

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091919\
 Data File : VX012523.D
 Acq On : 19 Sep 2019 13:14
 Operator : JC/SP
 Sample : K4888-01
 Misc : 6.64g/10mL/100uL/10mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 979-S-1-(18-19)

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.064	25	29	41	rBV	332055	385791	12.94%	3.246%
2	1.655	106	126	128	rBV2	33071	125655	4.21%	1.057%
3	3.015	340	349	357	rBV	12282	31720	1.06%	0.267%
4	5.490	745	755	769	rBV	92415	261994	8.79%	2.204%
5	5.642	769	780	793	rBV	197377	553094	18.55%	4.654%
6	6.051	835	847	859	rBV	118092	312013	10.46%	2.625%
7	6.849	967	978	996	rVB	279806	672142	22.54%	5.655%
8	8.709	1274	1283	1290	rBV	558174	883852	29.64%	7.436%
9	9.331	1376	1385	1405	rBV	2074982	2981529	100.00%	25.085%
10	10.111	1507	1513	1522	rBV	535954	741730	24.88%	6.241%
11	11.135	1675	1681	1691	rBV	461175	581449	19.50%	4.892%
12	11.525	1740	1745	1752	rVB	25824	36843	1.24%	0.310%
13	12.074	1830	1835	1841	rBV	558592	698026	23.41%	5.873%
14	12.470	1891	1900	1905	rBV	64497	84522	2.83%	0.711%
15	12.940	1972	1977	1983	rBV4	18461	40906	1.37%	0.344%
16	13.318	2035	2039	2042	rBV	84935	101208	3.39%	0.852%
17	13.348	2042	2044	2049	rVB3	29149	34179	1.15%	0.288%
18	13.470	2061	2064	2073	rVB8	22953	55805	1.87%	0.470%
19	13.891	2129	2133	2141	rVB6	29212	59175	1.98%	0.498%
20	14.086	2161	2165	2169	rVB	123415	140924	4.73%	1.186%
21	14.281	2192	2197	2203	rVB7	22679	43920	1.47%	0.370%
22	14.525	2234	2237	2239	rBV3	28511	37246	1.25%	0.313%
23	14.555	2239	2242	2247	rVB3	45272	65428	2.19%	0.550%
24	14.616	2247	2252	2257	rBV5	40615	70298	2.36%	0.591%
25	14.665	2257	2260	2267	rBV2	80767	105411	3.54%	0.887%
26	14.805	2276	2283	2287	rBV	311571	378576	12.70%	3.185%
27	14.848	2287	2290	2293	rVV5	30524	41659	1.40%	0.351%
28	14.897	2293	2298	2301	rVV5	38636	75578	2.53%	0.636%
29	15.159	2336	2341	2344	rBV5	47232	92959	3.12%	0.782%
30	15.238	2350	2354	2356	rBV3	67656	95660	3.21%	0.805%
31	15.269	2356	2359	2363	rVV	174887	230639	7.74%	1.941%
32	15.336	2367	2370	2374	rVB3	82307	107117	3.59%	0.901%
33	15.439	2383	2387	2392	rBV5	41868	65200	2.19%	0.549%
34	15.555	2401	2406	2412	rBV	542440	732728	24.58%	6.165%

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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_X\METHOD\82X091719W.M
Title : SW846 8260

35	15.634	2417	2419	2423	rVV4	25723	35392	1.19%	0.298%
36	15.958	2468	2472	2478	rVB3	47960	90029	3.02%	0.757%
37	16.067	2487	2490	2493	rBV5	23346	31305	1.05%	0.263%
38	16.104	2493	2496	2501	rVB	74976	115736	3.88%	0.974%
39	16.183	2502	2509	2513	rBV7	51969	152751	5.12%	1.285%
40	16.457	2548	2554	2560	rVB	311664	535347	17.96%	4.504%

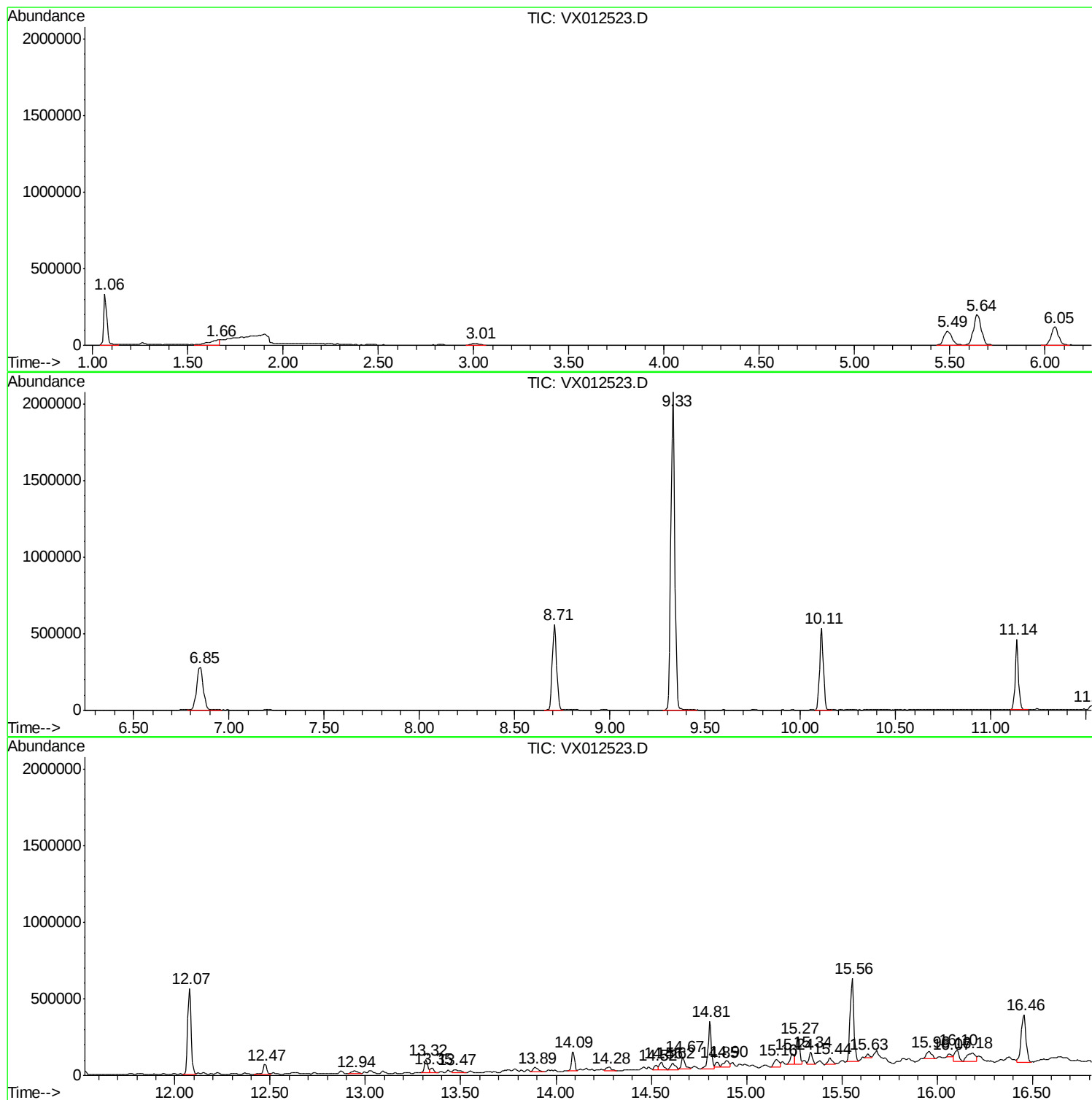
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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



