

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
 Data File : VN065626.D
 Acq On : 27 Jan 2021 13:46
 Operator : JC/MD
 Sample : M1190-05
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41053

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_N\methods\82N012521W.M
 Title : SW846 8260

Signal : TIC: VN065626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.251	451	470	504	rBV	347659	910737	23.57%	4.251%
2	3.782	622	635	656	rVB	50889	129568	3.35%	0.605%
3	7.550	1789	1807	1818	rBV2	131438	333450	8.63%	1.556%
4	7.624	1818	1830	1850	rVB	264813	632643	16.37%	2.953%
5	7.997	1926	1946	1972	rBV3	376290	971602	25.14%	4.535%
6	8.547	2102	2117	2141	rBV	403298	847825	21.94%	3.957%
7	10.058	2571	2587	2596	rBV	643675	1193286	30.88%	5.570%
8	10.122	2596	2607	2637	rVB	2140272	3864625	100.00%	18.039%
9	11.376	2983	2997	3016	rBV	546753	966196	25.00%	4.510%
10	11.479	3017	3029	3045	rVB	282007	470232	12.17%	2.195%
11	11.589	3048	3063	3083	rVV	1108870	2093850	54.18%	9.773%
12	11.917	3151	3165	3187	rVB	928993	1551816	40.15%	7.243%
13	12.373	3284	3307	3328	rBV	401182	733666	18.98%	3.424%
14	12.563	3355	3366	3375	rBV	42877	70897	1.83%	0.331%
15	12.624	3375	3385	3392	rBV	303988	500226	12.94%	2.335%
16	12.704	3402	3410	3427	rVB	173378	279995	7.25%	1.307%
17	12.862	3446	3459	3474	rBV	179455	290461	7.52%	1.356%
18	13.010	3492	3505	3519	rBV	575097	903538	23.38%	4.217%
19	13.315	3587	3600	3605	rBV	477251	825044	21.35%	3.851%
20	13.511	3643	3661	3669	rBV	263261	476352	12.33%	2.223%
21	13.553	3670	3674	3693	rVB2	81770	132542	3.43%	0.619%
22	13.708	3711	3722	3732	rVB3	22924	39657	1.03%	0.185%
23	13.772	3733	3742	3747	rBV	52938	83400	2.16%	0.389%
24	13.859	3760	3769	3779	rVB	93550	142765	3.69%	0.666%
25	13.965	3793	3802	3815	rVB2	87667	142580	3.69%	0.666%
26	14.097	3834	3843	3853	rBV	36374	56377	1.46%	0.263%
27	14.180	3853	3869	3874	rBV	77918	121767	3.15%	0.568%
28	14.219	3874	3881	3890	rVB	115210	174717	4.52%	0.816%
29	14.444	3943	3951	3961	rBV	102156	155963	4.04%	0.728%
30	14.563	3974	3988	4000	rBV3	230345	457376	11.83%	2.135%
31	14.711	4024	4034	4043	rBV	65730	111313	2.88%	0.520%
32	14.820	4050	4068	4074	rBV6	52272	124982	3.23%	0.583%
33	14.923	4090	4100	4121	rVB2	58139	128064	3.31%	0.598%
34	15.100	4134	4155	4166	rBV	179002	340977	8.82%	1.592%
35	15.209	4180	4189	4198	rBV6	29799	61491	1.59%	0.287%
36	15.380	4230	4242	4258	rBV	52997	104411	2.70%	0.487%

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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

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37	15.540	4273	4292	4295	rBV5	42294	86305	2.23%	0.403%
38	15.572	4296	4302	4319	rVB2	85553	159079	4.12%	0.743%
39	15.659	4319	4329	4339	rBV2	22663	40914	1.06%	0.191%
40	15.730	4339	4351	4364	rBV4	34994	73565	1.90%	0.343%
41	15.868	4379	4394	4414	rBV3	62145	139382	3.61%	0.651%
42	16.058	4435	4453	4462	rBV5	53206	126561	3.27%	0.591%
43	16.119	4462	4472	4498	rVB	79573	189463	4.90%	0.884%
44	16.306	4516	4530	4542	rBV5	57041	139590	3.61%	0.652%
45	16.441	4563	4572	4586	rVB6	19148	44814	1.16%	0.209%

