

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
 Data File : VN065633.D
 Acq On : 27 Jan 2021 16:37
 Operator : JC/MD
 Sample : M1190-02ME
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 20796ME

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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_N\methods\82N012521W.M
 Title : SW846 8260

Signal : TIC: VN065633.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.788	617	637	705	rVB	730506	2315596	20.65%	4.076%
2	7.338	1721	1741	1762	rVB3	45331	135248	1.21%	0.238%
3	7.586	1786	1818	1841	rBV3	593394	2537374	22.63%	4.467%
4	7.698	1842	1853	1873	rVV	198976	508488	4.53%	0.895%
5	7.830	1873	1894	1927	rVV	771999	1892700	16.88%	3.332%
6	7.987	1927	1943	1962	rVV2	177376	421363	3.76%	0.742%
7	8.110	1962	1981	1990	rVV4	121641	320192	2.86%	0.564%
8	8.171	1991	2000	2017	rVV3	108222	330246	2.94%	0.581%
9	8.258	2017	2027	2045	rVB2	57808	135325	1.21%	0.238%
10	8.396	2053	2070	2099	rBV	711317	1454945	12.97%	2.561%
11	8.547	2099	2117	2140	rBV	423379	888771	7.93%	1.565%
12	9.042	2247	2271	2283	rBV2	180350	468627	4.18%	0.825%
13	9.483	2388	2408	2425	rBV4	53666	113052	1.01%	0.199%
14	9.621	2429	2451	2463	rBV3	63226	158230	1.41%	0.279%
15	9.695	2463	2474	2499	rVV2	64518	164578	1.47%	0.290%
16	9.833	2499	2517	2540	rVB2	56496	142392	1.27%	0.251%
17	10.058	2573	2587	2595	rBV	694438	1270908	11.33%	2.237%
18	10.122	2595	2607	2632	rVB	5979089	11214309	100.00%	19.742%
19	10.251	2638	2647	2662	rVB	119671	212756	1.90%	0.375%
20	11.171	2917	2933	2953	rVB5	123645	290920	2.59%	0.512%
21	11.270	2953	2964	2985	rBV2	105582	199747	1.78%	0.352%
22	11.376	2985	2997	3017	rVV	532592	970954	8.66%	1.709%
23	11.482	3018	3030	3045	rVV	109767	244758	2.18%	0.431%
24	11.601	3045	3067	3081	rVV5	597792	1446800	12.90%	2.547%
25	11.917	3143	3165	3182	rBV3	201236	583049	5.20%	1.026%
26	12.016	3188	3196	3204	rBV	90126	127424	1.14%	0.224%
27	12.132	3225	3232	3250	rVB6	140753	292100	2.60%	0.514%
28	12.373	3299	3307	3316	rVV	345282	530180	4.73%	0.933%
29	12.418	3316	3321	3329	rVB	100510	130539	1.16%	0.230%
30	12.560	3361	3365	3373	rVB	92004	119924	1.07%	0.211%
31	12.624	3374	3385	3392	rBV	311515	552290	4.92%	0.972%
32	12.698	3400	3408	3418	rVB3	841502	1347249	12.01%	2.372%
33	12.749	3419	3424	3434	rVB2	105448	157664	1.41%	0.278%
34	12.862	3449	3459	3467	rBV	147171	259702	2.32%	0.457%
35	12.933	3475	3481	3493	rVB4	154279	259616	2.32%	0.457%
36	13.010	3494	3505	3516	rBV	510606	870220	7.76%	1.532%

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37	13.138	3535	3545	3553	rVB3	109734	194874	1.74%	0.343%
38	13.206	3554	3566	3575	rBV4	255096	495202	4.42%	0.872%
39	13.315	3589	3600	3607	rBV	485855	931533	8.31%	1.640%
40	13.511	3646	3661	3668	rBV2	575514	1063516	9.48%	1.872%
41	13.556	3668	3675	3690	rVV4	645775	1275829	11.38%	2.246%
42	13.640	3691	3701	3710	rVV4	502499	824861	7.36%	1.452%
43	13.711	3716	3723	3733	rVB	253681	392603	3.50%	0.691%
44	13.772	3734	3742	3746	rVV	528747	771067	6.88%	1.357%
45	13.801	3747	3751	3760	rVV	650329	942486	8.40%	1.659%
46	13.859	3760	3769	3780	rVB	1304178	1981419	17.67%	3.488%
47	13.965	3792	3802	3812	rVB2	424141	705274	6.29%	1.242%
48	14.097	3835	3843	3849	rBV	238929	369017	3.29%	0.650%
49	14.135	3849	3855	3861	rVV3	270599	444827	3.97%	0.783%
50	14.180	3861	3869	3874	rVV	883225	1408156	12.56%	2.479%
51	14.219	3874	3881	3890	rVV	1919024	2928924	26.12%	5.156%
52	14.264	3890	3895	3901	rVV2	198235	257760	2.30%	0.454%
53	14.302	3901	3907	3916	rVB2	240230	328376	2.93%	0.578%
54	14.360	3920	3925	3931	rVV4	83310	115498	1.03%	0.203%
55	14.405	3934	3939	3944	rVV2	119408	146783	1.31%	0.258%
56	14.444	3944	3951	3960	rVV2	367605	660677	5.89%	1.163%
57	14.492	3961	3966	3974	rVB	356785	506306	4.51%	0.891%
58	14.553	3974	3985	3998	rBV4	1105662	2288429	20.41%	4.029%
59	14.614	3999	4004	4015	rVB2	199878	327301	2.92%	0.576%
60	14.711	4026	4034	4051	rVB2	213187	376228	3.35%	0.662%
61	14.820	4061	4068	4088	rVB3	191274	439347	3.92%	0.773%
62	14.923	4093	4100	4113	rVB4	148635	303688	2.71%	0.535%
63	15.100	4145	4155	4165	rVB	211636	403763	3.60%	0.711%
64	15.154	4166	4172	4180	rVV	137111	198130	1.77%	0.349%
65	15.212	4181	4190	4208	rVV8	174403	461527	4.12%	0.812%
66	15.293	4209	4215	4230	rVB6	128379	254049	2.27%	0.447%
67	15.379	4232	4242	4256	rVB3	97496	224572	2.00%	0.395%
68	15.576	4295	4303	4319	rVB2	281166	532295	4.75%	0.937%
69	15.730	4344	4351	4374	rVB7	77946	239837	2.14%	0.422%
70	15.868	4383	4394	4406	rBV2	159445	309237	2.76%	0.544%
71	16.058	4442	4453	4464	rVB2	194283	373510	3.33%	0.658%
72	16.119	4465	4472	4489	rVB7	65972	130159	1.16%	0.229%
73	16.437	4565	4571	4588	rVB5	59377	130111	1.16%	0.229%

