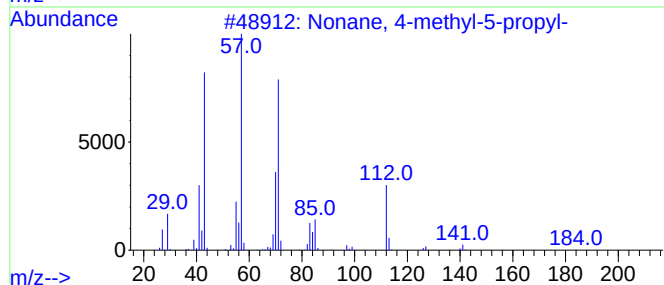
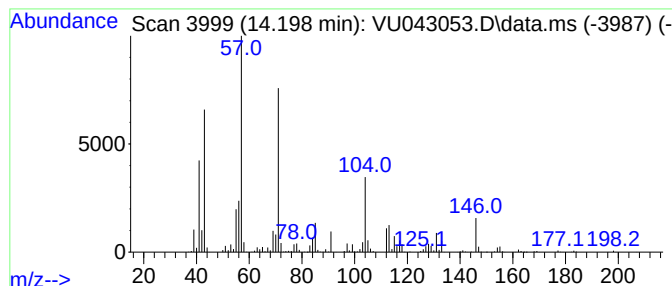
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Nonane, 4-methyl-5-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	173.22 ug/l	2635400	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	52
2			Tridecane, 2-methyl-	198	C14H30	001560-96-9	52
3			Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	50
4			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	50
5			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043053.D
Acq On : 13 Apr 2021 15:50
Operator : SY/MD
Sample : M1983-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31019

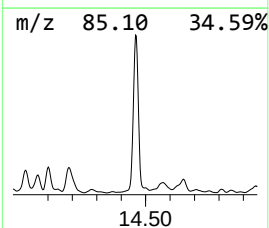
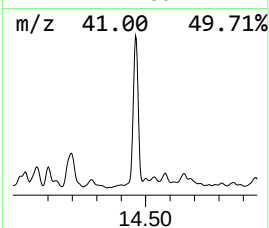
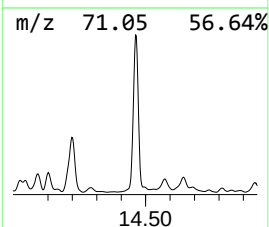
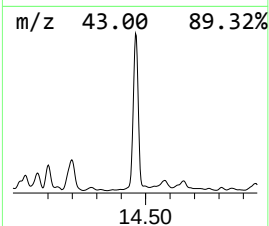
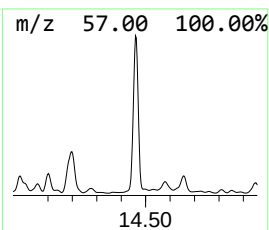
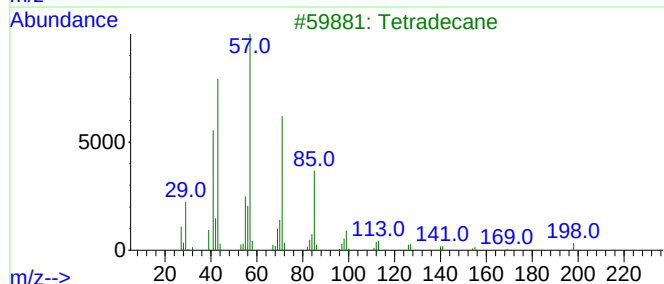
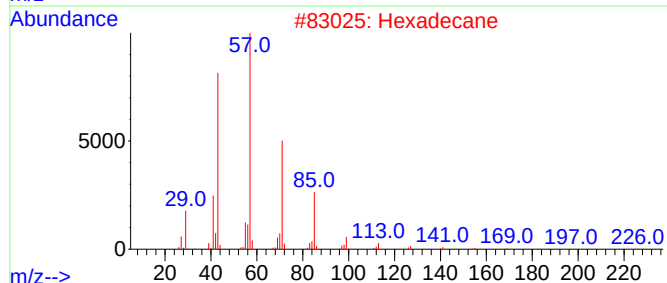
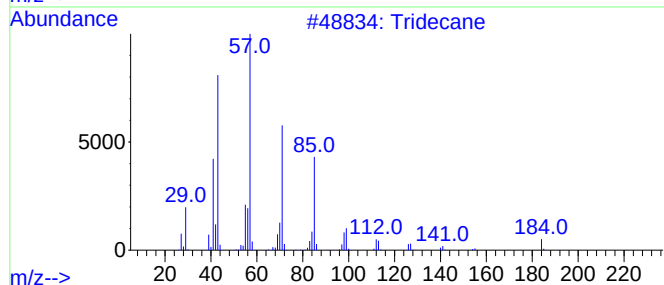
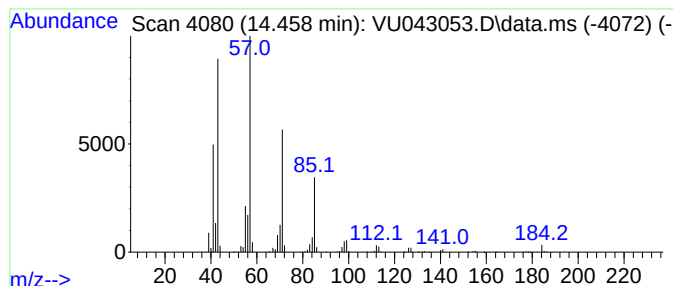
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tridecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.458	307.88 ug/l	4684180	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Hexadecane	226	C16H34	000544-76-3	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Undecane	156	C11H24	001120-21-4	83