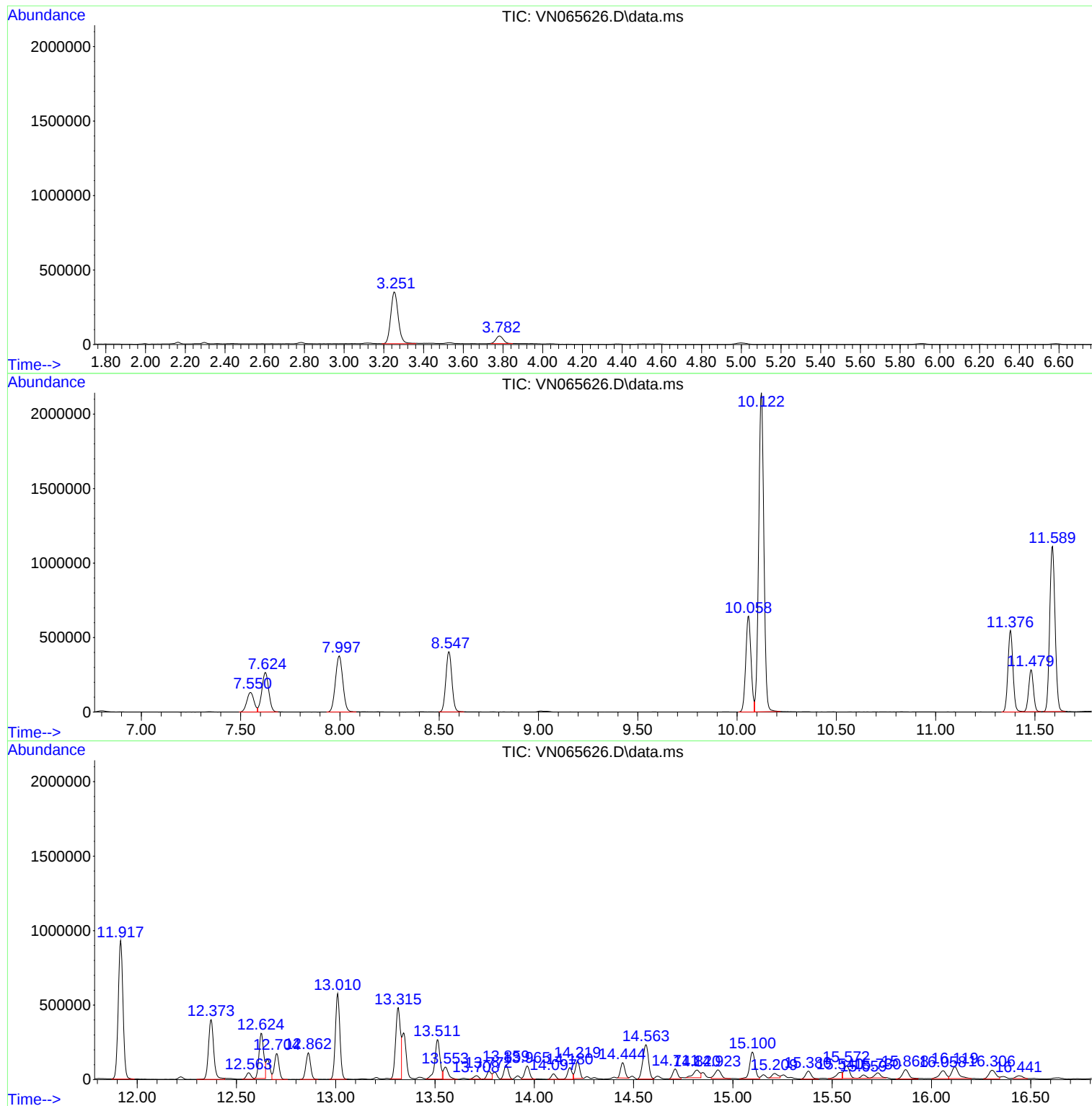
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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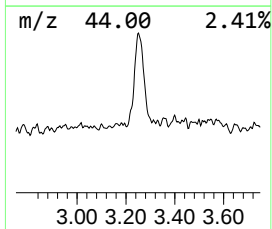
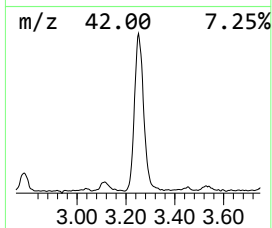
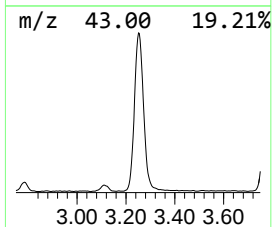
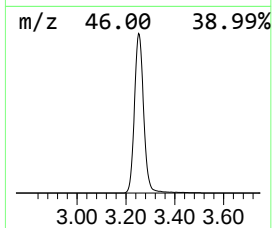
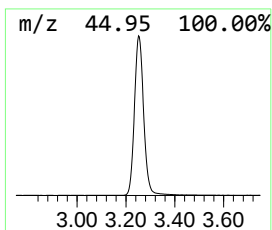
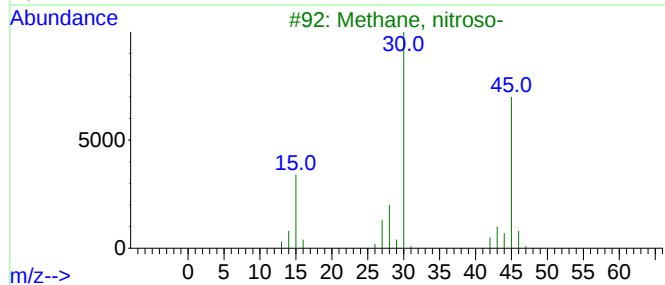
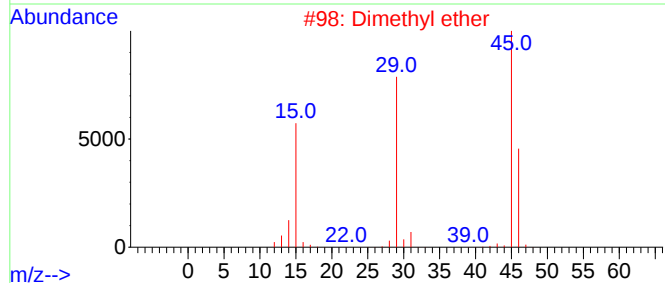
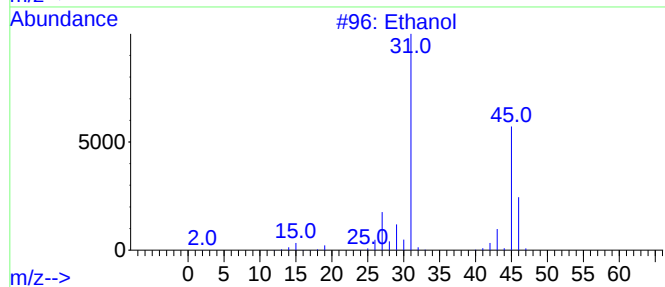
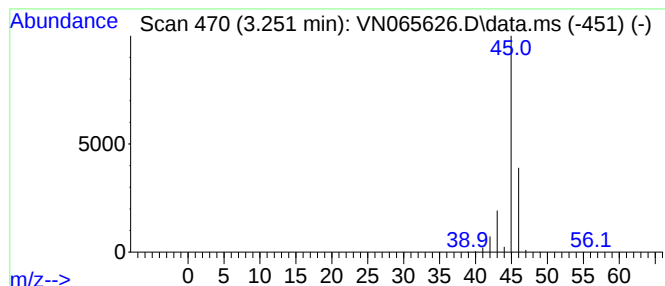