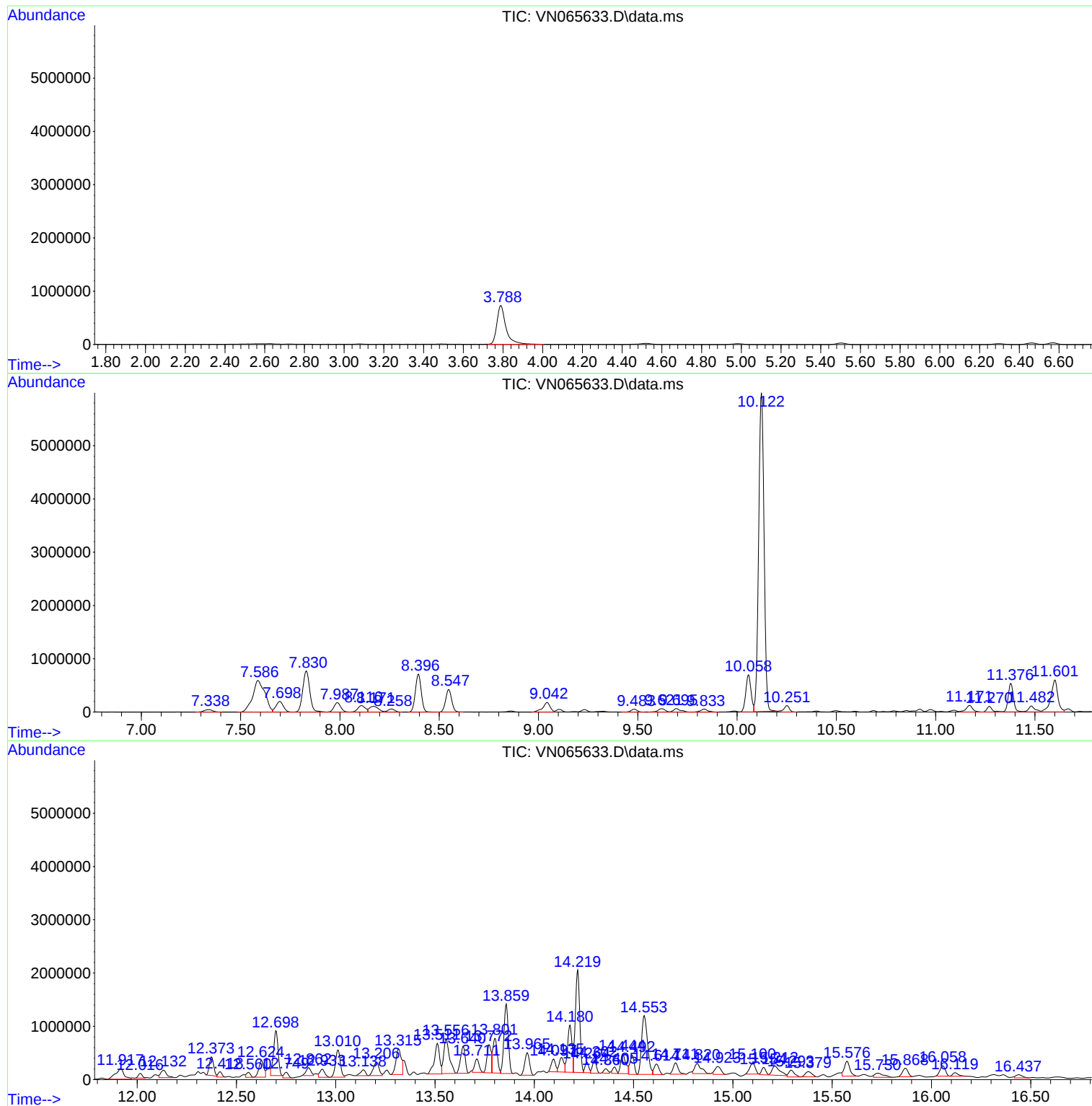
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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Instrument :
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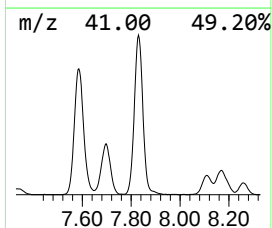
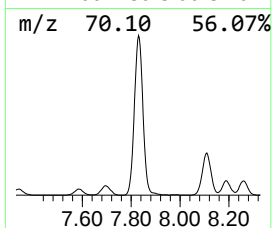
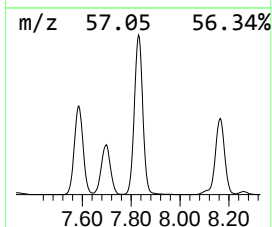
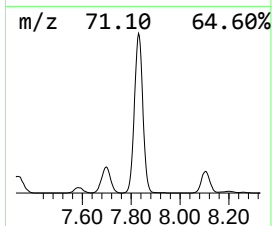
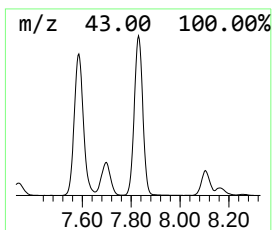
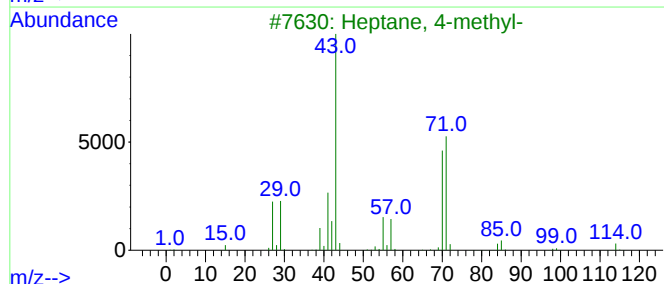
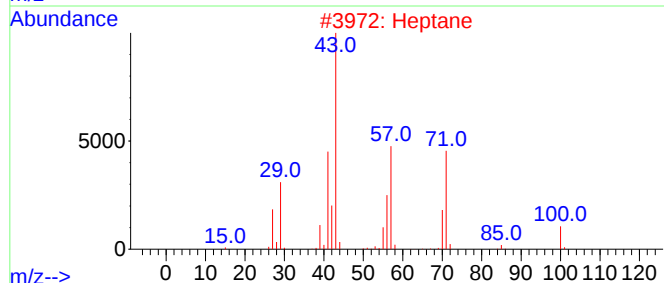
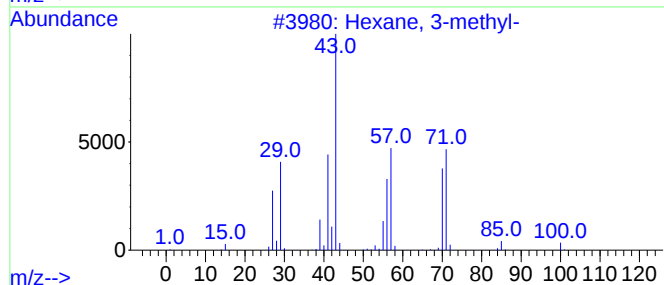
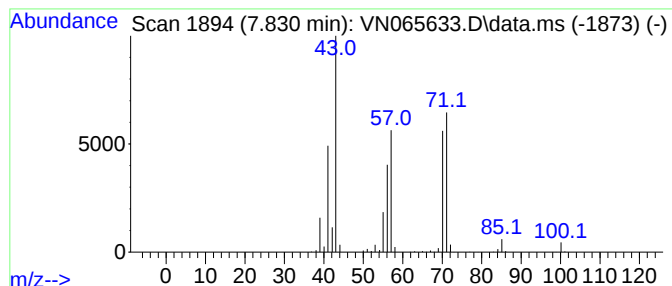
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.830	37.30 ug/l	1892700	Pentafluorobenzene	7.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	64
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	53
5			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	50



