

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032019\
 Data File : VN054473.D
 Acq On : 20 Mar 2019 19:40
 Operator : JC/SP
 Sample : K1994-05
 Misc : 4.34g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 40021

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_N\METHODS\82N032019W.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	2.516	204	231	232	rBV5	39906	115157	1.37%	0.125%
2	2.555	236	243	254	rVB5	50999	102159	1.22%	0.111%
3	7.590	1789	1809	1819	rBV	408750	1008638	12.00%	1.097%
4	7.664	1820	1832	1861	rVB	745445	1823880	21.70%	1.983%
5	8.027	1927	1945	1964	rBV	460318	1073543	12.77%	1.167%
6	8.583	2103	2118	2167	rVB	1092725	2423420	28.84%	2.635%
7	10.091	2570	2587	2620	rBV	1618445	3295900	39.22%	3.584%
8	11.406	2983	2996	3024	rBV	1370233	2604906	30.99%	2.833%
9	11.632	3057	3066	3080	rVB3	101930	174582	2.08%	0.190%
10	12.043	3186	3194	3202	rVB	67520	94528	1.12%	0.103%
11	12.159	3223	3230	3240	rVB8	50674	92661	1.10%	0.101%
12	12.400	3296	3305	3315	rBV	1020659	1642442	19.54%	1.786%
13	12.561	3351	3355	3370	rVB6	46628	94140	1.12%	0.102%
14	12.654	3371	3384	3390	rBV3	112811	224711	2.67%	0.244%
15	12.725	3397	3406	3417	rVV2	1063730	1672336	19.90%	1.819%
16	12.779	3418	3423	3432	rVB4	102975	159269	1.90%	0.173%
17	12.879	3446	3454	3463	rBV5	71814	187155	2.23%	0.204%
18	12.959	3472	3479	3490	rVB	423405	670175	7.97%	0.729%
19	13.037	3493	3503	3512	rVB3	180465	334074	3.97%	0.363%
20	13.088	3514	3519	3529	rVB2	79936	112391	1.34%	0.122%
21	13.146	3530	3537	3551	rVB7	128764	316641	3.77%	0.344%
22	13.236	3551	3565	3573	rBV6	401774	879716	10.47%	0.957%
23	13.284	3573	3580	3585	rVV2	329482	480688	5.72%	0.523%
24	13.345	3586	3599	3615	rVV3	1553789	3116483	37.08%	3.389%
25	13.422	3616	3623	3631	rVV	313922	421255	5.01%	0.458%
26	13.541	3654	3660	3666	rVB2	315072	423057	5.03%	0.460%
27	13.583	3667	3673	3688	rVB4	341437	631338	7.51%	0.687%
28	13.670	3689	3700	3709	rBV	2993829	4713177	56.08%	5.126%
29	13.831	3745	3750	3760	rVB5	517537	730259	8.69%	0.794%
30	13.889	3761	3768	3775	rVB	501119	695878	8.28%	0.757%
31	13.930	3776	3781	3791	rVB3	394545	602677	7.17%	0.655%
32	13.995	3792	3801	3810	rBV3	783947	1277071	15.20%	1.389%
33	14.059	3812	3821	3831	rBV7	346368	787204	9.37%	0.856%
34	14.162	3843	3853	3868	rBV9	1045834	2843467	33.83%	3.092%

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35	14.294	3887	3894	3900	rBV2	1032300	1419912	16.89%	1.544%
36	14.332	3901	3906	3914	rVB2	798571	1059266	12.60%	1.152%
37	14.432	3932	3937	3944	rVB2	412524	477694	5.68%	0.519%
38	14.477	3945	3951	3955	rVV2	459260	662654	7.88%	0.721%
39	14.522	3957	3965	3975	rVB	4898558	7000503	83.30%	7.613%
40	14.590	3976	3986	3994	rBV6	1762417	3557250	42.33%	3.869%
41	14.641	3995	4002	4014	rVB2	2055247	3445042	40.99%	3.746%
42	14.847	4061	4066	4073	rVB3	850078	1099382	13.08%	1.196%
43	14.956	4091	4100	4110	rBV5	1186354	2456956	29.23%	2.672%
44	15.110	4139	4148	4156	rBV2	2102220	3630315	43.20%	3.948%
45	15.188	4166	4172	4179	rVB2	852581	1155869	13.75%	1.257%
46	15.242	4181	4189	4199	rBV5	1257581	2582261	30.73%	2.808%
47	15.329	4208	4216	4230	rVB	5160436	8404424	100.00%	9.140%
48	15.416	4233	4243	4256	rVV6	1255969	3220350	38.32%	3.502%
49	15.612	4298	4304	4317	rVB	2382246	4070715	48.44%	4.427%
50	15.908	4386	4396	4406	rBV5	1532546	3040609	36.18%	3.307%
51	16.030	4429	4434	4442	rBV	552752	704069	8.38%	0.766%
52	16.101	4447	4456	4466	rVB2	2096436	3954804	47.06%	4.301%
53	16.229	4488	4496	4513	rVB	2272576	4186678	49.82%	4.553%