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.251	71.98 ug/l	910737	Pentafluorobenzene	7.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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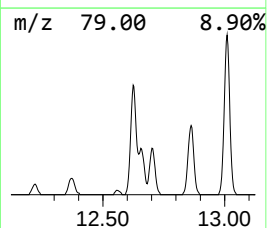
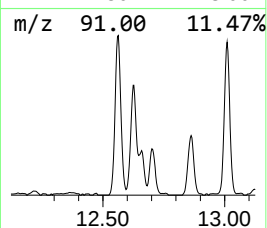
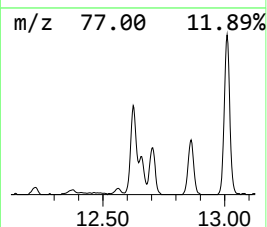
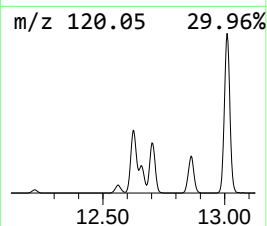
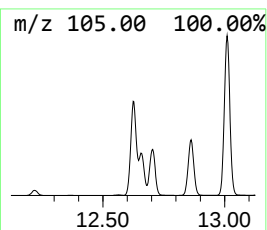
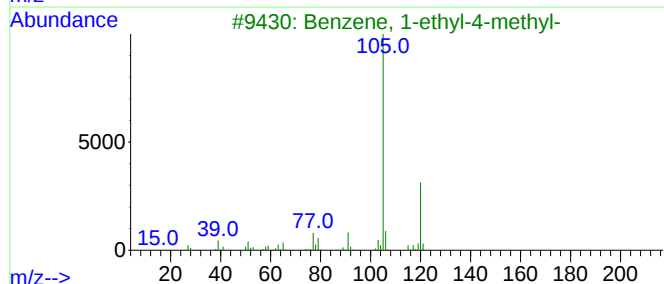
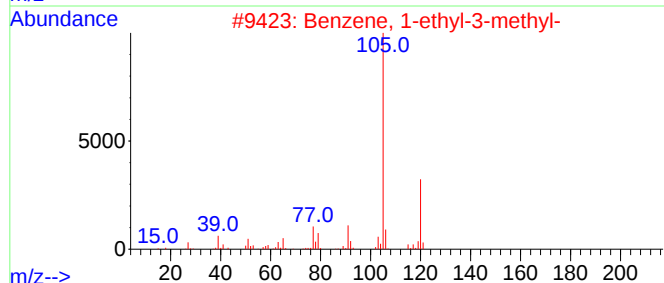
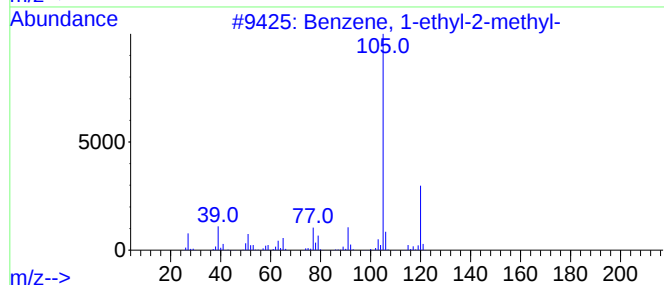
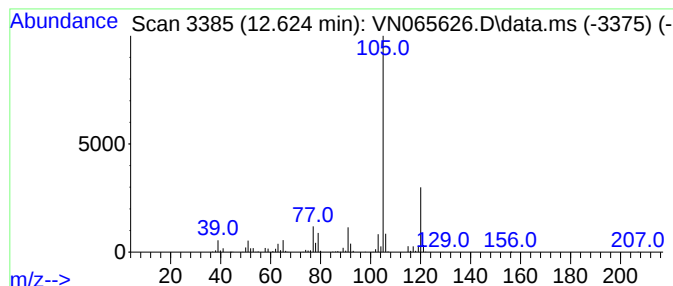
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.624	30.32 ug/l	500226	1,4-Dichlorobenzene-d4	13.315