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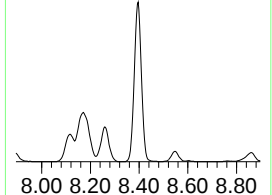
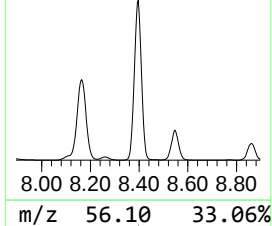
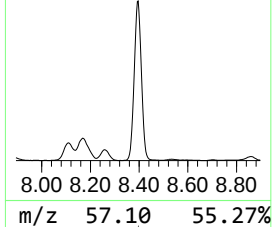
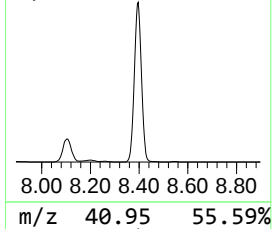
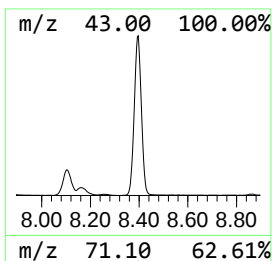
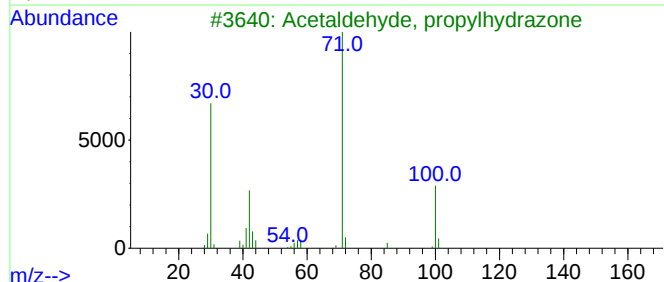
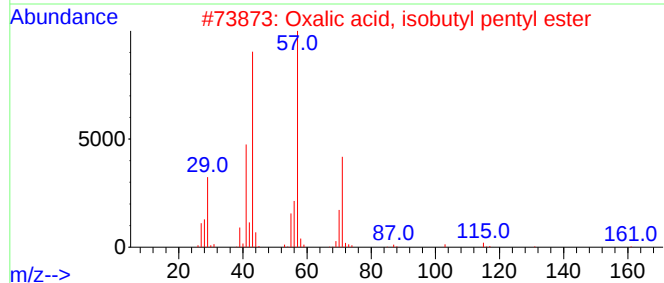
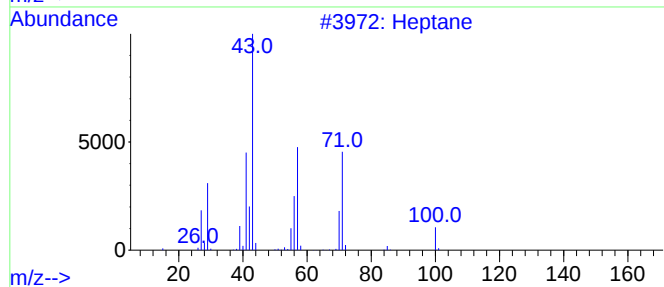
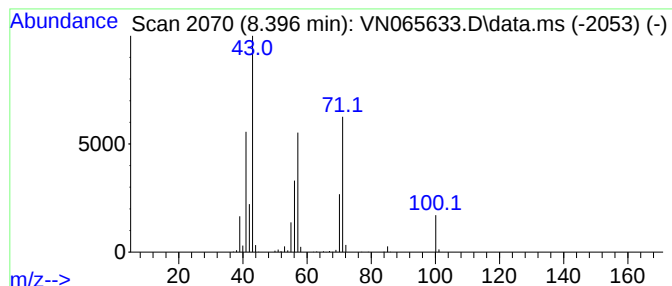
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.396	81.85 ug/l	1454950	1,4-Difluorobenzene	8.547

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	59
3			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	46
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	40