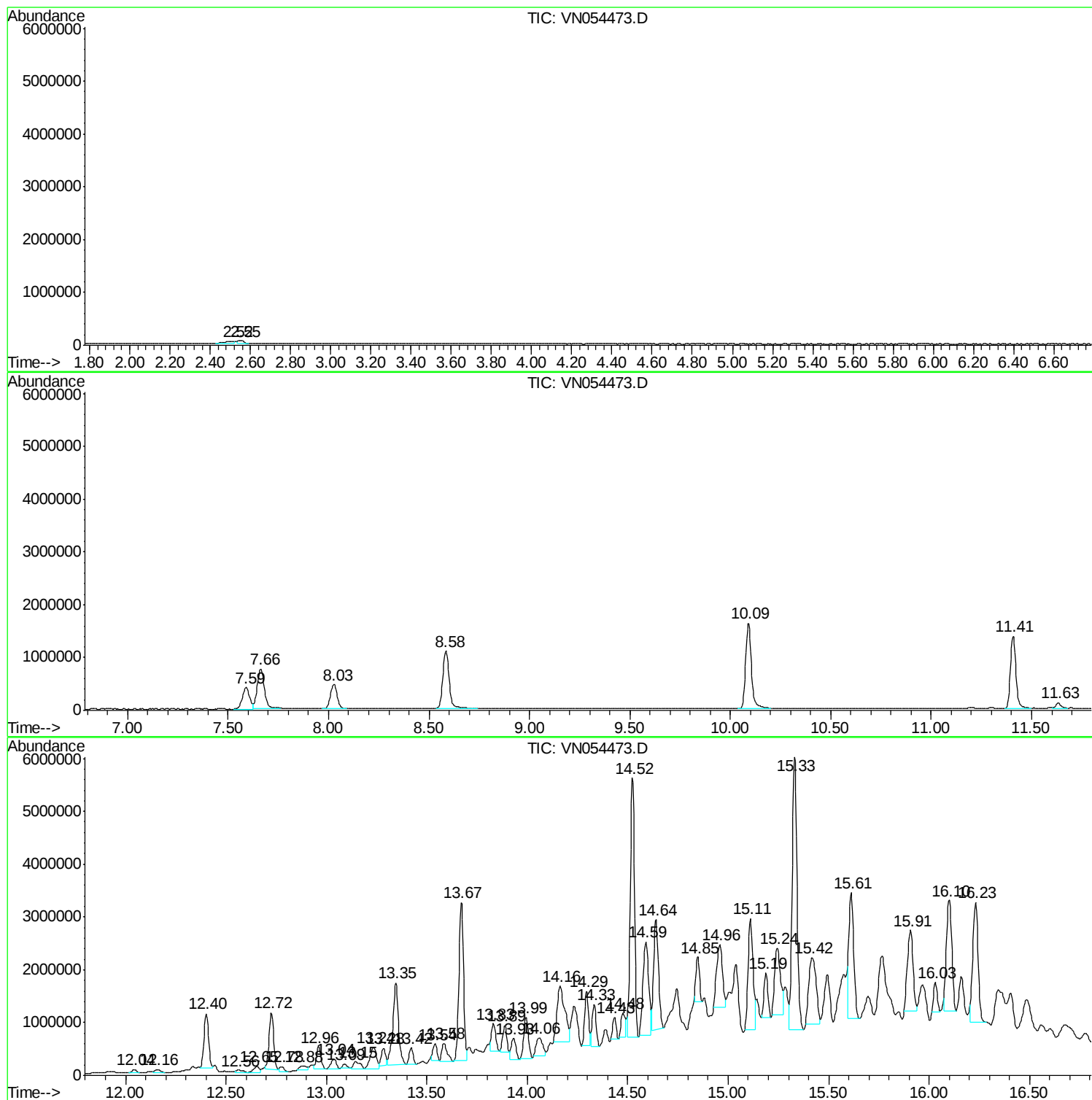
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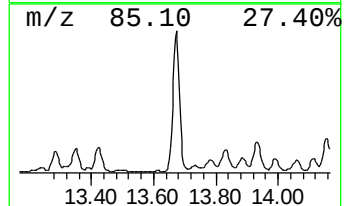
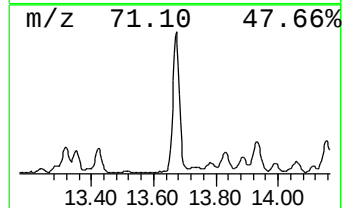
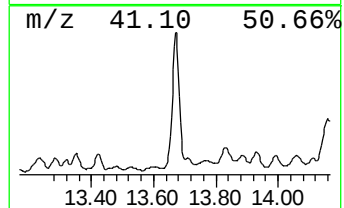
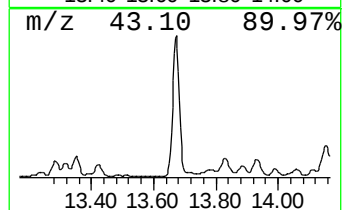
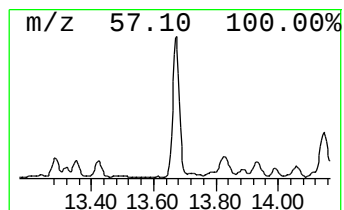
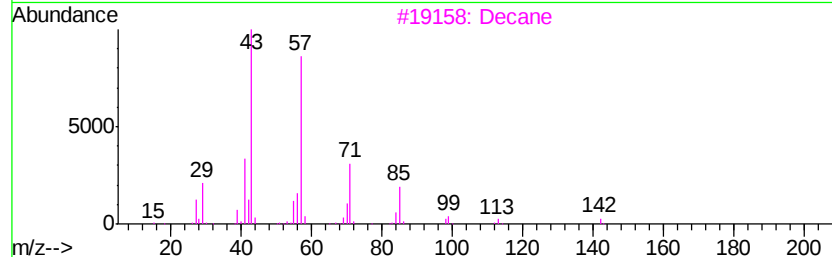
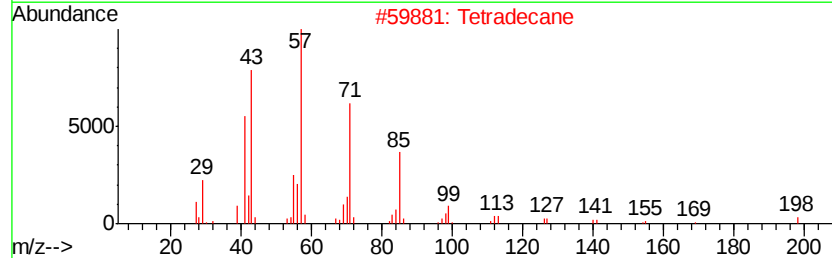
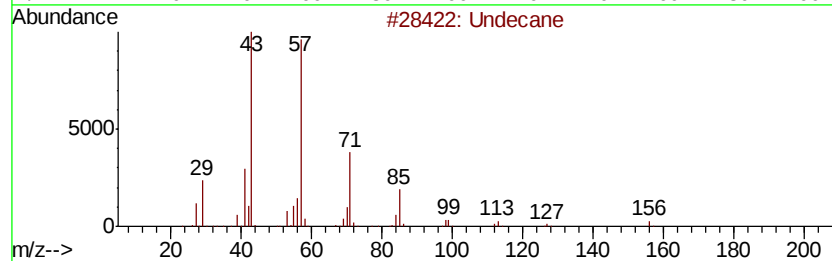
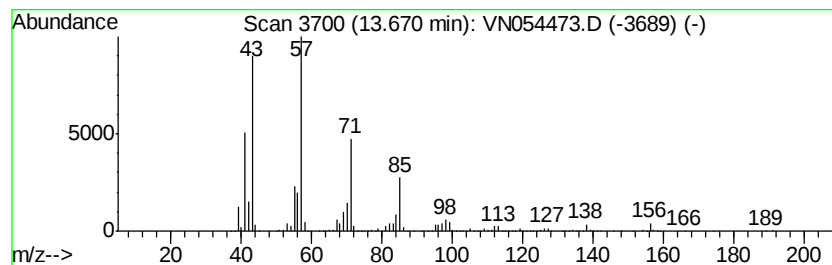
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	75.62 ug/l	4713180	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane		156	C11H24	001120-21-4	90
2	Tetradecane		198	C14H30	000629-59-4	80
3	Decane		142	C10H22	000124-18-5	80
4	Tridecane		184	C13H28	000629-50-5	78
5	Undecane, 2,3-dimethyl-		184	C13H28	017312-77-5	59