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



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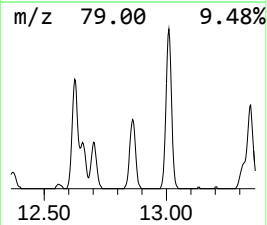
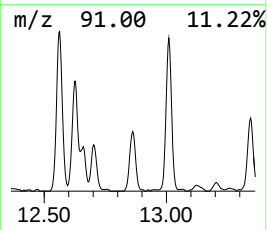
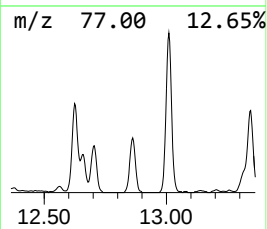
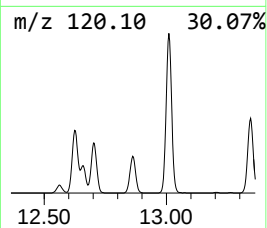
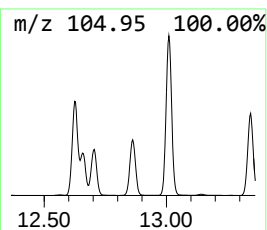
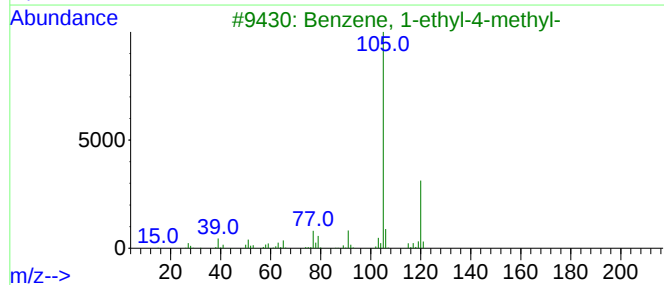
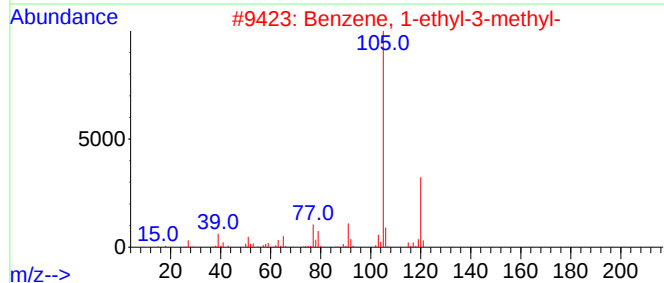
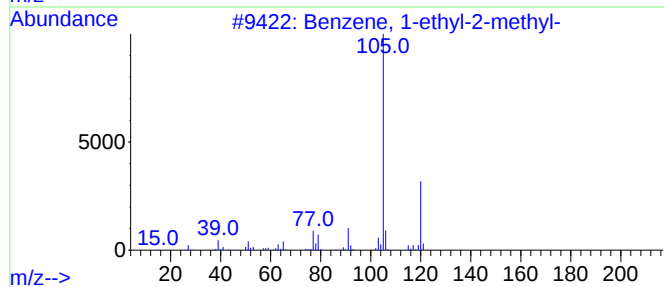
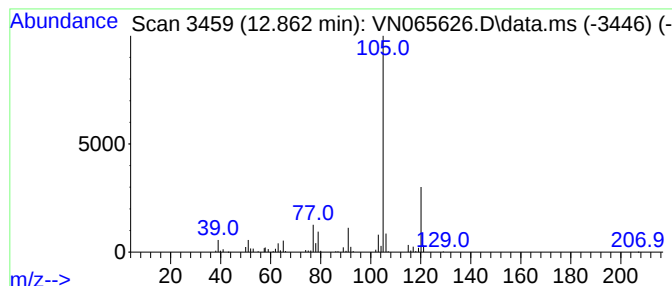
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.862	17.60 ug/l	290461	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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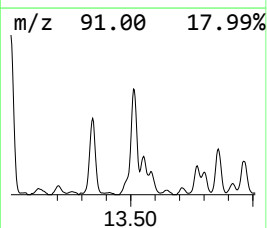
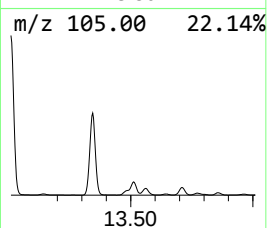
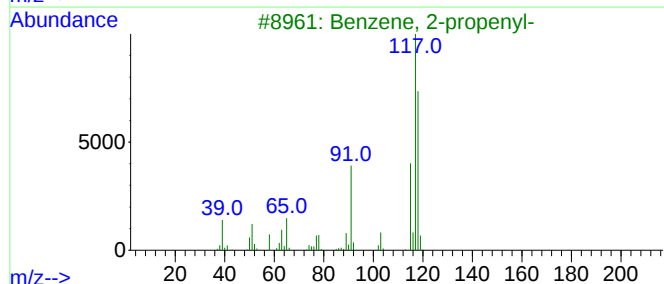
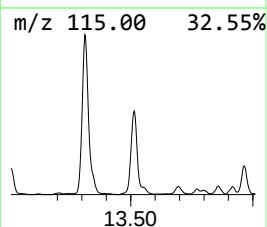
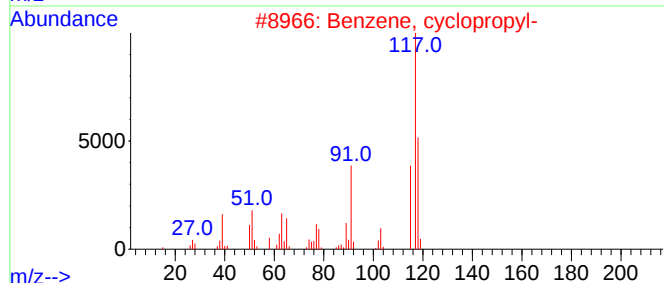
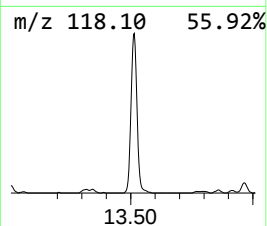
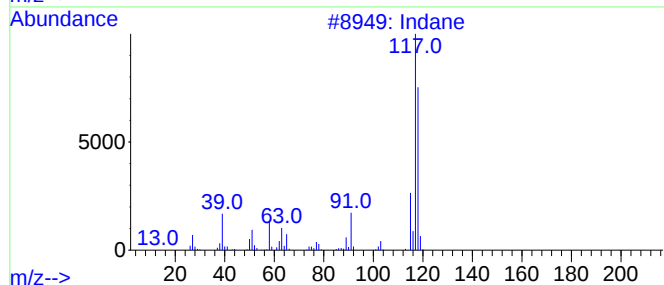
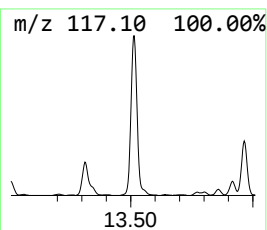
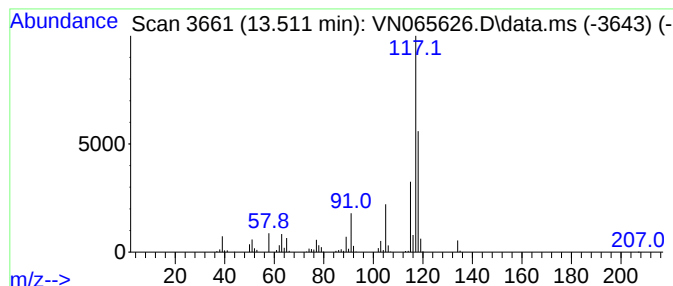
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Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.511	28.87 ug/l	476352	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
3			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	68
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64