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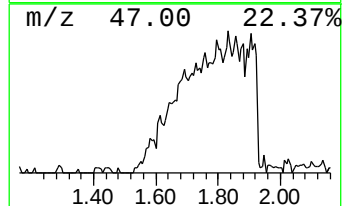
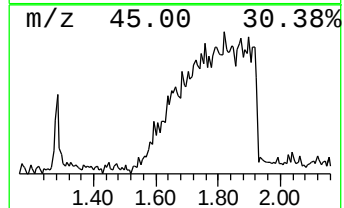
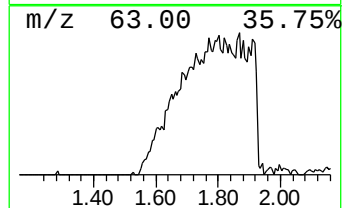
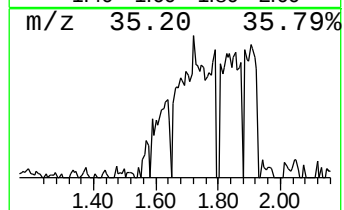
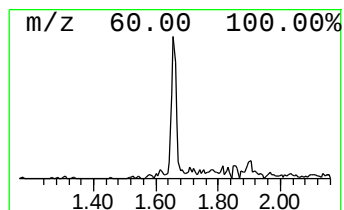
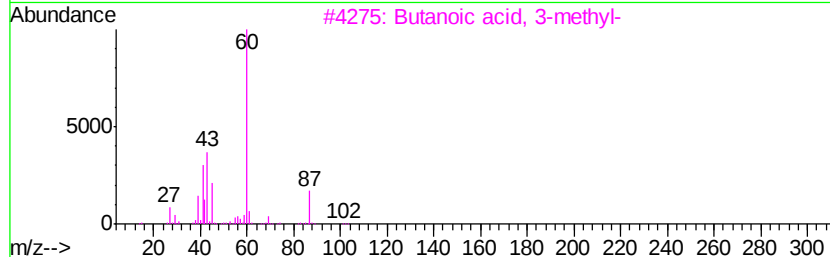
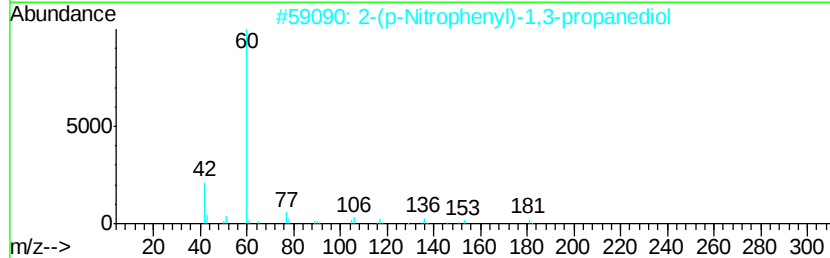
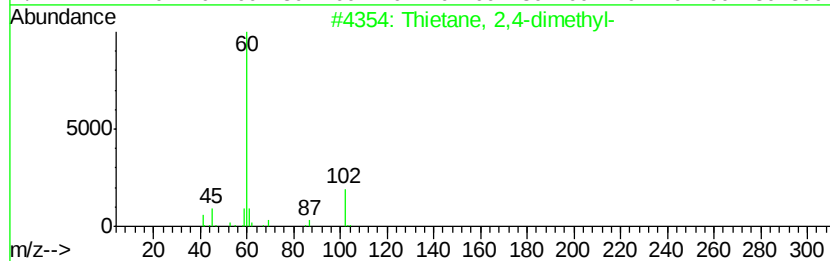
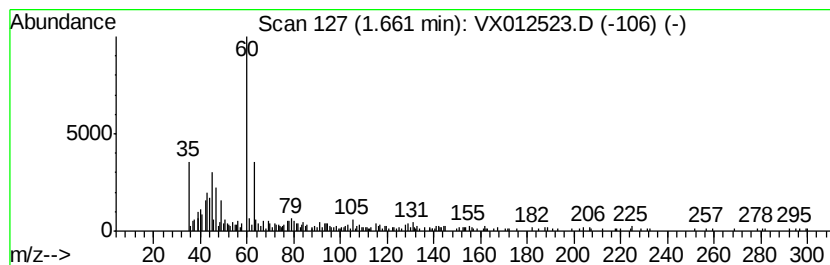
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown1.66 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	11.36 ug/l	125655	Pentafluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	37
2		2-(p-Nitrophenyl)-1,3-propanediol	197	C9H11N04	091748-03-7	35
3		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	27
4		1,3-Propanediol, 2-amino-1-(4-ni...	212	C9H12N2O4	000119-62-0	25
5		N-(4-Methylcyclohexyl)acetamide,...	155	C9H17NO	060504-06-5	25