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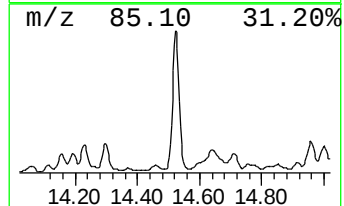
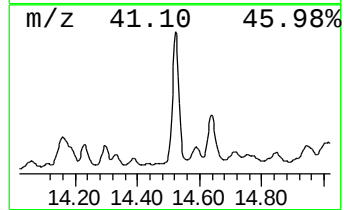
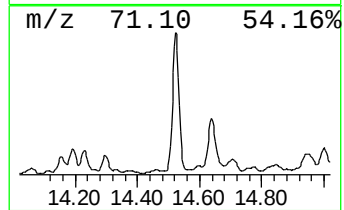
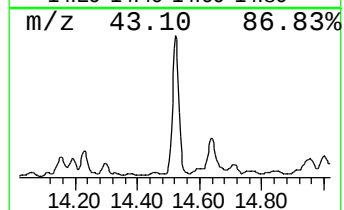
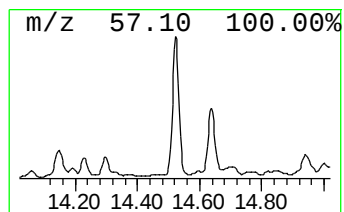
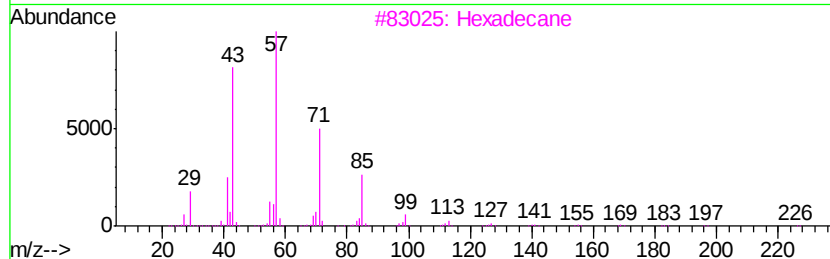
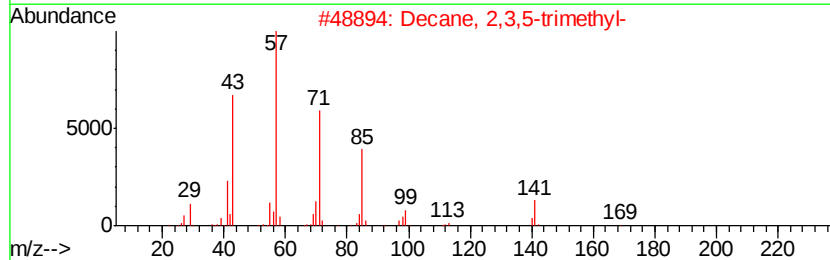
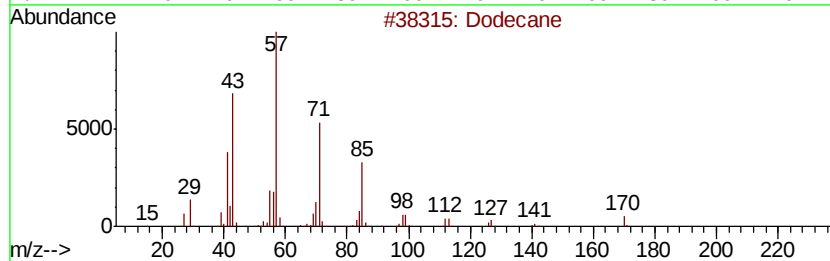
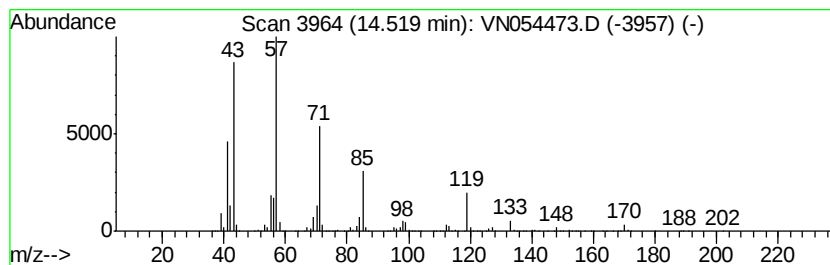
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	112.31 ug/l	7000500	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane	170	C12H26	000112-40-3	95
2		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64
3		Hexadecane	226	C16H34	000544-76-3	64
4		Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	59
5		Tridecane	184	C13H28	000629-50-5	59



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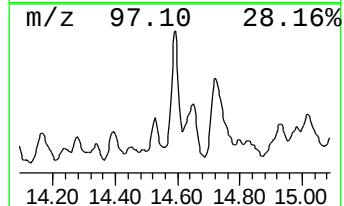
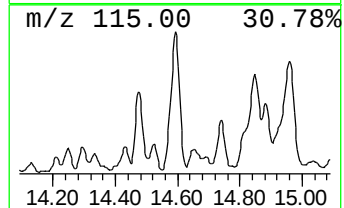
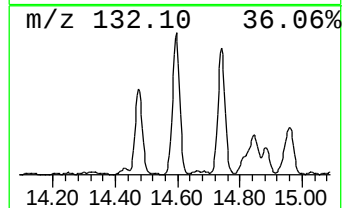
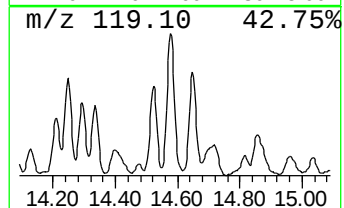
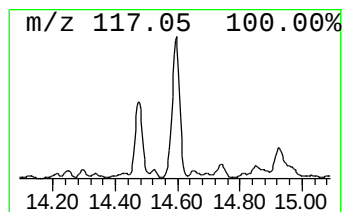
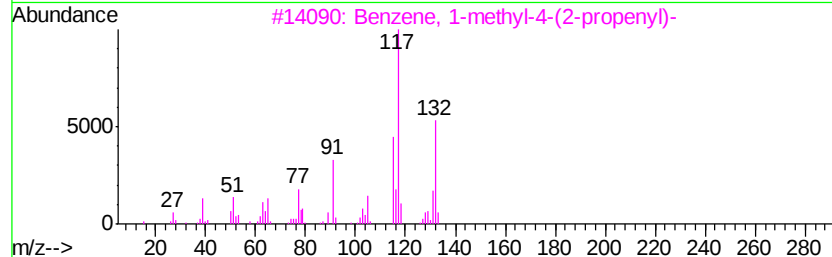
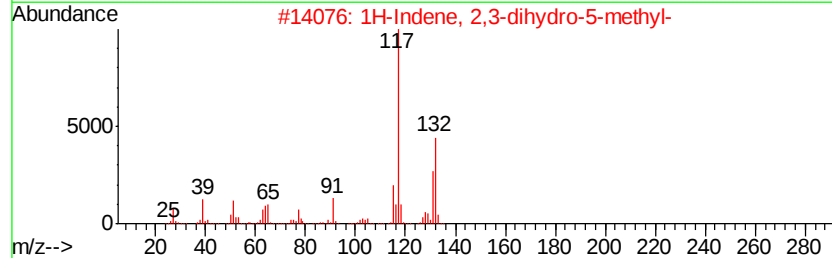
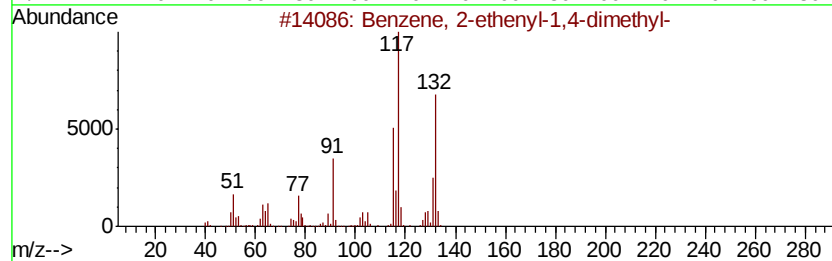
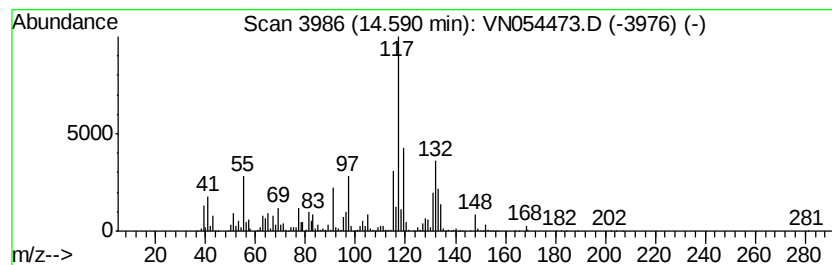
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	57.07 ug/l	3557250	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
3		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	83
4		2,4-Dimethylstyrene	132	C10H12	002234-20-0	83
5		3-Phenylbut-1-ene	132	C10H12	000934-10-1	64