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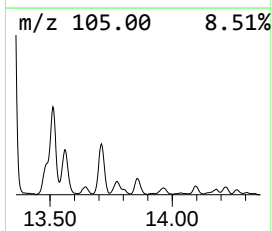
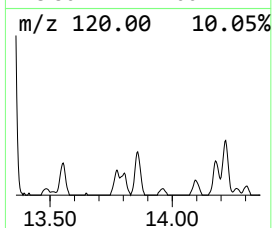
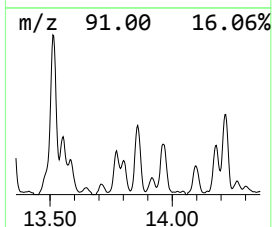
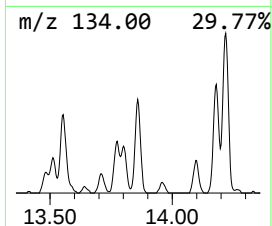
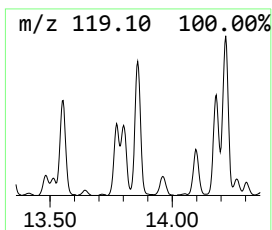
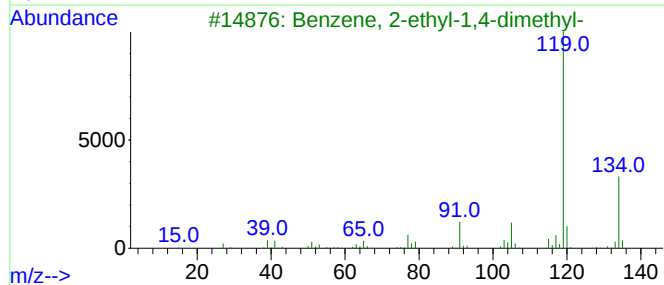
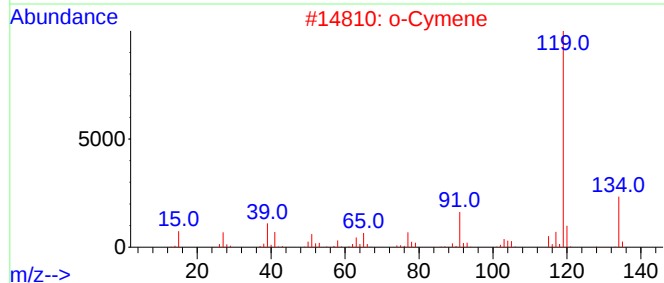
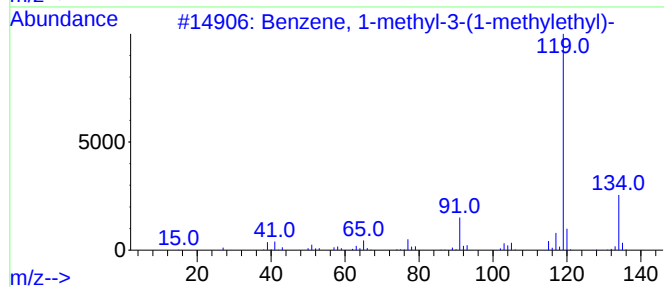
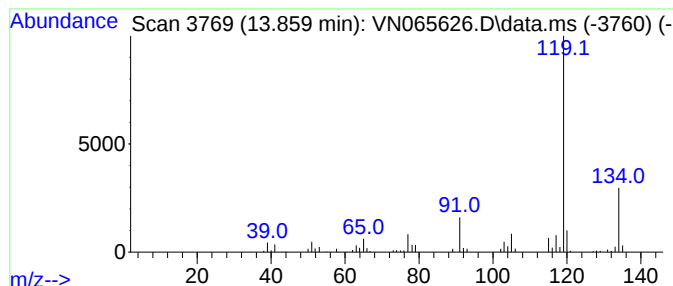
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-methyl-3-(1-meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.859	8.65 ug/l	142765	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	97
2			o-Cymene	134	C10H14	000527-84-4	97
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5			p-Cymene	134	C10H14	000099-87-6	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065626.D
Acq On : 27 Jan 2021 13:46
Operator : JC/MD
Sample : M1190-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41053