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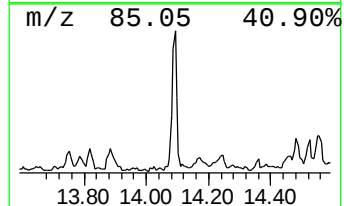
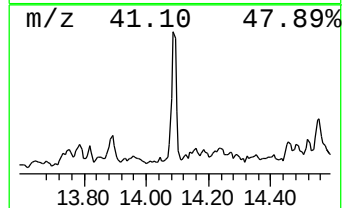
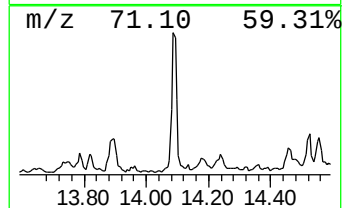
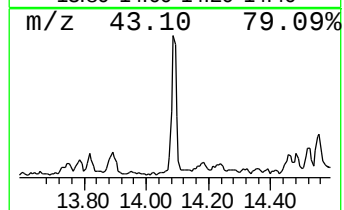
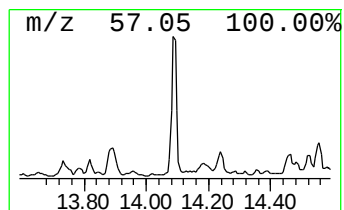
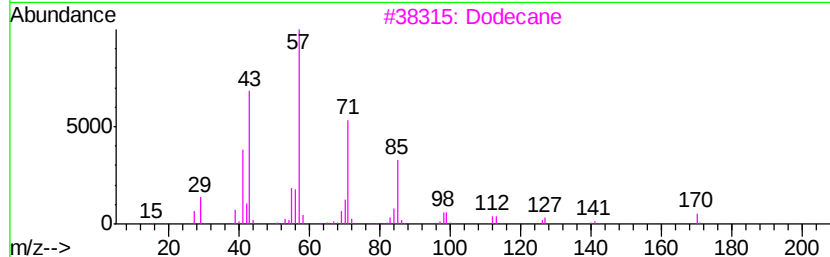
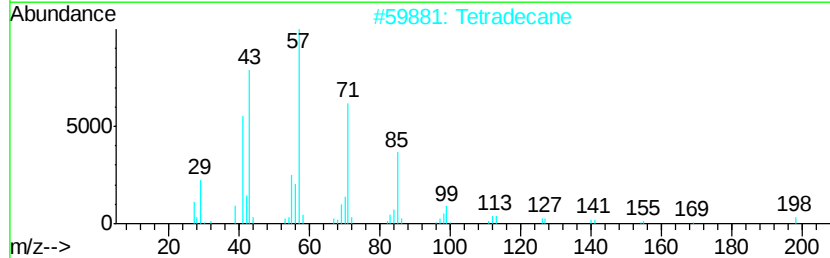
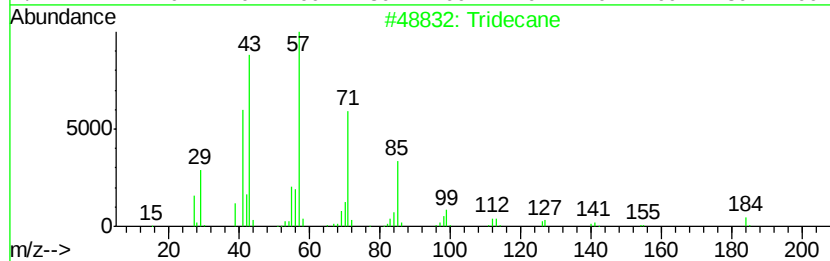
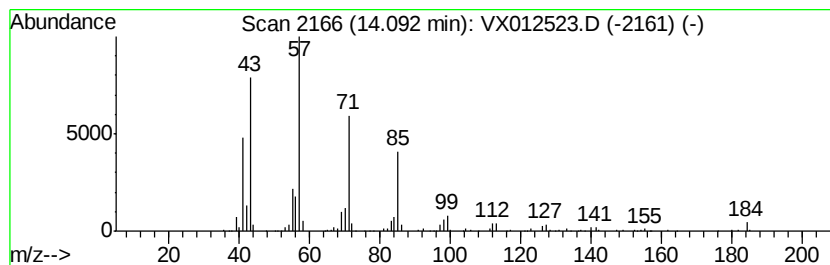
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	10.09 ug/l	140924	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane		184	C13H28	000629-50-5	97
2	Tetradecane		198	C14H30	000629-59-4	87
3	Dodecane		170	C12H26	000112-40-3	86
4	Hexadecane		226	C16H34	000544-76-3	83
5	Pentadecane		212	C15H32	000629-62-9	72