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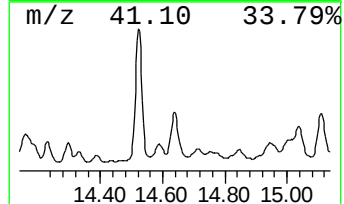
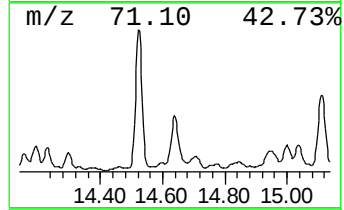
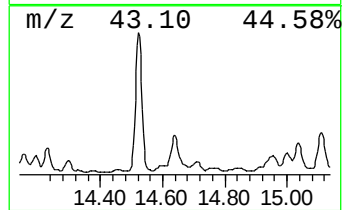
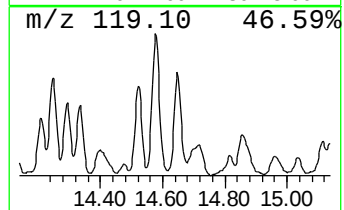
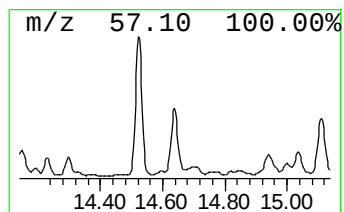
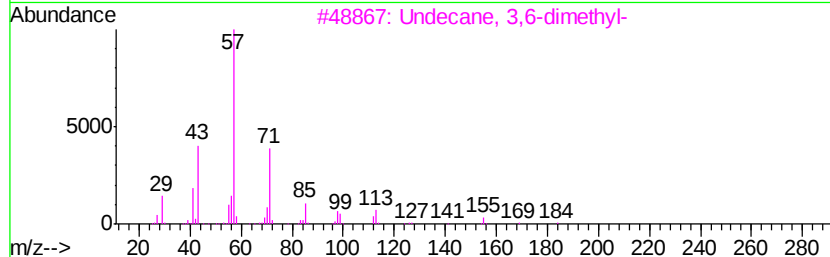
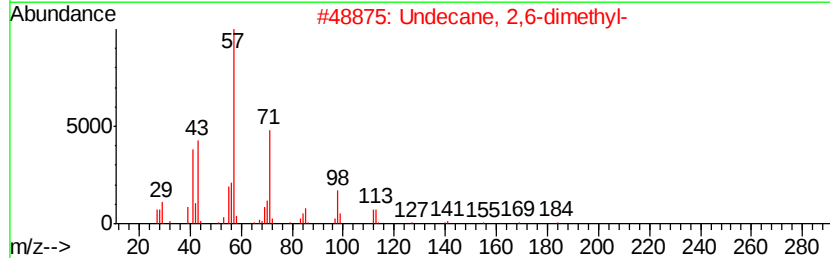
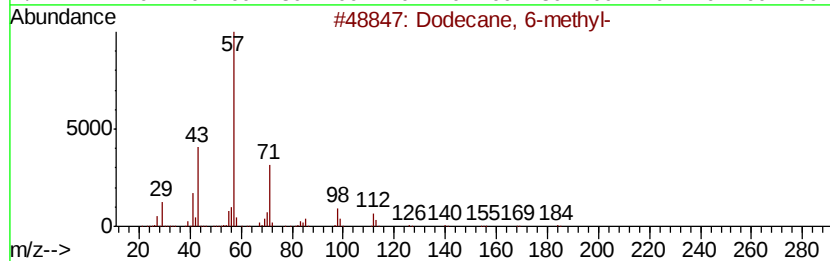
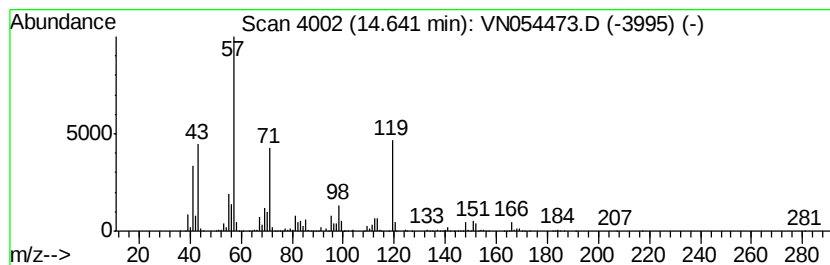
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Dodecane, 6-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	55.27 ug/l	3445040	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 6-methyl-	184	C13H28	006044-71-9	86
2		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64
3		Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	50
4		Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	45
5		Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	38