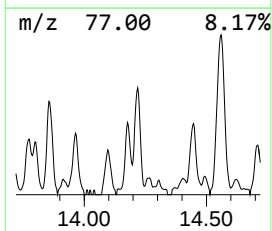
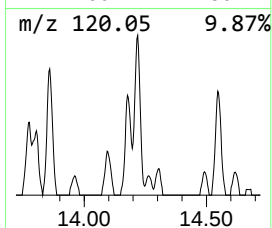
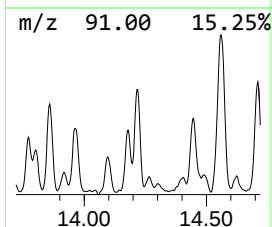
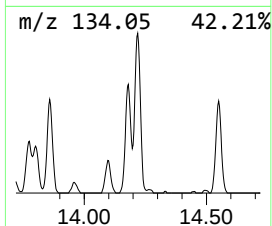
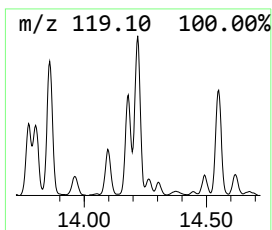
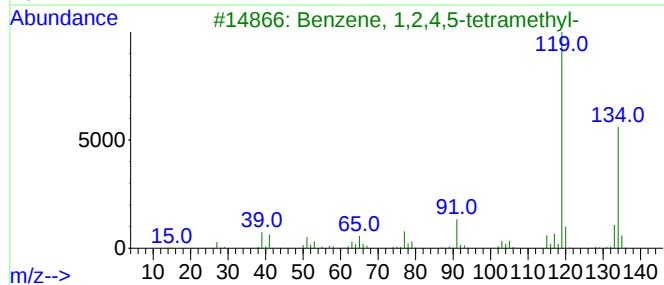
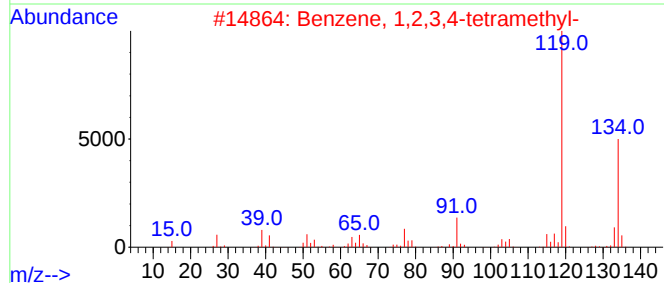
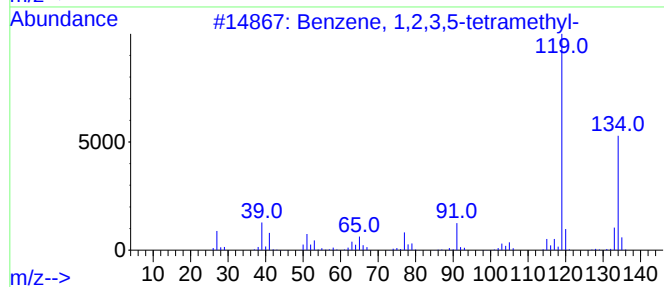
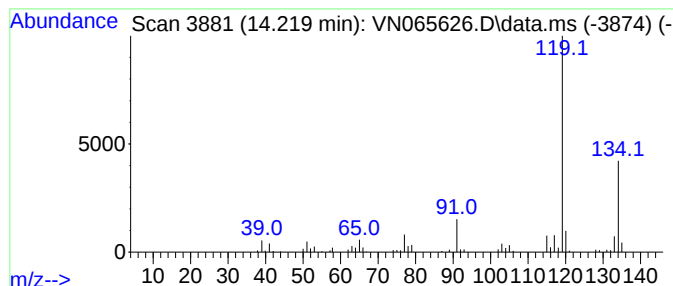
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	10.59 ug/l	174717	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	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4			o-Cymene	134	C10H14	000527-84-4	93
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065626.D
Acq On : 27 Jan 2021 13:46
Operator : JC/MD
Sample : M1190-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41053