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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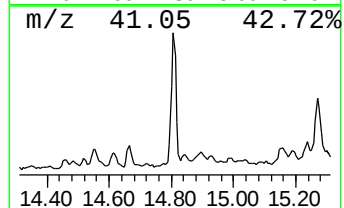
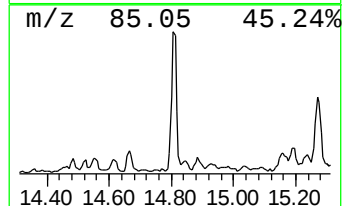
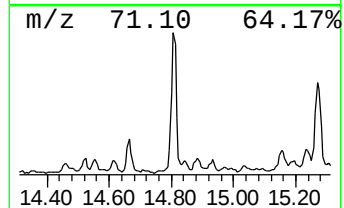
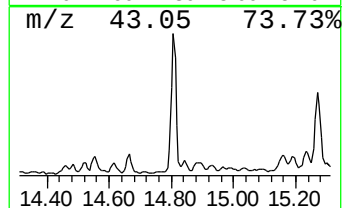
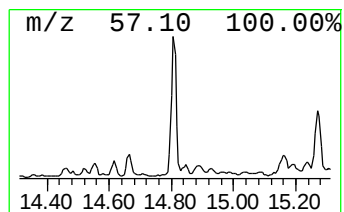
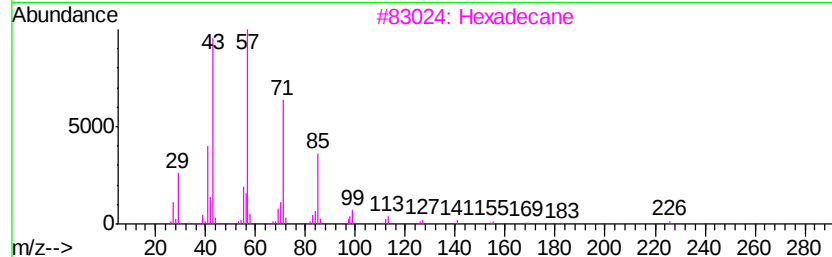
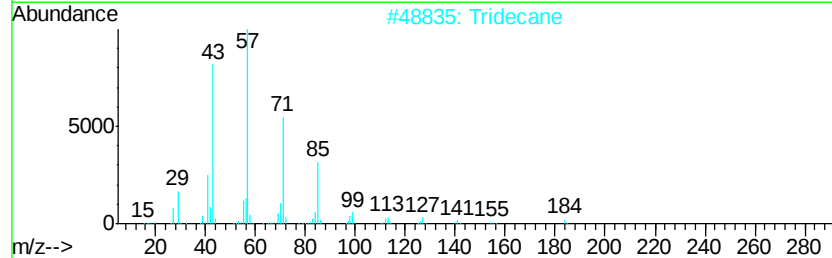
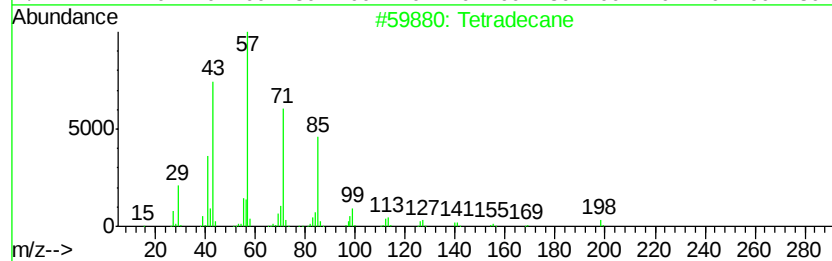
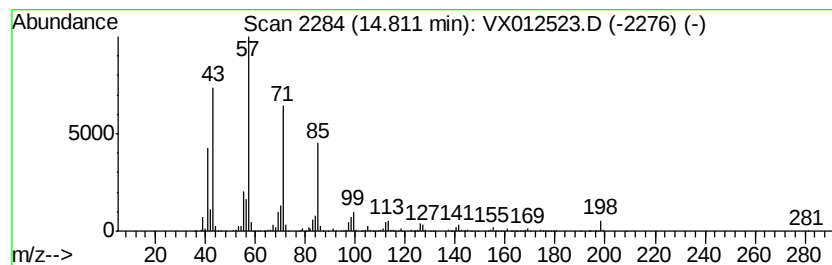
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 4 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	27.12 ug/l	378576	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	98
2		Tridecane	184	C13H28	000629-50-5	90
3		Hexadecane	226	C16H34	000544-76-3	87
4		Pentadecane	212	C15H32	000629-62-9	86
5		Dodecane	170	C12H26	000112-40-3	86



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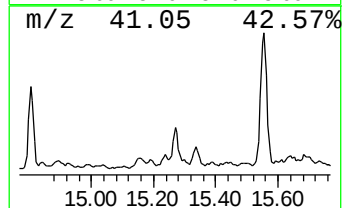
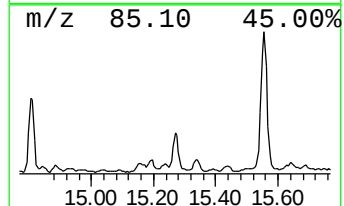
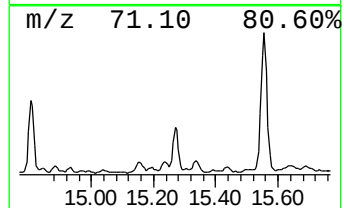
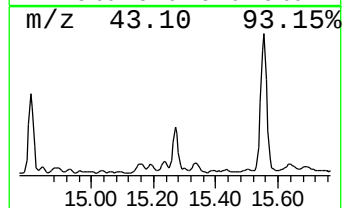
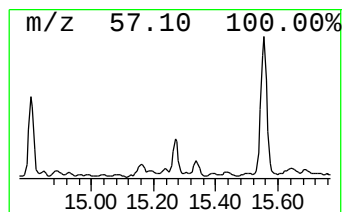
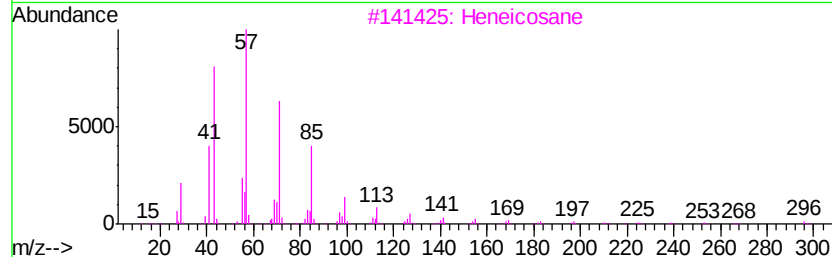
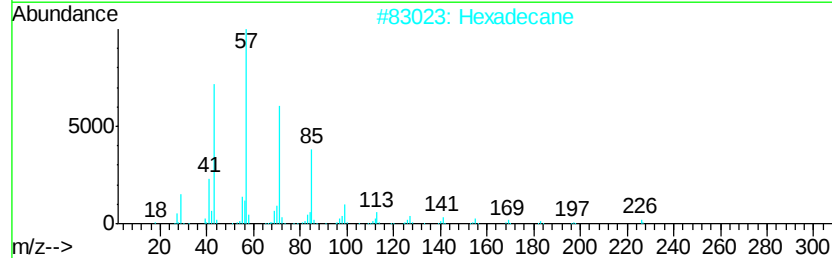
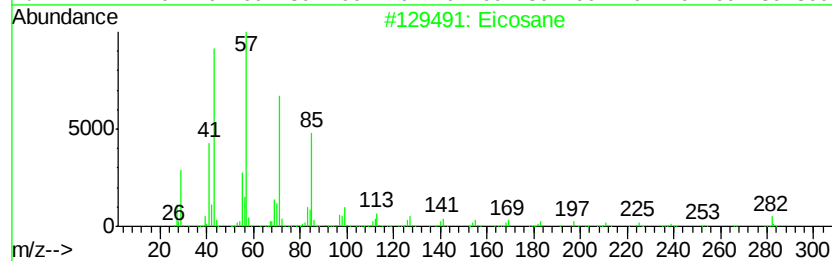
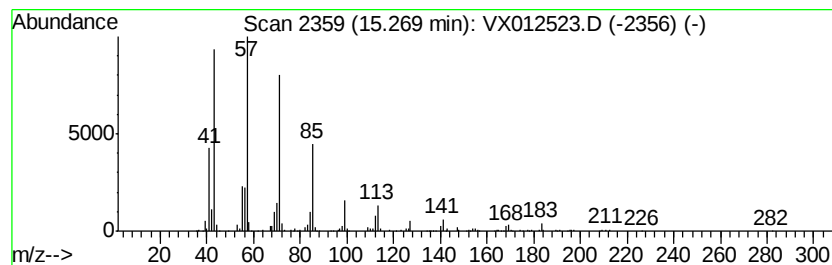
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	16.52 ug/l	230639	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Heneicosane		296	C21H44	000629-94-7	90
4	Octadecane, 2-methyl-		268	C19H40	001560-88-9	90
5	Decane, 2-methyl-		156	C11H24	006975-98-0	90