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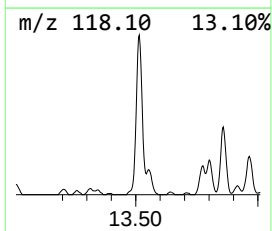
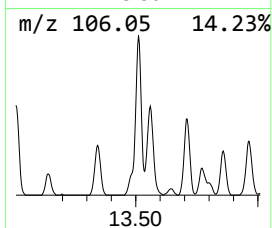
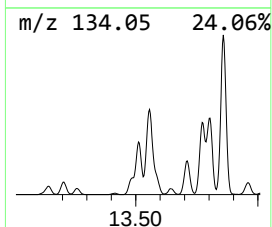
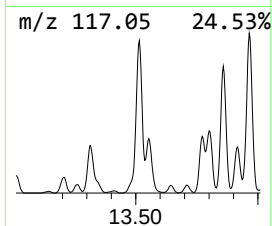
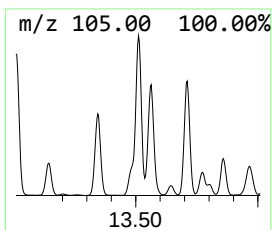
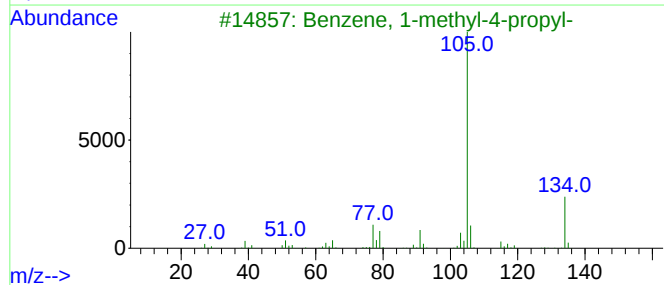
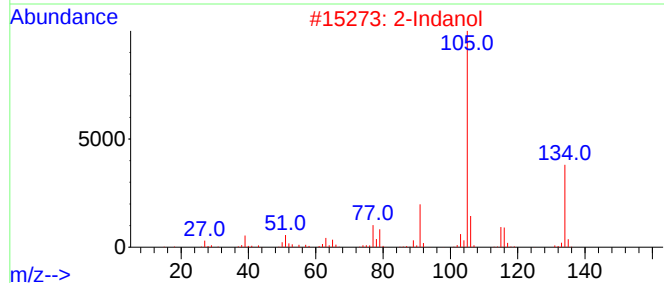
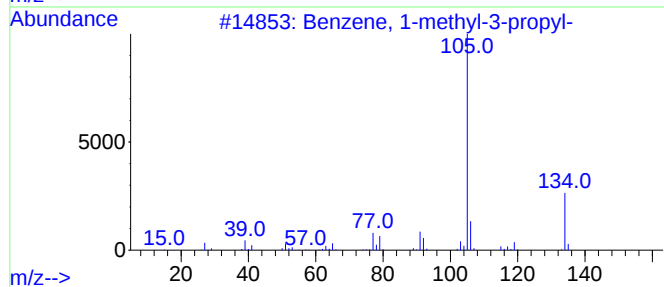
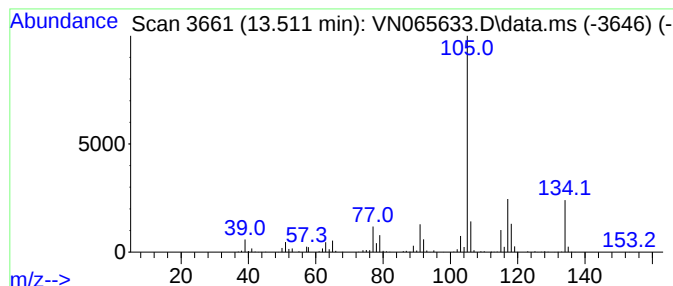
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Benzene, 1-methyl-3-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.511	57.08 ug/l	1063520	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	70
2			2-Indanol	134	C9H10O	004254-29-9	68
3			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	64
4			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	64
5			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	64



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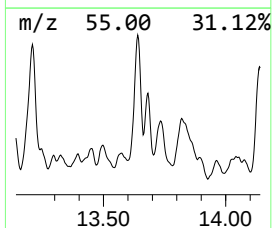
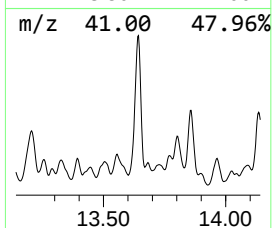
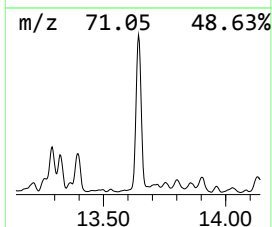
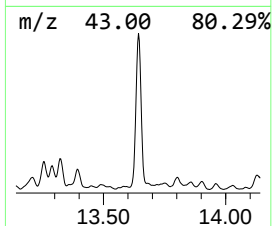
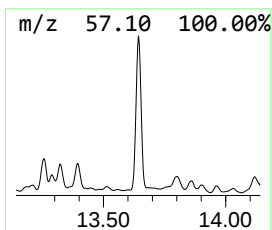
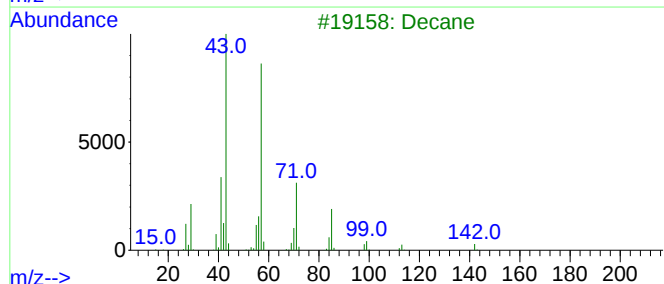
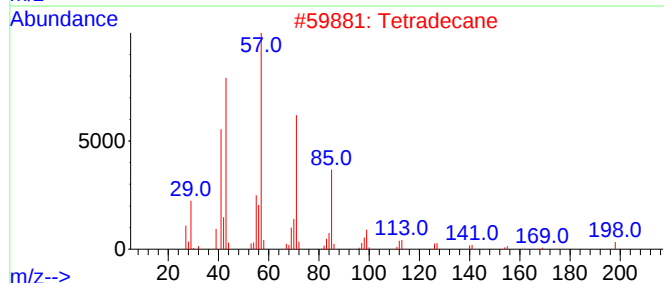
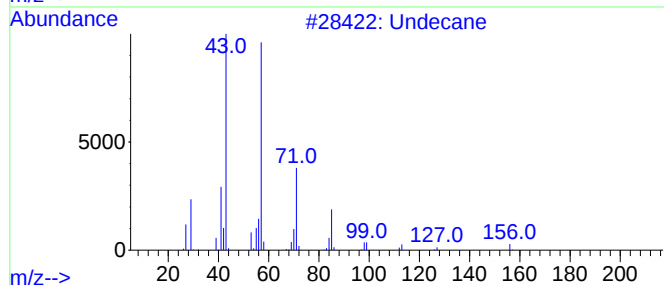
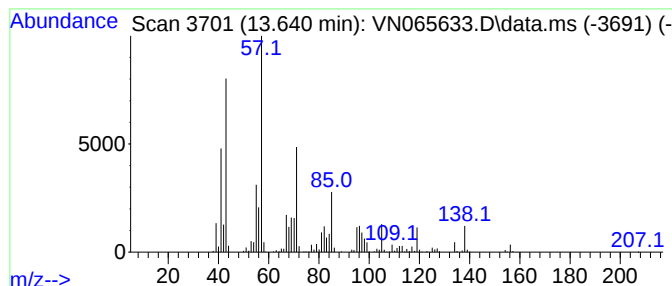
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Quant Title : SW846 8260