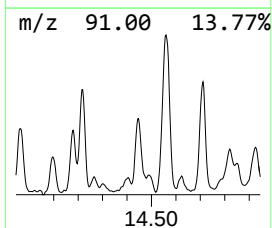
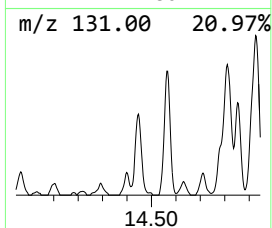
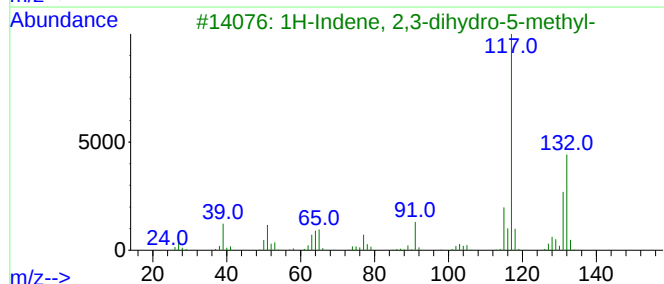
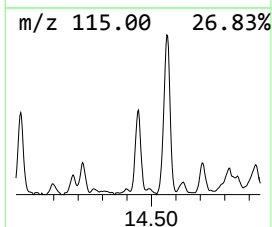
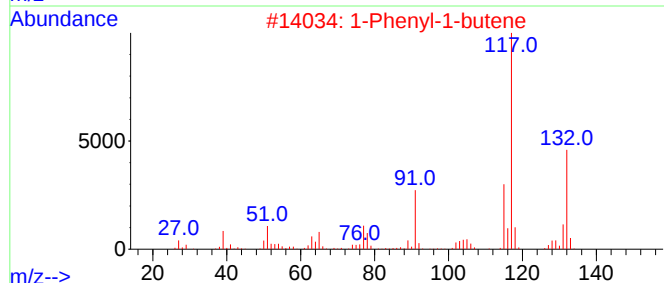
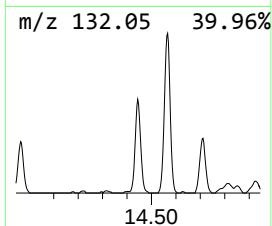
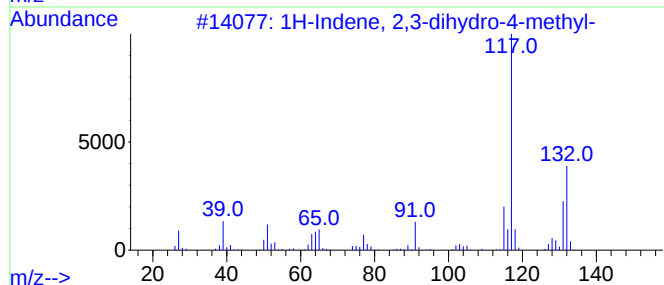
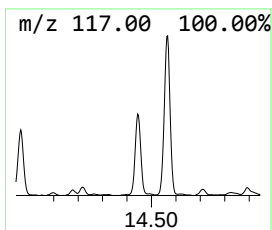
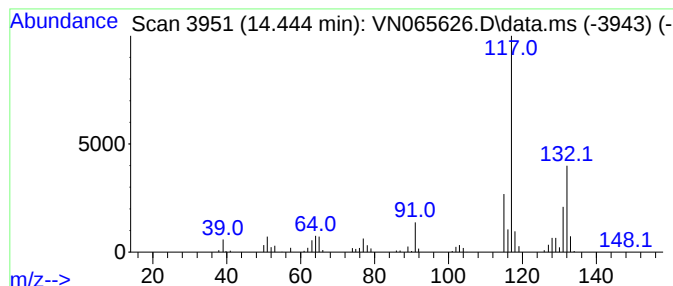
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Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.444	9.45 ug/l	155963	1,4-Dichlorobenzene-d4	13.315

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	94
2		1-Phenyl-1-butene	132	C10H12	000824-90-8	90
3		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
5		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065626.D
Acq On : 27 Jan 2021 13:46
Operator : JC/MD
Sample : M1190-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41053

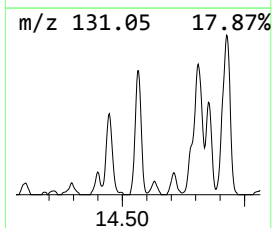
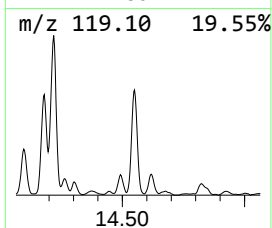
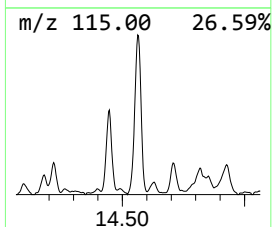
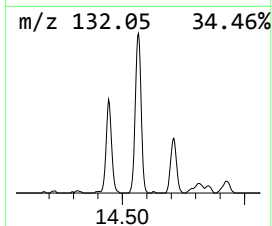
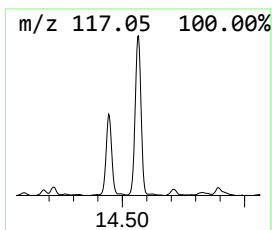
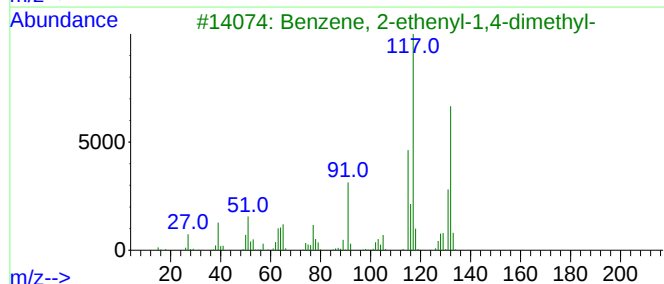
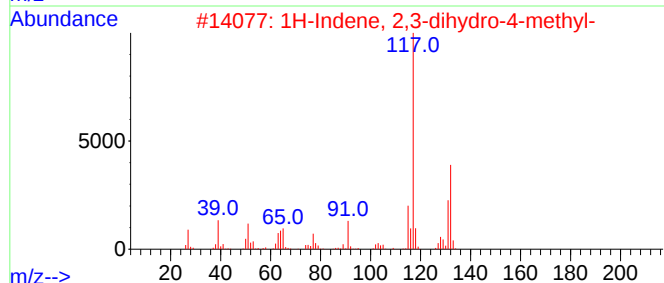
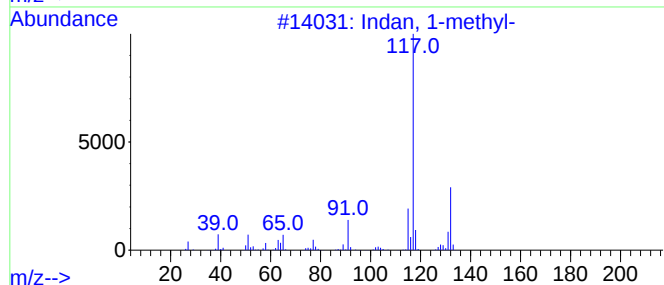
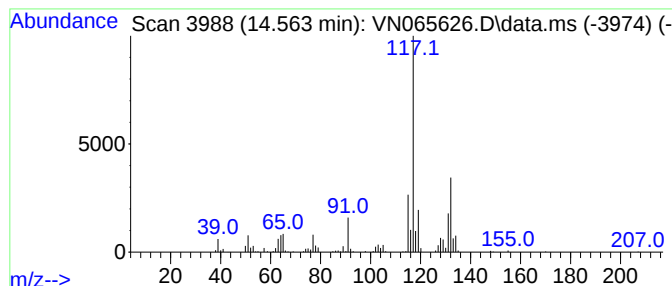
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Quant Title : SW846 8260