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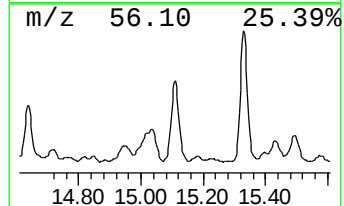
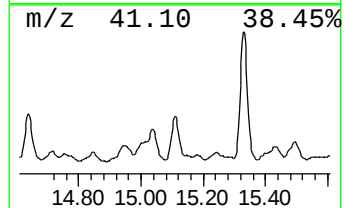
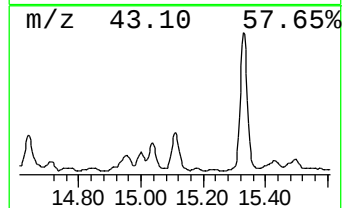
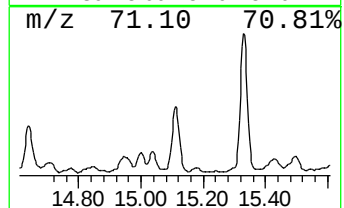
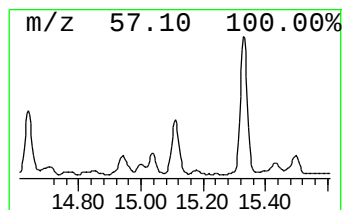
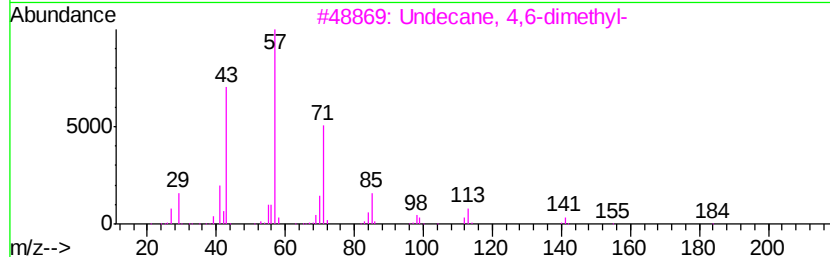
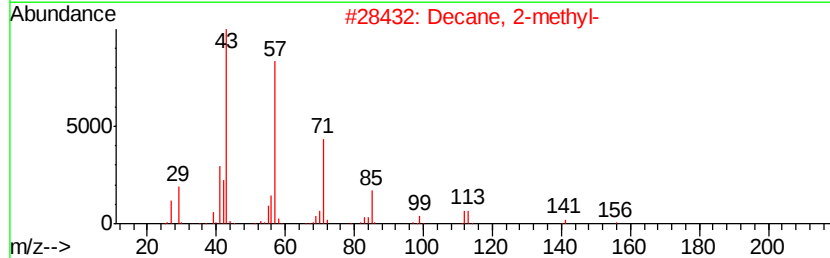
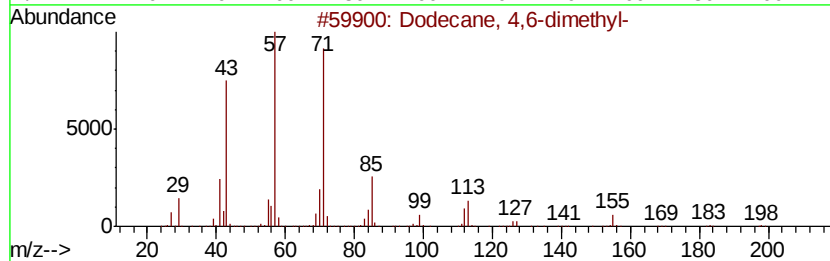
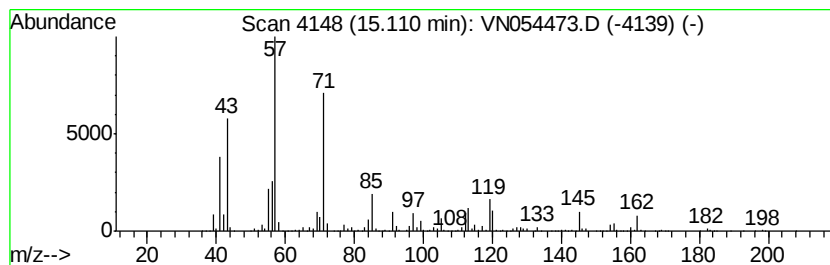
Instrument :
MSVOA_N
ClientSampleID :
40021

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 5 Dodecane, 4,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.11	58.24 ug/l	3630320	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Dodecane, 4,6-dimethyl-	198 C14H30	061141-72-8 78
2		Decane, 2-methyl-	156 C11H24	006975-98-0 58
3		Undecane, 4,6-dimethyl-	184 C13H28	017312-82-2 58
4		Octadecane, 2,6-dimethyl-	282 C20H42	075163-97-2 58
5		Sulfurous acid, decyl 2-ethylhex...	334 C18H38O3S	1000309-19-3 52



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN032019\
Data File : VN054473.D
Acq On : 20 Mar 2019 19:40
Operator : JC/SP
Sample : K1994-05
Misc : 4.34uL/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

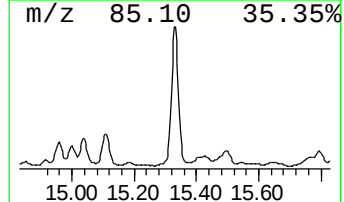
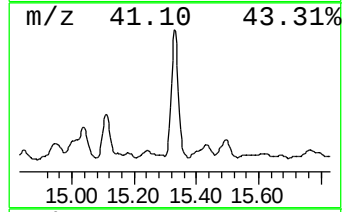
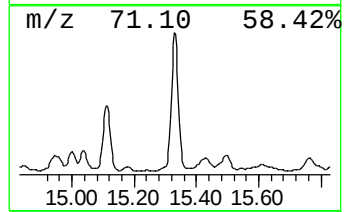
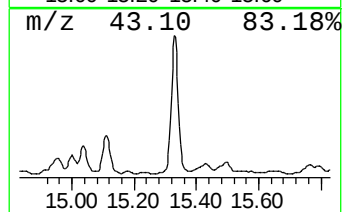
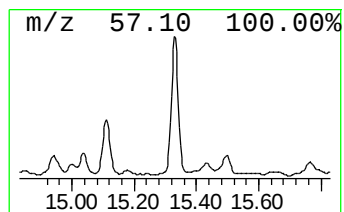
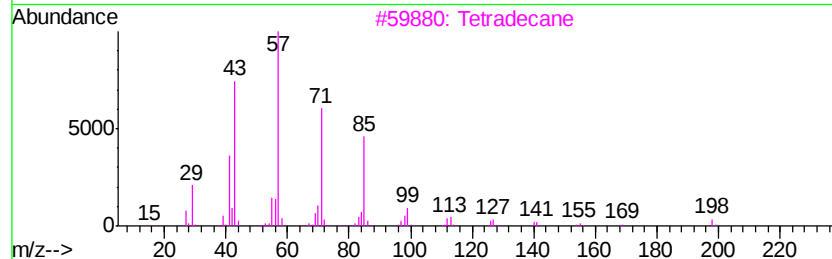
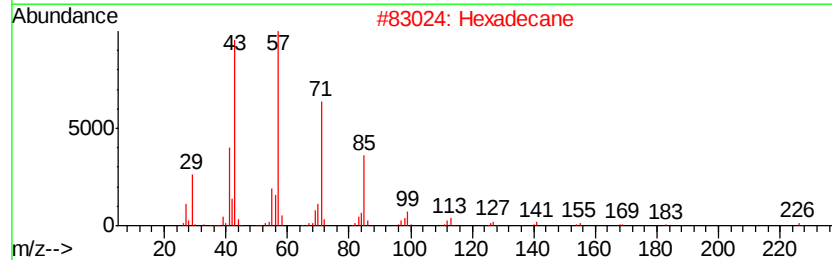
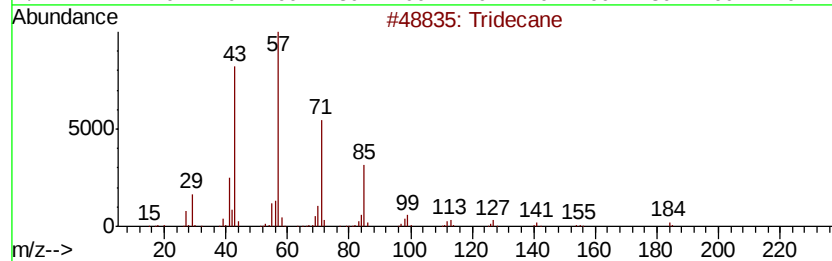
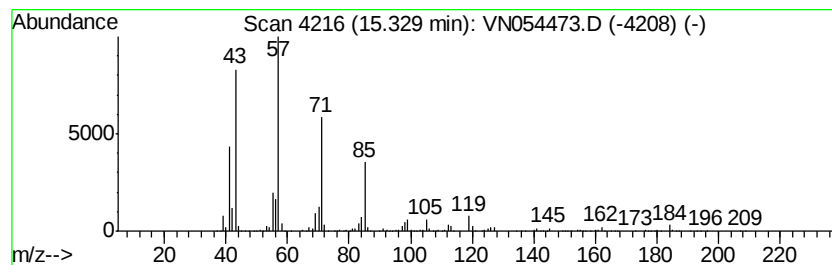
Instrument :
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ClientSampleId :
40021