5			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043053.D
Acq On : 13 Apr 2021 15:50
Operator : SY/MD
Sample : M1983-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31019

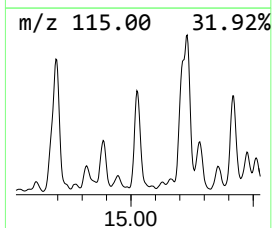
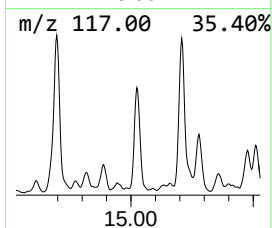
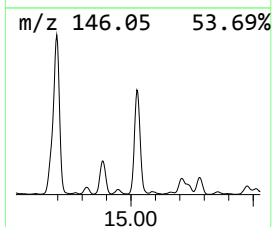
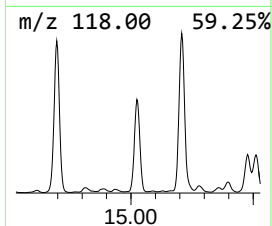
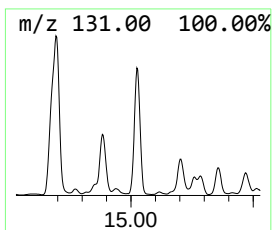
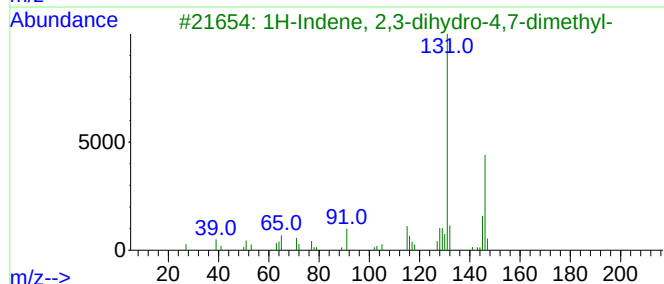
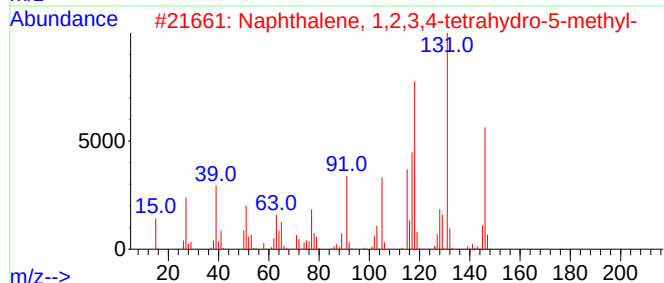
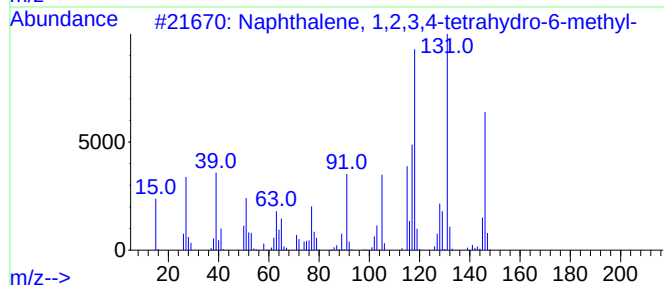
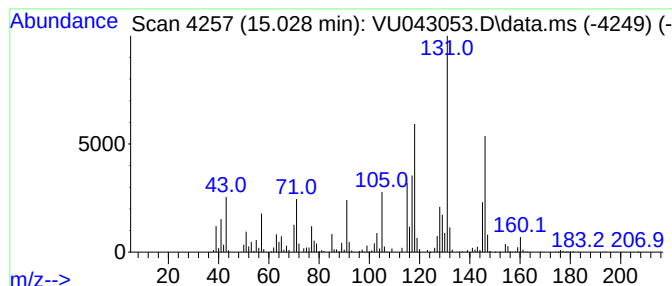
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.028	102.60 ug/l	1560990	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	95
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	95
3			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70
4			Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64
5			Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043053.D
Acq On : 13 Apr 2021 15:50
Operator : SY/MD
Sample : M1983-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31019