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Misc : 6.64µl/10mL/100µl/10mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

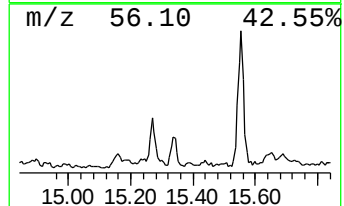
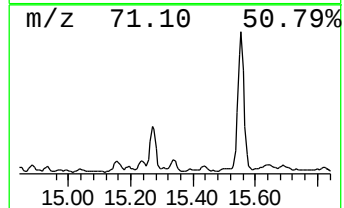
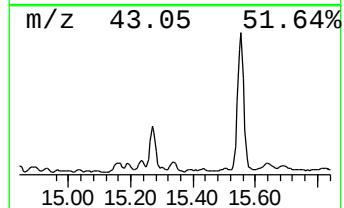
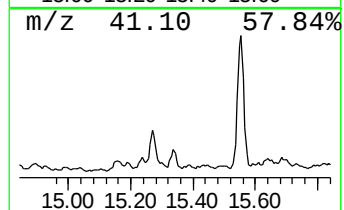
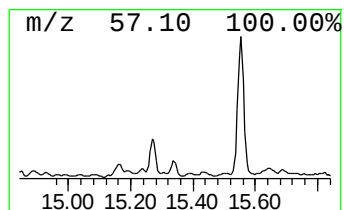
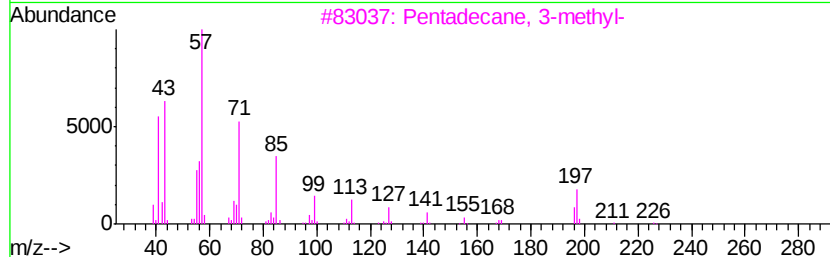
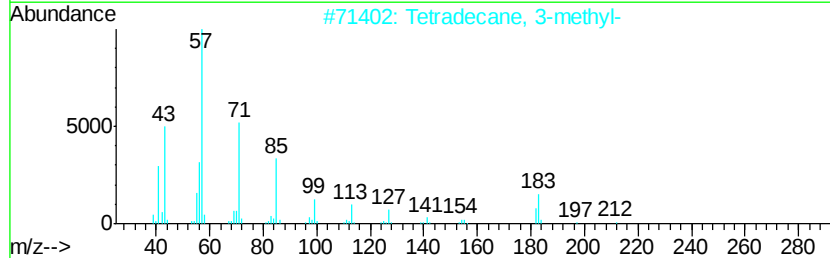
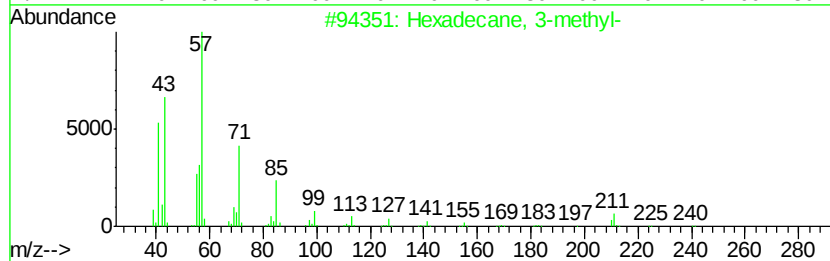
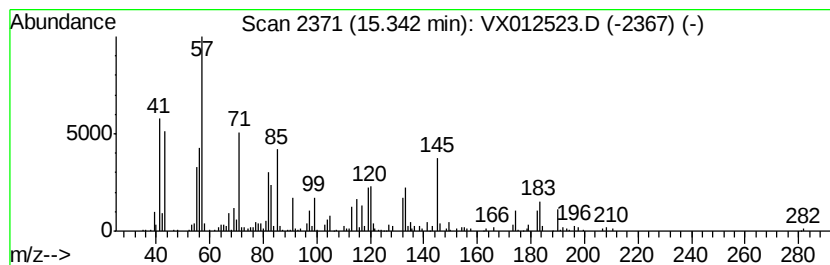
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ClientSampleId :
979-S-1-(18-19)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 6 unknown15.34 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.34	7.67 ug/l	107117	1,4-Dichlorobenzene-d4	12.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	30
2	Tetradecane, 3-methyl-	212	C15H32	018435-22-8	25
3	Pentadecane, 3-methyl-	226	C16H34	002882-96-4	25
4	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	22
5	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	22



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091919\
Data File : VX012523.D
Acq On : 19 Sep 2019 13:14
Operator : JC/SP
Sample : K4888-01
Misc : 6.64g/10mL/100uL/10mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
979-S-1-(18-19)