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

Peak Number 4 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.640	44.27 ug/l	824861	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	70
2	Tetradecane			198	C14H30	000629-59-4	50
3	Decane			142	C10H22	000124-18-5	47
4	Undecane, 2,4-dimethyl-			184	C13H28	017312-80-0	47
5	Decane, 2,3,5-trimethyl-			184	C13H28	062238-11-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065633.D
Acq On : 27 Jan 2021 16:37
Operator : JC/MD
Sample : M1190-02ME
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20796ME

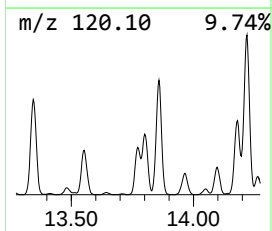
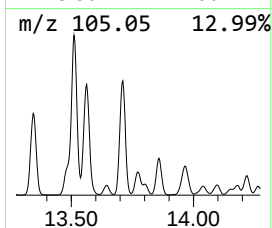
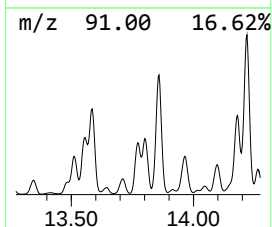
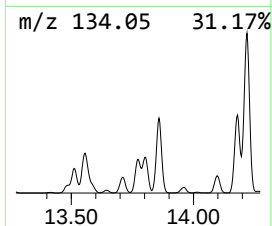
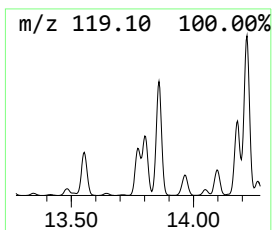
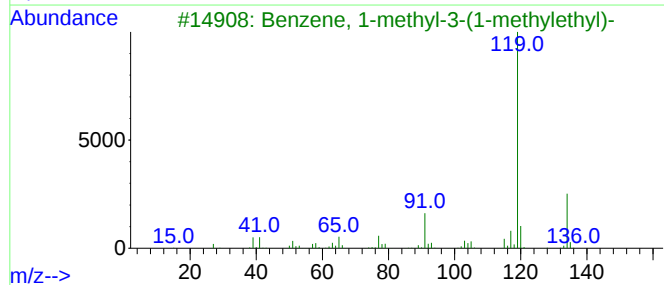
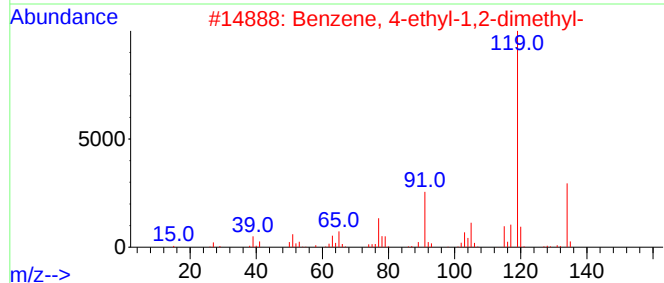
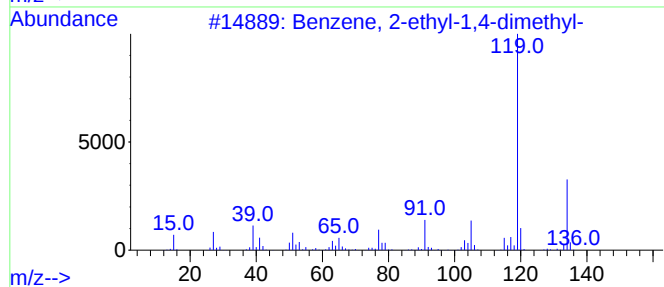
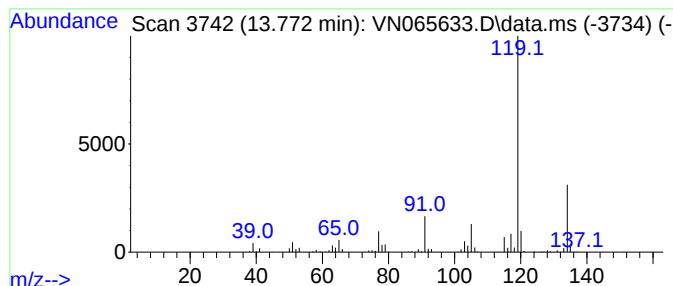
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.772	41.39 ug/l	771067	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065633.D
Acq On : 27 Jan 2021 16:37
Operator : JC/MD
Sample : M1190-02ME
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20796ME