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 6 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	134.84 ug/l	8404420	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tridecane	184 C13H28	000629-50-5	94
2	Hexadecane	226 C16H34	000544-76-3	87
3	Tetradecane	198 C14H30	000629-59-4	86
4	Undecane	156 C11H24	001120-21-4	80
5	Decane, 2,3,5-trimethyl-	184 C13H28	062238-11-3	78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN032019\
Data File : VN054473.D
Acq On : 20 Mar 2019 19:40
Operator : JC/SP
Sample : K1994-05
Misc : 4.34uL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

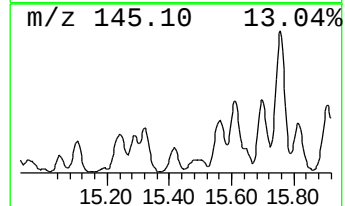
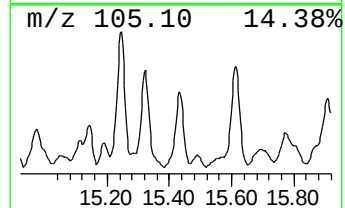
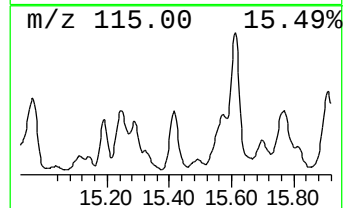
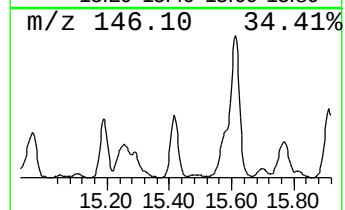
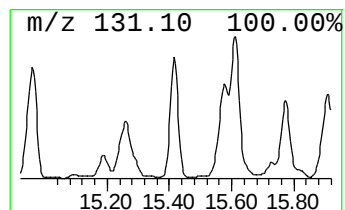
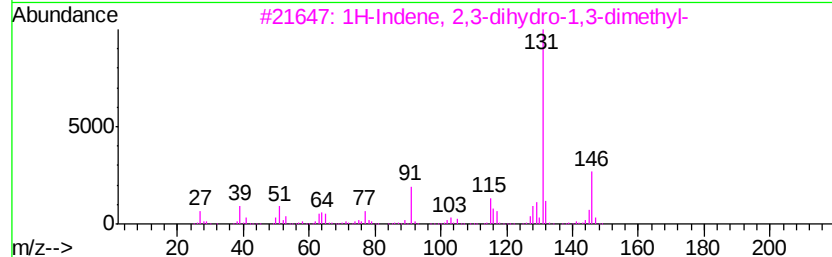
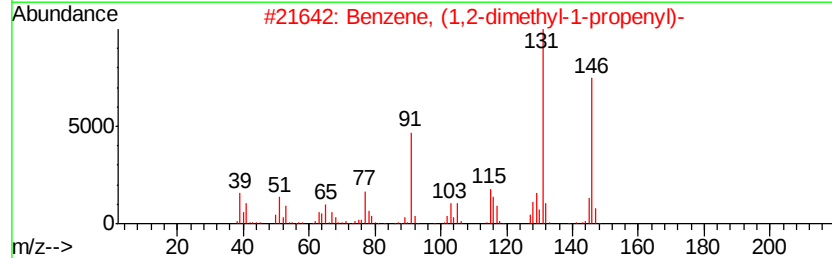
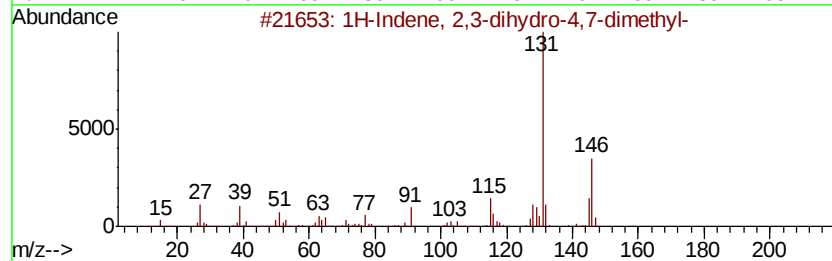
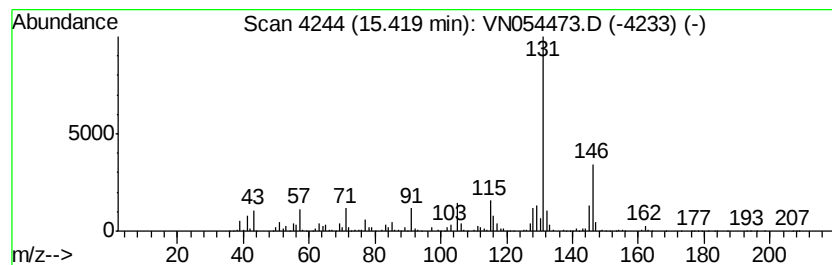
Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	51.67 ug/l	3220350	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146 C11H14	006682-71-9	95
2	Benzene, (1,2-dimethyl-1-propenyl)-	146 C11H14	000769-57-3	94
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146 C11H14	004175-53-5	94
4	Benzene, 1-methyl-3-(1-methyl-2-...	146 C11H14	052161-57-6	91
5	Benzene, 1-methyl-4-(1-methyl-2-...	146 C11H14	097664-18-1	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_N\DATA\VN032019\
Data File : VN054473.D
Acq On : 20 Mar 2019 19:40
Operator : JC/SP
Sample : K1994-05
Misc : 4.34uL/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
40021