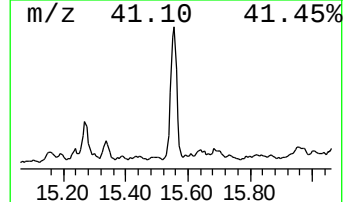
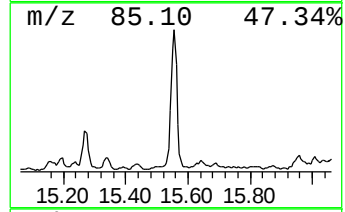
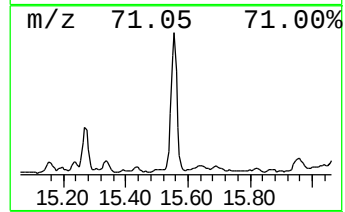
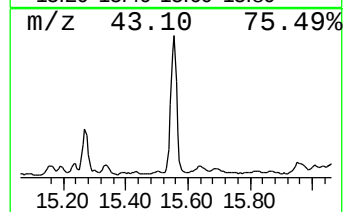
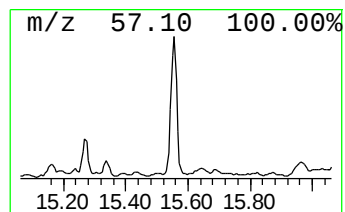
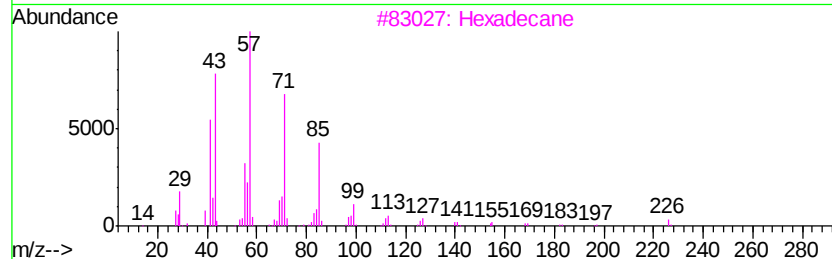
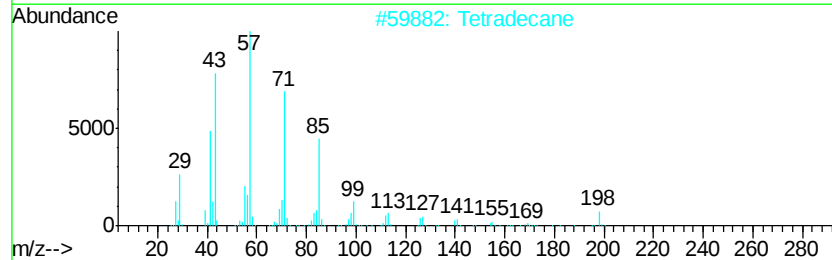
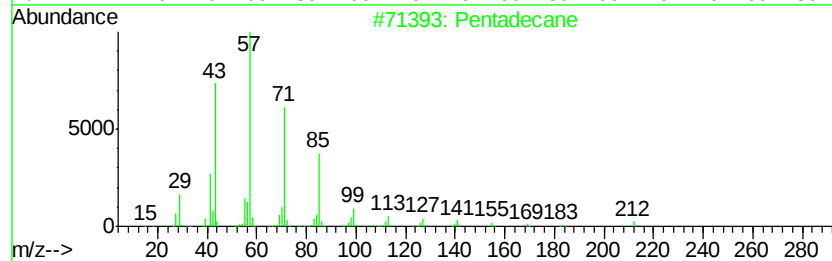
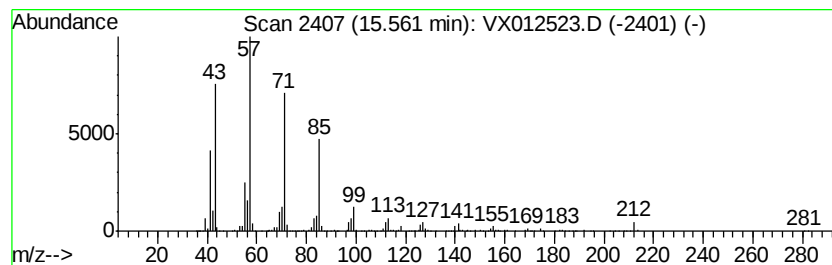
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Quant Title : SW846 8260

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

Peak Number 7 Pentadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	52.49 ug/l	732728	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	97
2	Tetradecane		198	C14H30	000629-59-4	91
3	Hexadecane		226	C16H34	000544-76-3	90
4	Tridecane		184	C13H28	000629-50-5	90
5	Nonane, 4,5-dimethyl-		156	C11H24	017302-23-7	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091919\
Data File : VX012523.D
Acq On : 19 Sep 2019 13:14
Operator : JC/SP
Sample : K4888-01
Misc : 6.64g/10mL/100uL/10mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

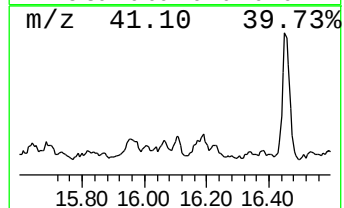
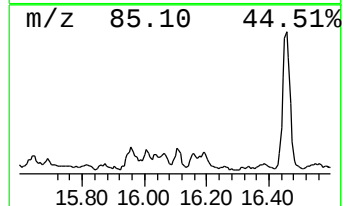
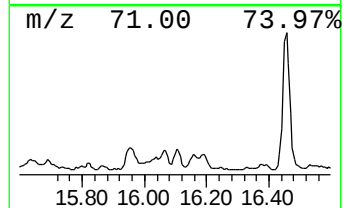
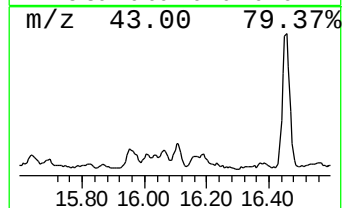
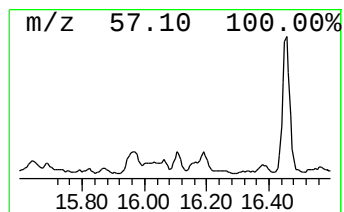
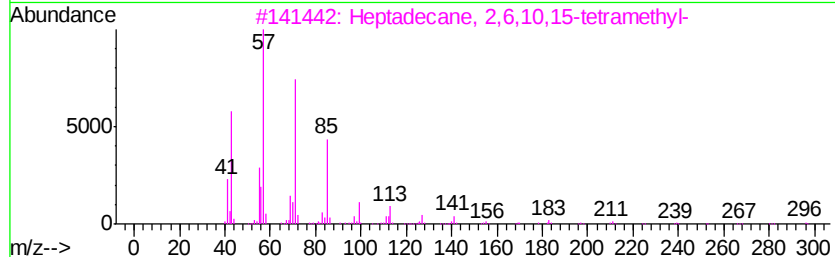
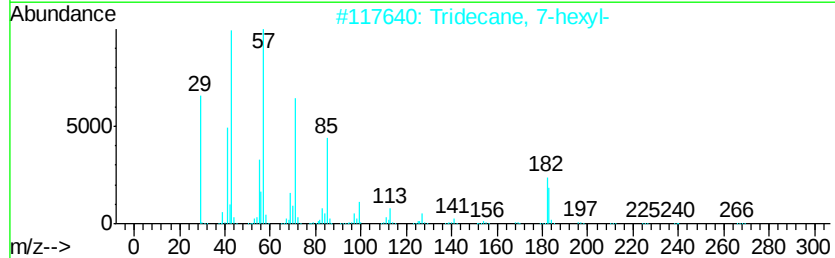
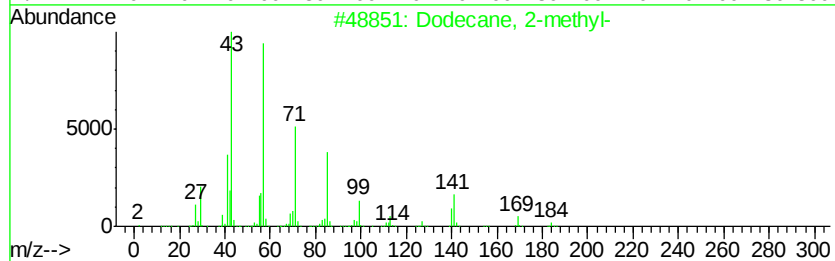
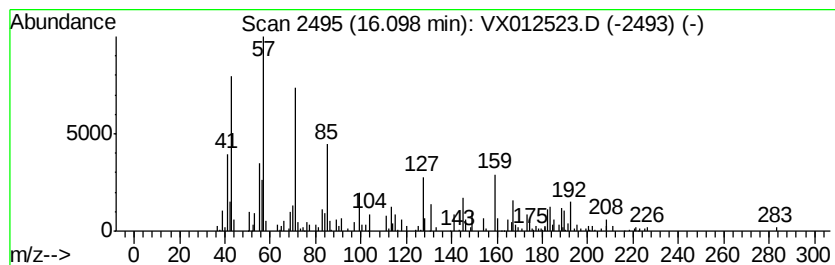
Instrument :
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ClientSampleId :
979-S-1-(18-19)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 8 Dodecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.10	8.29 ug/l	115736	1,4-Dichlorobenzene-d4	12.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-	184	C13H28	001560-97-0	64
2	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	64
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	62
4	Hexacosane	366	C26H54	000630-01-3	62
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX091919\
Data File : VX012523.D
Acq On : 19 Sep 2019 13:14
Operator : JC/SP
Sample : K4888-01
Misc : 6.64g/10mL/100uL/10mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
979-S-1-(18-19)