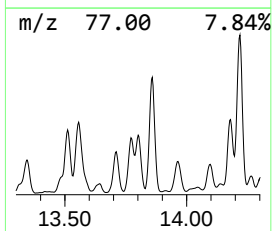
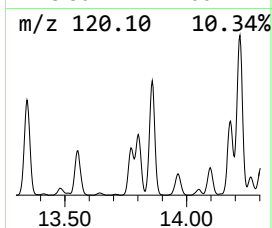
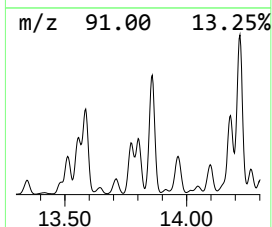
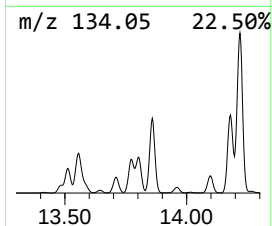
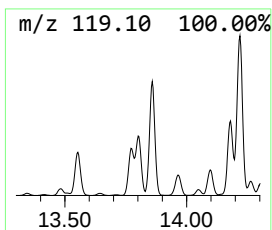
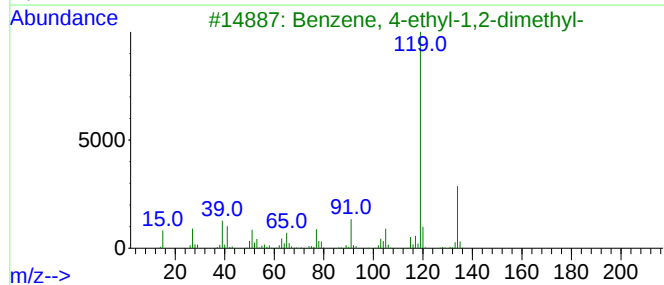
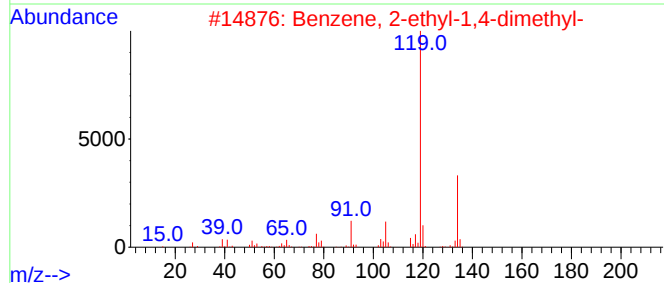
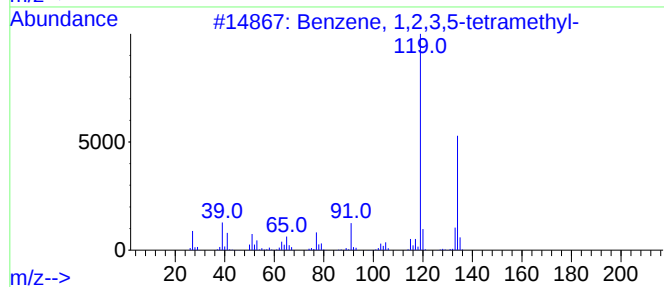
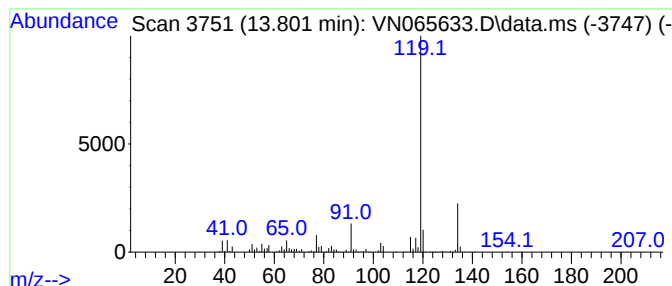
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.801	50.59 ug/l	942486	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065633.D
Acq On : 27 Jan 2021 16:37
Operator : JC/MD
Sample : M1190-02ME
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20796ME

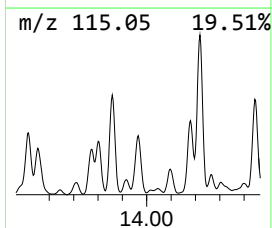
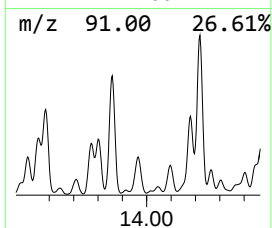
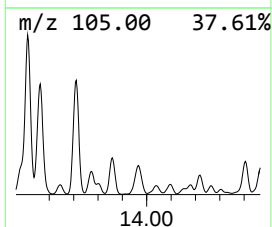
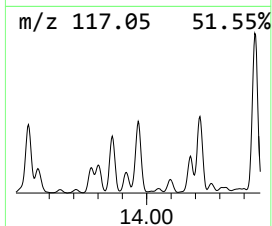
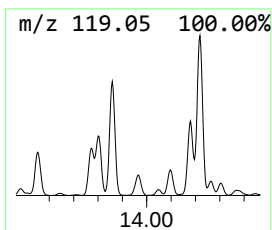
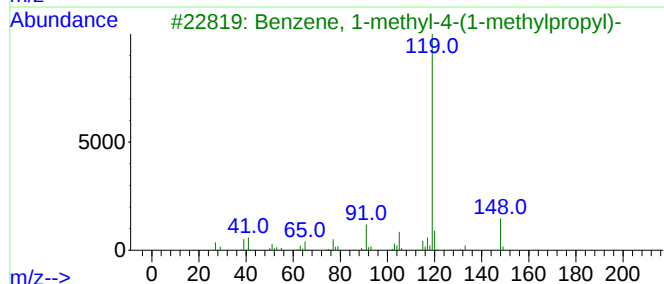
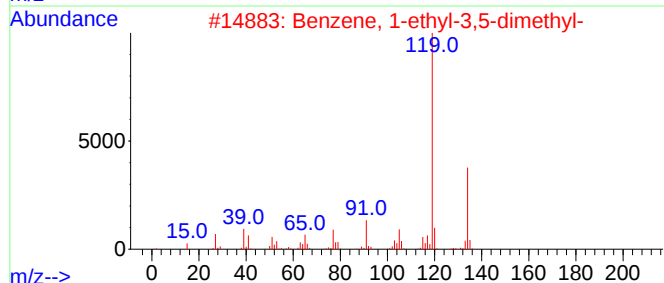
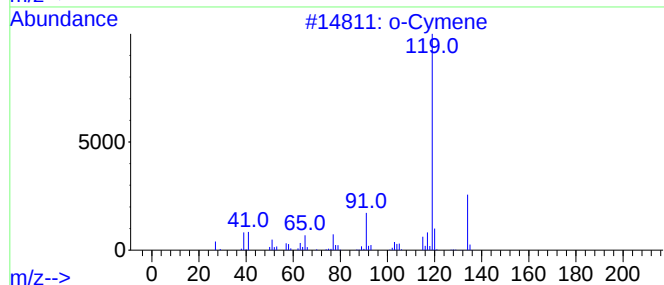
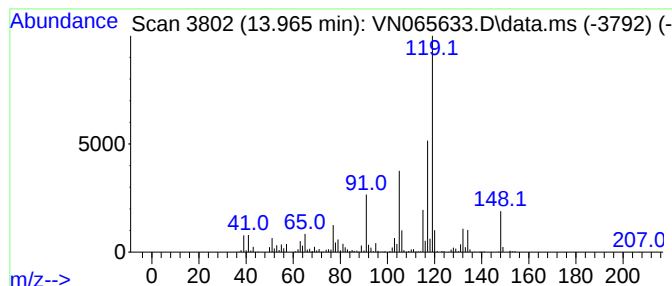
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Quant Title : SW846 8260