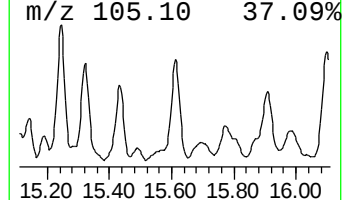
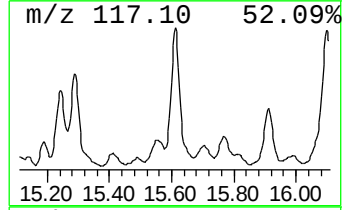
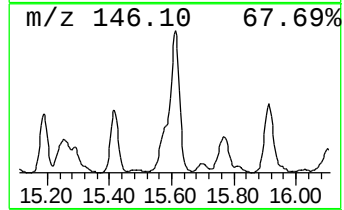
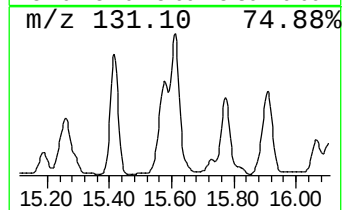
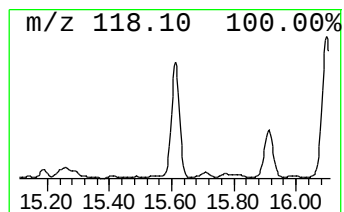
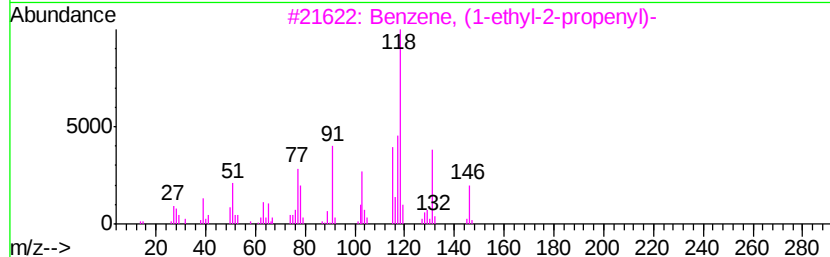
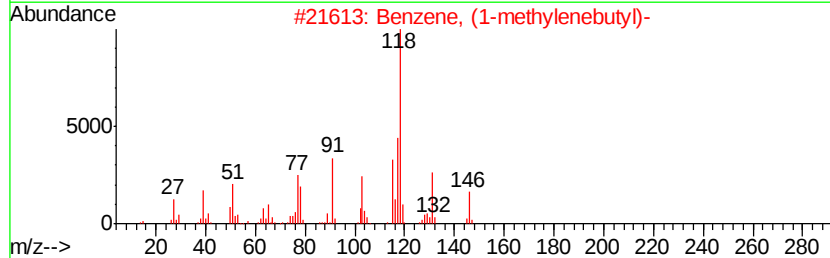
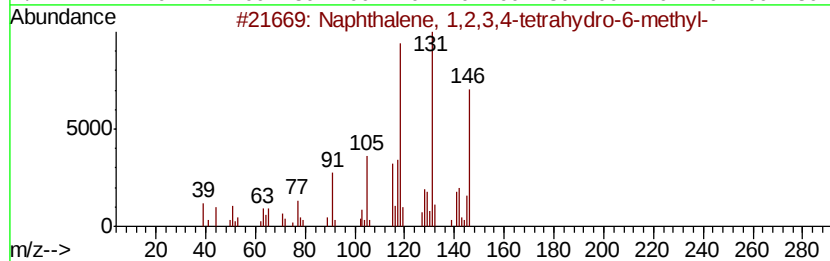
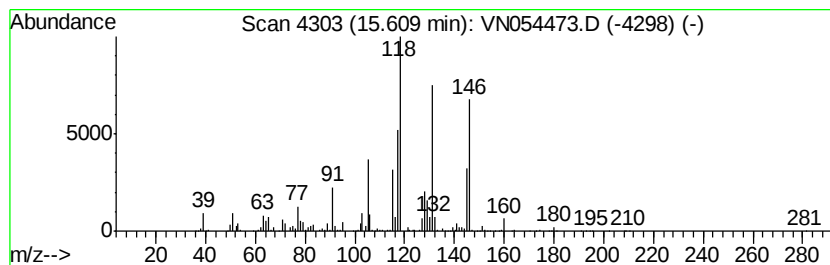
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 1,2,3,4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	65.31 ug/l	4070720	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	83
2		Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	72
3		Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	72
4		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	68
5		2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	49



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN032019\
Data File : VN054473.D
Acq On : 20 Mar 2019 19:40
Operator : JC/SP
Sample : K1994-05
Misc : 4.34u/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
40021

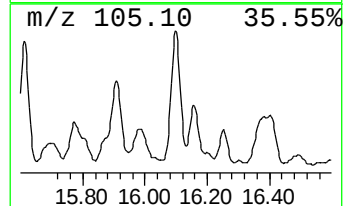
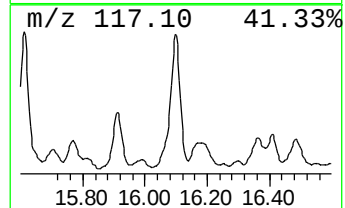
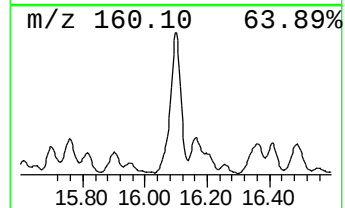
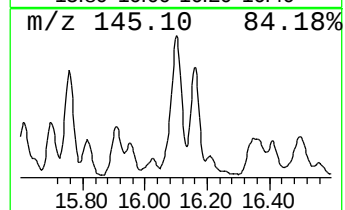
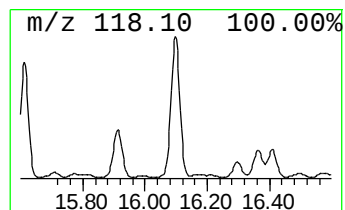
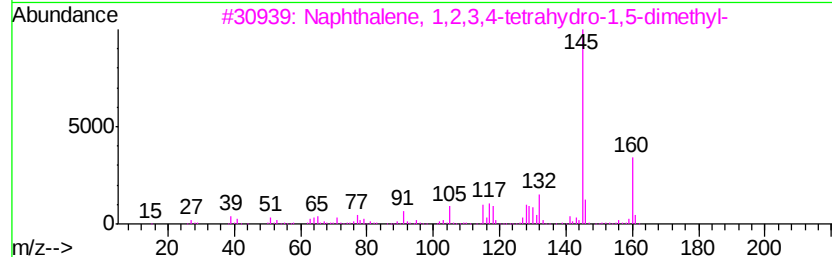
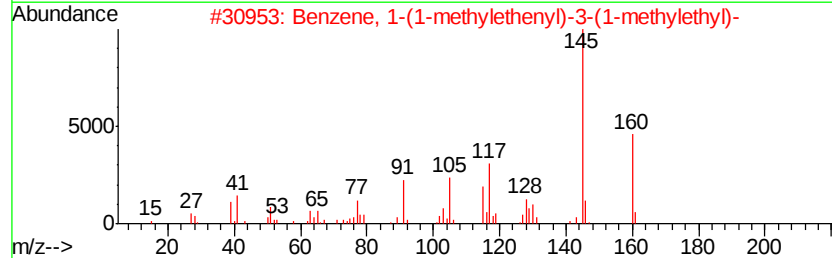
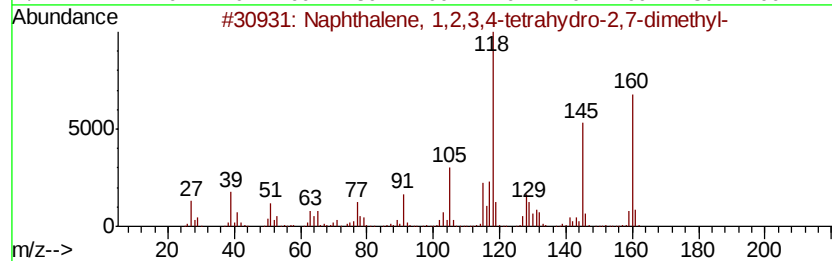
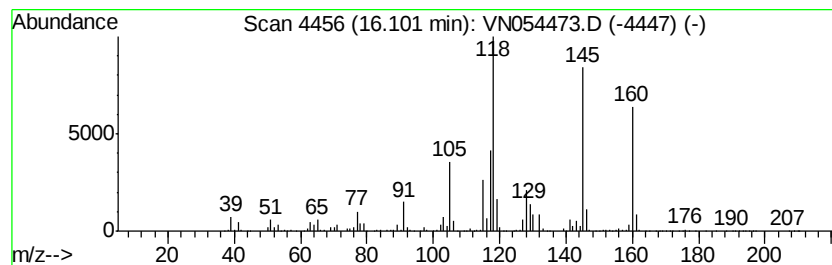
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	63.45 ug/l	3954800	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	90
2		Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	70
3		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	53
4		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	025419-33-4	52
5		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	49