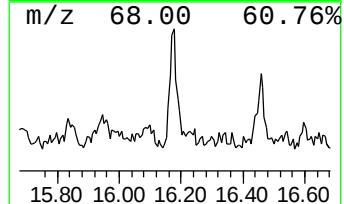
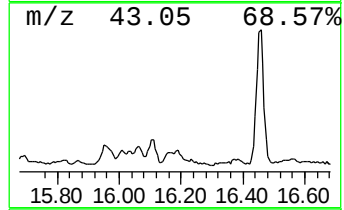
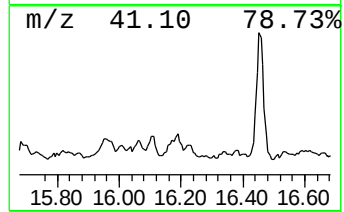
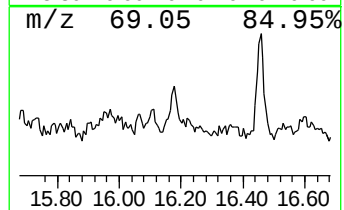
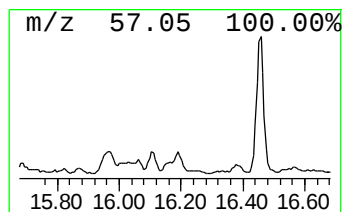
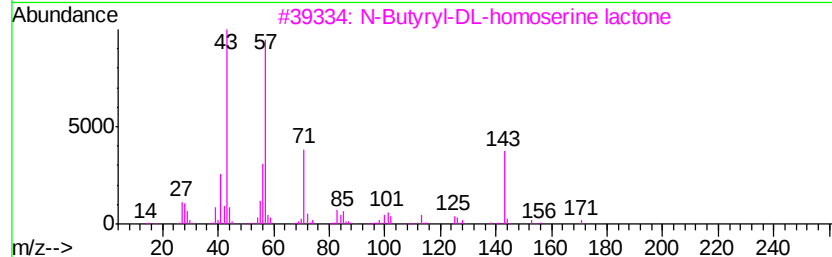
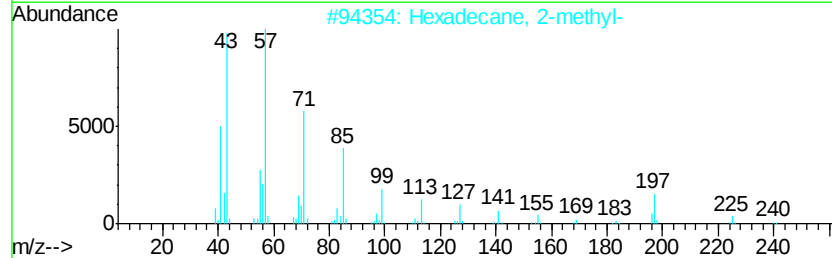
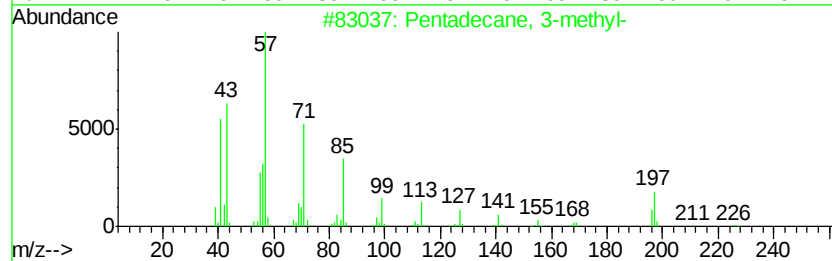
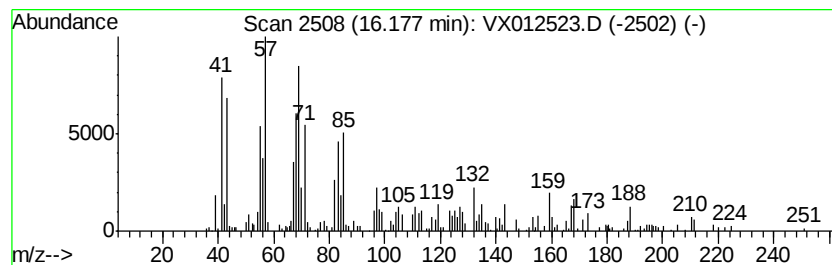
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.18 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	10.94 ug/l	152751	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 3-methyl-	226	C16H34	002882-96-4	49
2		Hexadecane, 2-methyl-	240	C17H36	001560-92-5	46
3		N-Butyryl-DL-homoserine lactone	171	C8H13NO3	098426-48-3	46
4		Decane	142	C10H22	000124-18-5	45
5		2,2-Dimethyloctadecane	282	C20H42	1000360-43-2	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091919\
Data File : VX012523.D
Acq On : 19 Sep 2019 13:14
Operator : JC/SP
Sample : K4888-01
Misc : 6.64g/10mL/100uL/10mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
979-S-1-(18-19)