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

Peak Number 7 o-Cymene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	37.86 ug/l	705274	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	50
2			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	49
3			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	49
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	49
5			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065633.D
Acq On : 27 Jan 2021 16:37
Operator : JC/MD
Sample : M1190-02ME
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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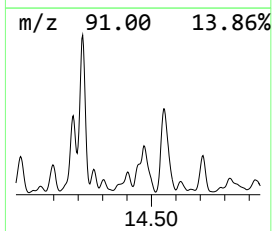
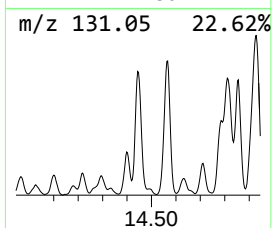
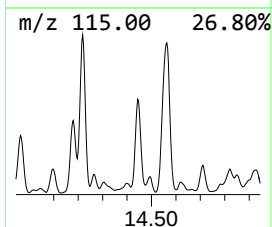
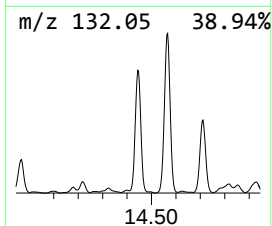
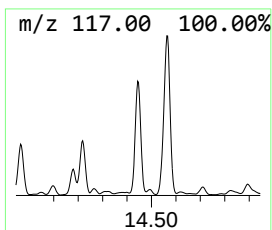
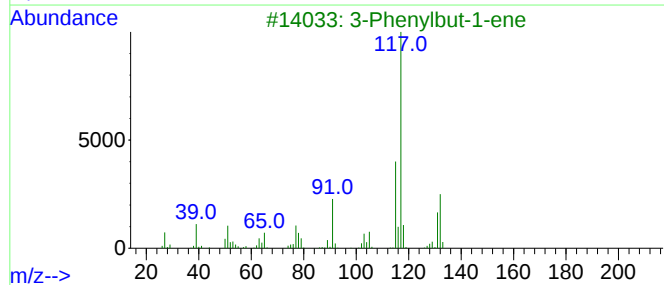
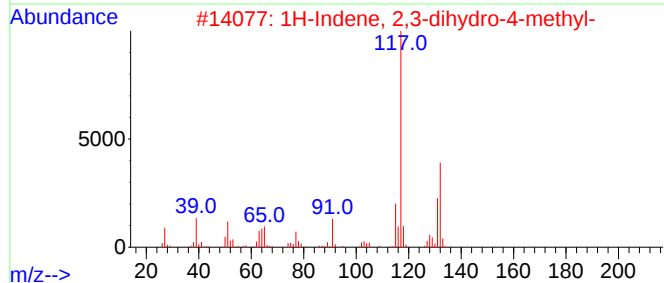
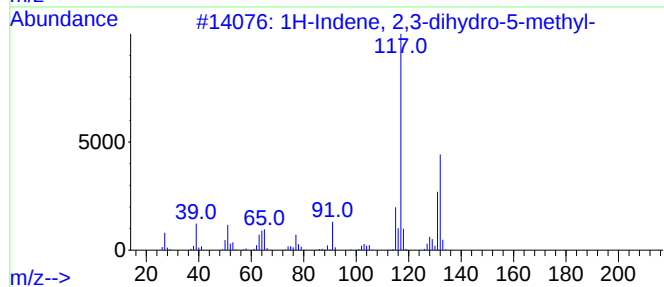
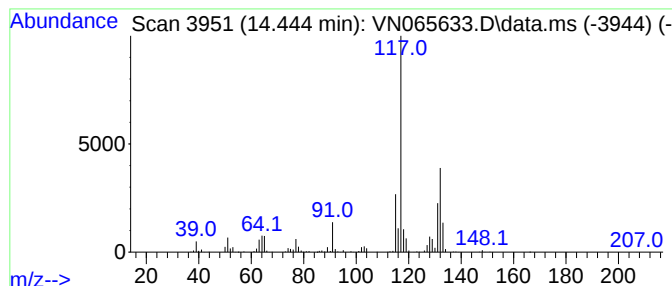
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Quant Title : SW846 8260