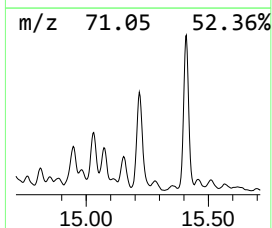
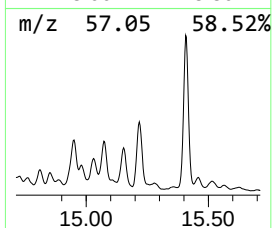
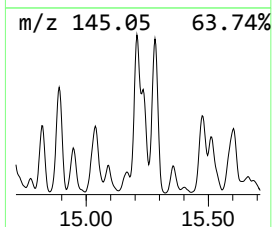
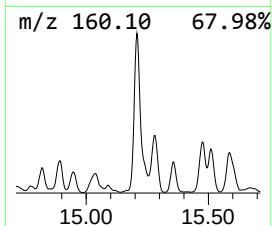
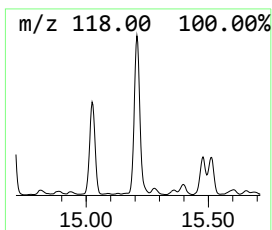
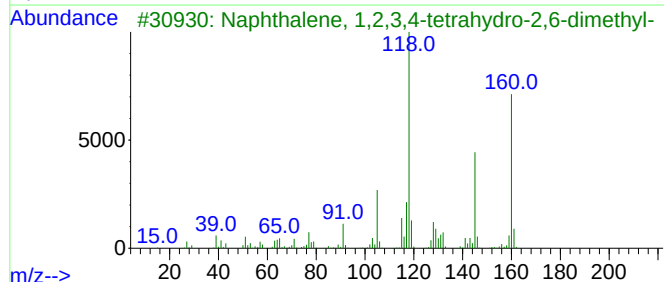
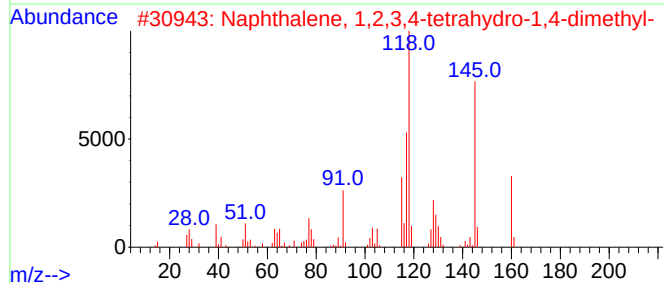
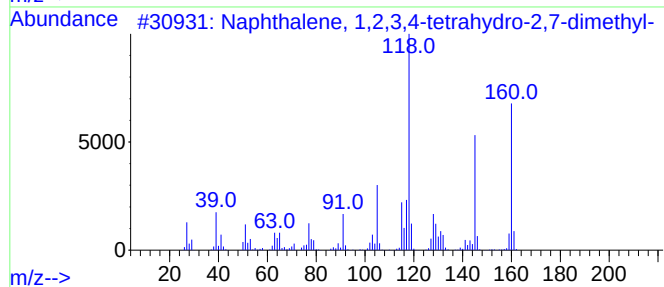
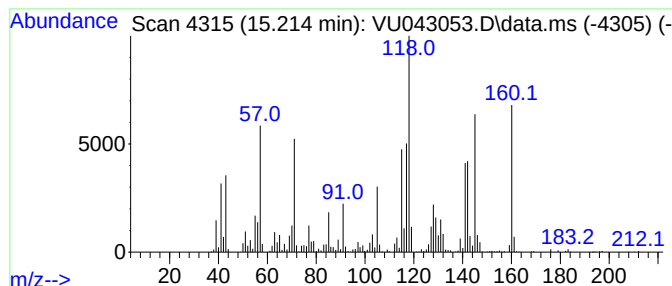
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.214	201.79 ug/l	3070050	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	70
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	64
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	43
4			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	43
5			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043053.D
Acq On : 13 Apr 2021 15:50
Operator : SY/MD
Sample : M1983-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31019

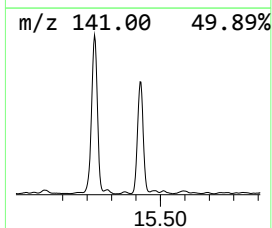
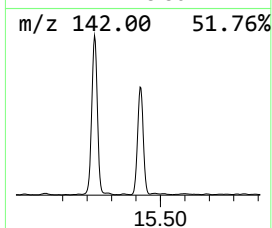
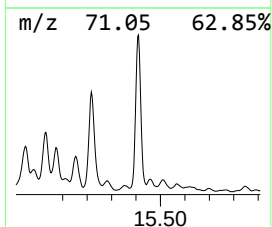
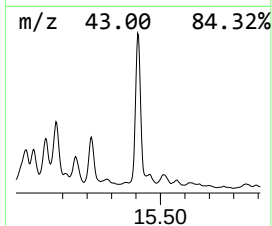
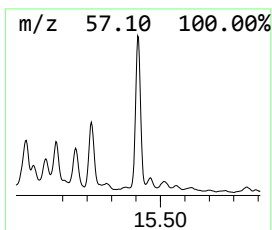
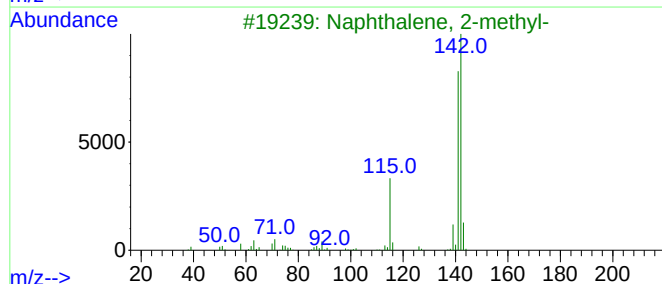
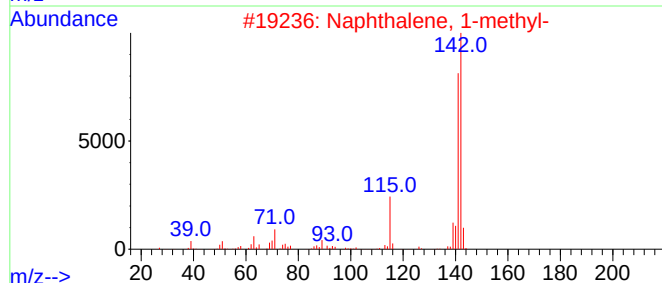
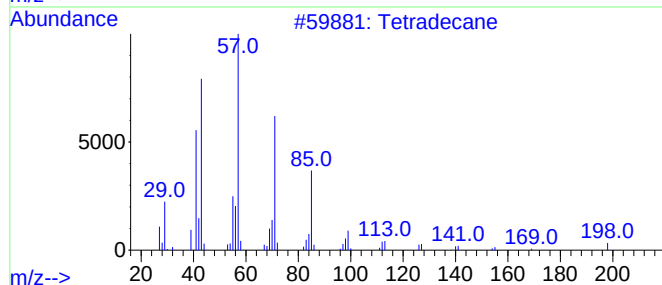
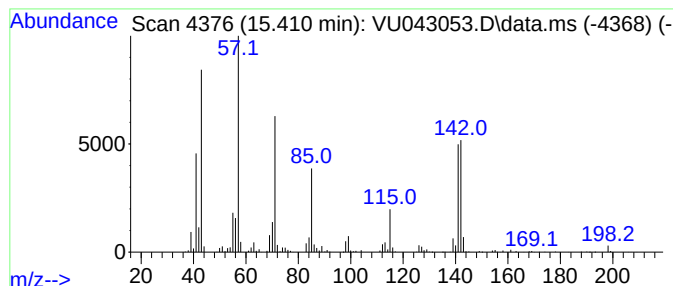
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	105.91 ug/l	1611360	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	94
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	58
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	50
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	43
5			Dodecane	170	C12H26	000112-40-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041321\
Data File : VU043053.D
Acq On : 13 Apr 2021 15:50
Operator : SY/MD
Sample : M1983-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
31019

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U041221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol	2.407	541.1	ug/l	4518080	1	5.382	417525	50.0
Hexanal	8.793	102.2	ug/l	1429150	3	9.423	699474	50.0
1-Hexanol	10.005	70.6	ug/l	987212	3	9.423	699474	50.0
Dodecane	13.439	307.3	ug/l	4675970	4	11.819	760707	50.0
Nonane, 4-methy...	14.198	173.2	ug/l	2635400	4	11.819	760707	50.0
Tridecane	14.458	307.9	ug/l	4684180	4	11.819	760707	50.0
Naphthalene, 1,...	15.028	102.6	ug/l	1560990	4	11.819	760707	50.0
Naphthalene, 1,...	15.214	201.8	ug/l	3070050	4	11.819	760707	50.0
Tetradecane	15.410	105.9	ug/l	1611360	4	11.819	760707	50.0