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032019\
 Data File : VN054473.D
 Acq On : 20 Mar 2019 19:40
 Operator : JC/SP
 Sample : K1994-05
 Misc : 4.34uL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 40021

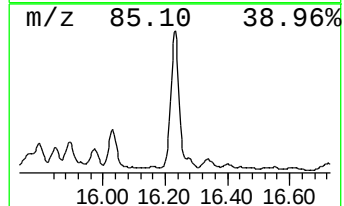
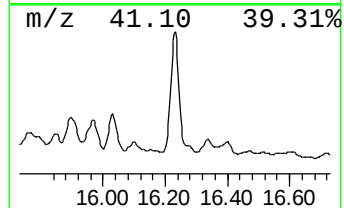
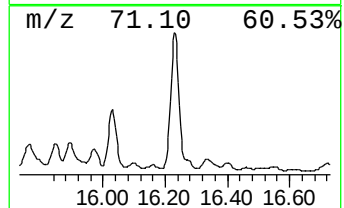
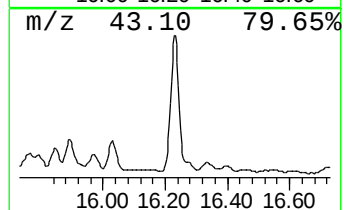
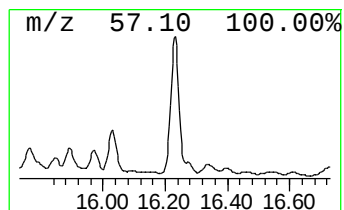
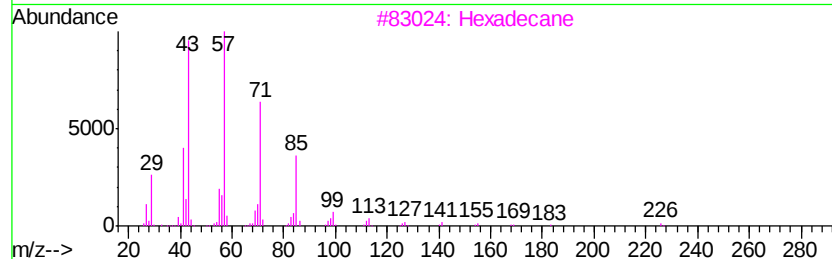
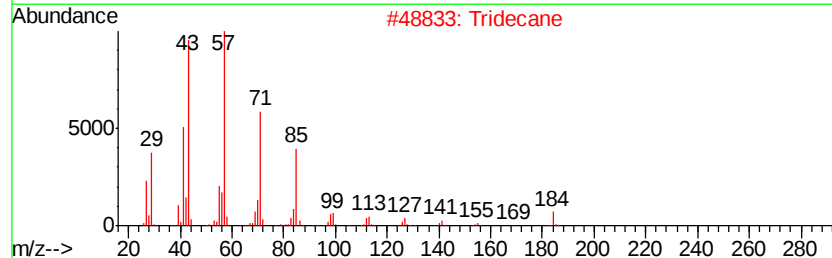
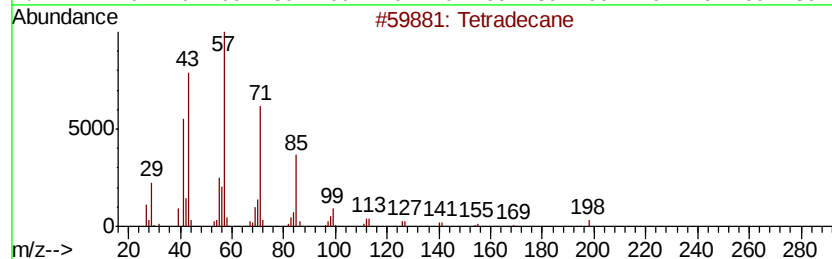
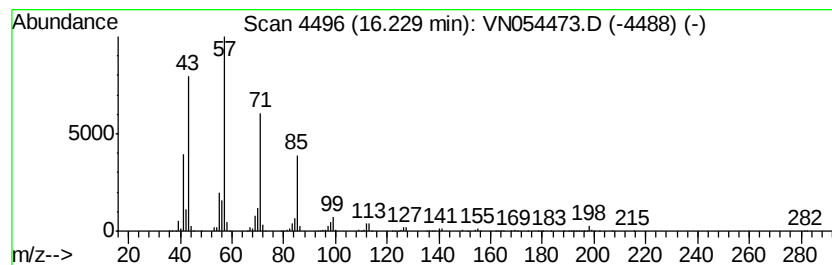
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
 Quant Title : SW846 8260

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

 Peak Number 10 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	67.17 ug/l	4186680	1,4-Dichlorobenzene-d4	13.35

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	90
4		Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	83
5		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032019\
 Data File : VN054473.D
 Acq On : 20 Mar 2019 19:40
 Operator : JC/SP
 Sample : K1994-05
 Misc : 4.34g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.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
Undecane	13.67	75.6	ug/l	4713180	4	13.35	3116480	50.0
Dodecane	14.52	112.3	ug/l	7000500	4	13.35	3116480	50.0
Benzene, 2-etheny...	14.59	57.1	ug/l	3557250	4	13.35	3116480	50.0
Dodecane, 6-methyl-	14.64	55.3	ug/l	3445040	4	13.35	3116480	50.0
Dodecane, 4,6-dim...	15.11	58.2	ug/l	3630320	4	13.35	3116480	50.0
Tridecane	15.33	134.8	ug/l	8404420	4	13.35	3116480	50.0
1H-Indene, 2,3-di...	15.42	51.7	ug/l	3220350	4	13.35	3116480	50.0
Naphthalene, 1,2,...	15.61	65.3	ug/l	4070720	4	13.35	3116480	50.0
Naphthalene, 1,2,...	16.10	63.5	ug/l	3954800	4	13.35	3116480	50.0
Tetradecane	16.23	67.2	ug/l	4186680	4	13.35	3116480	50.0