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

Peak Number 8 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.444	35.46 ug/l	660677	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	86
4			Indan, 1-methyl-	132	C10H12	000767-58-8	81
5			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065633.D
Acq On : 27 Jan 2021 16:37
Operator : JC/MD
Sample : M1190-02ME
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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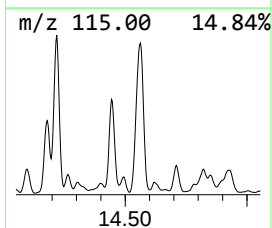
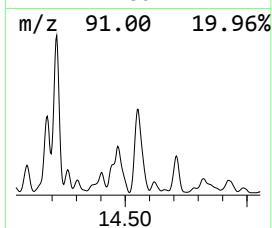
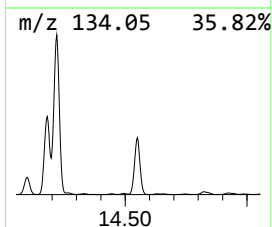
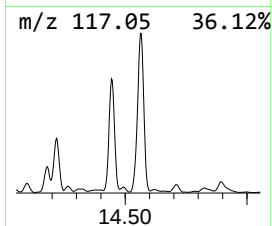
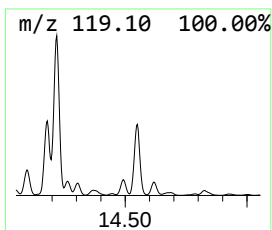
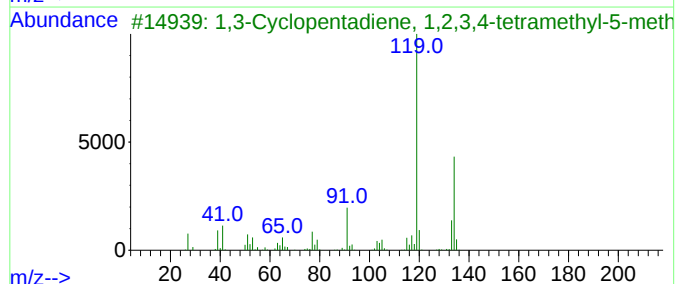
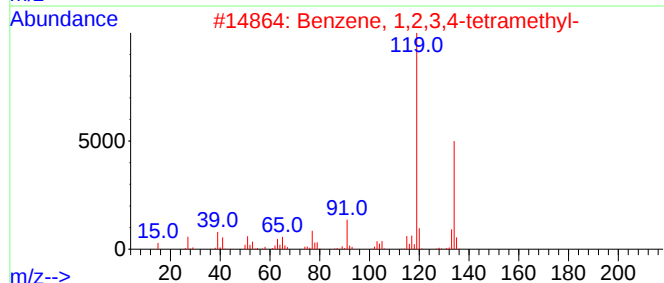
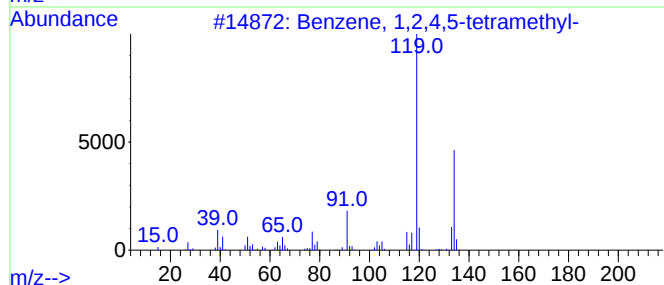
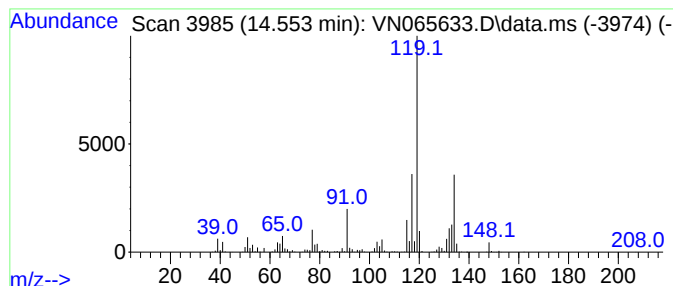
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.553	122.83 ug/l	2288430	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
3			1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	81
4			o-Cymene	134	C10H14	000527-84-4	76
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065633.D
Acq On : 27 Jan 2021 16:37
Operator : JC/MD
Sample : M1190-02ME
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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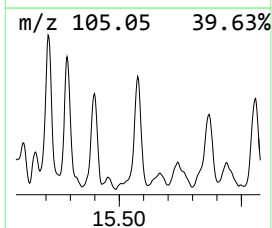
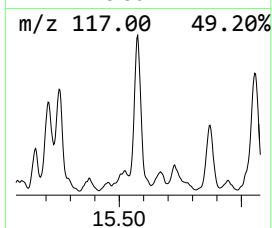
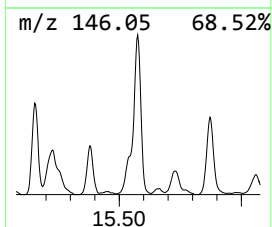
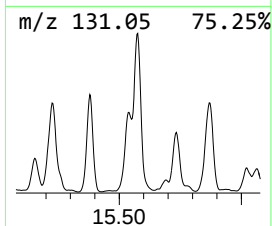
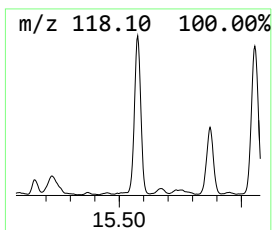
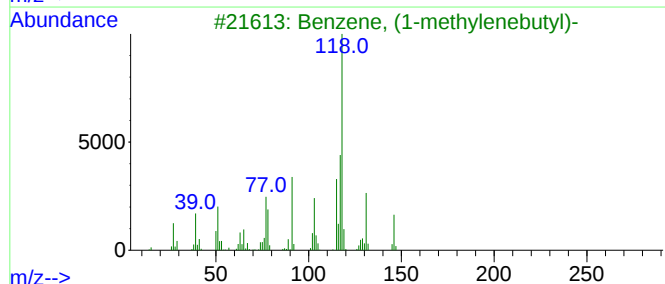
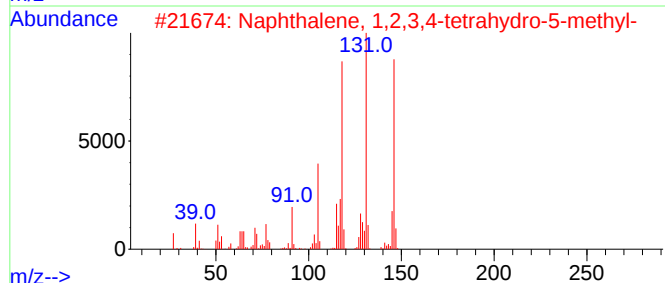
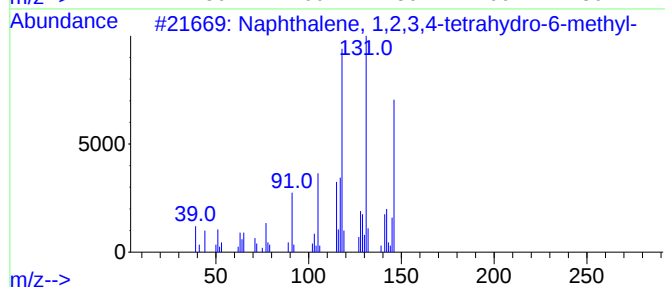
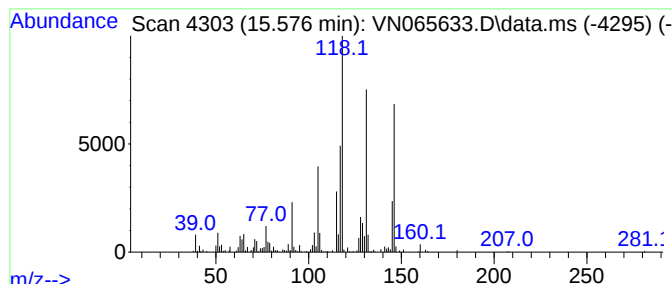
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.576	28.57 ug/l	532295	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	91
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	87
3			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	87
4			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	74
5			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065633.D
Acq On : 27 Jan 2021 16:37
Operator : JC/MD
Sample : M1190-02ME
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20796ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.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
Hexane, 3-methyl-	7.830	37.3	ug/l	1892700	1	7.621	2537370	50.0
Heptane	8.396	81.9	ug/l	1454950	2	8.547	888771	50.0
Benzene, 1-meth...	13.511	57.1	ug/l	1063520	4	13.315	931533	50.0
Undecane	13.640	44.3	ug/l	824861	4	13.315	931533	50.0
Benzene, 2-ethy...	13.772	41.4	ug/l	771067	4	13.315	931533	50.0
Benzene, 1,2,3,...	13.801	50.6	ug/l	942486	4	13.315	931533	50.0
o-Cymene	13.965	37.9	ug/l	705274	4	13.315	931533	50.0
1H-Indene, 2,3-...	14.444	35.5	ug/l	660677	4	13.315	931533	50.0
Benzene, 1,2,4,...	14.553	122.8	ug/l	2288430	4	13.315	931533	50.0
Naphthalene, 1,...	15.576	28.6	ug/l	532295	4	13.315	931533	50.0