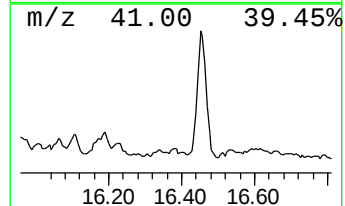
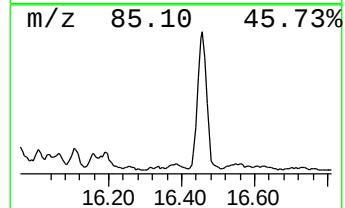
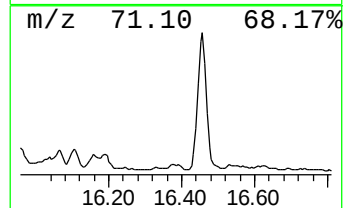
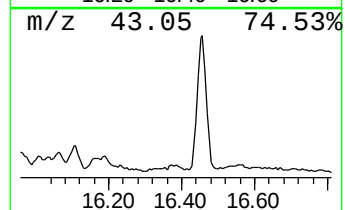
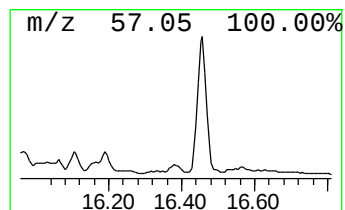
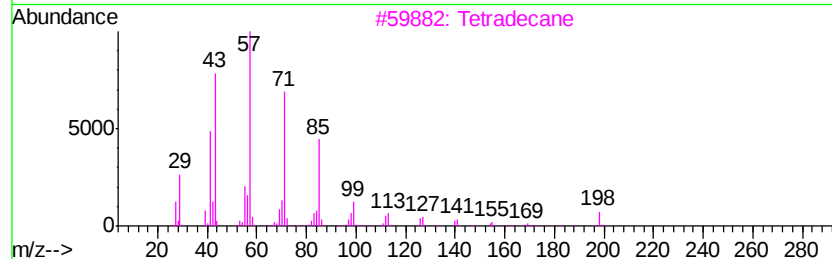
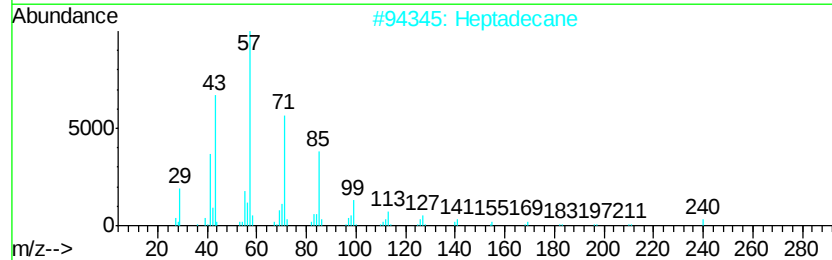
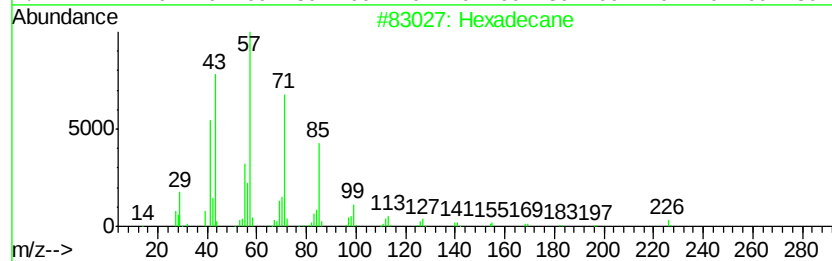
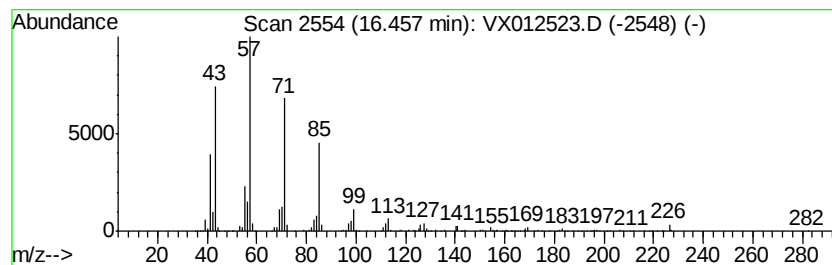
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 10 Hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	38.35 ug/l	535347	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	98
2		Heptadecane	240	C17H36	000629-78-7	91
3		Tetradecane	198	C14H30	000629-59-4	91
4		Pentadecane	212	C15H32	000629-62-9	90
5		Nonadecane	268	C19H40	000629-92-5	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX091919\
Data File : VX012523.D
Acq On : 19 Sep 2019 13:14
Operator : JC/SP
Sample : K4888-01
Misc : 6.64g/10mL/100uL/10mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
979-S-1-(18-19)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.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
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Tridecane	14.09	10.1	ug/l	140924	4	12.07	698026	50.0
Tetradecane	14.81	27.1	ug/l	378576	4	12.07	698026	50.0
Eicosane	15.27	16.5	ug/l	230639	4	12.07	698026	50.0
unknown15.34	15.34	7.7	ug/l	107117	4	12.07	698026	50.0
Pentadecane	15.56	52.5	ug/l	732728	4	12.07	698026	50.0
Dodecane, 2-methyl-	16.10	8.3	ug/l	115736	4	12.07	698026	50.0
unknown16.18	16.18	10.9	ug/l	152751	4	12.07	698026	50.0
Hexadecane	16.46	38.4	ug/l	535347	4	12.07	698026	50.0