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

Peak Number 8 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.563	27.72 ug/l	457376	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	93
2			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065626.D
Acq On : 27 Jan 2021 13:46
Operator : JC/MD
Sample : M1190-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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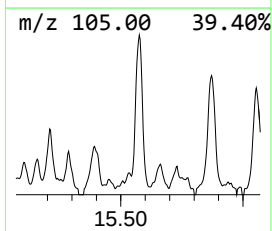
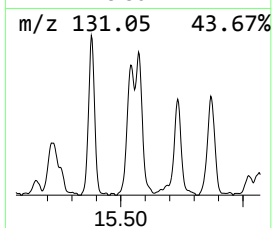
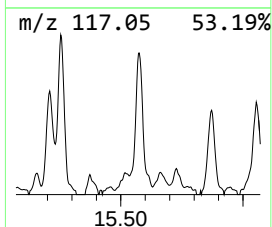
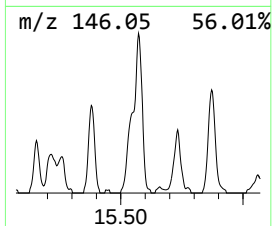
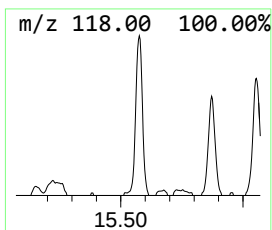
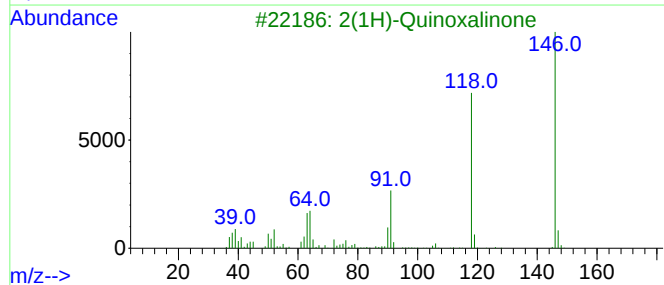
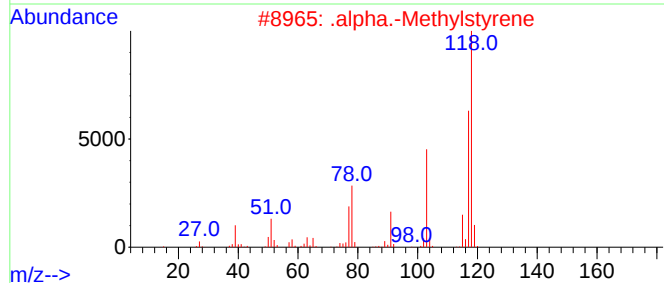
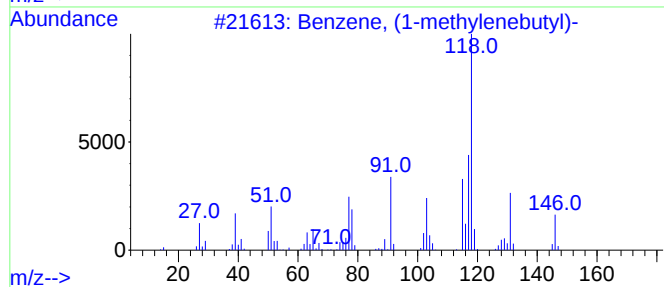
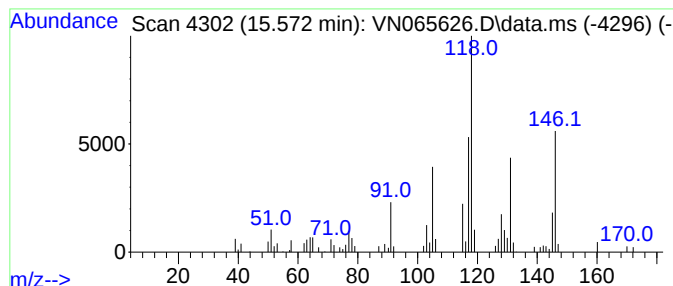
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, (1-methylenebutyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.572	9.64 ug/l	159079	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	83
2			.alpha.-Methylstyrene	118	C9H10	000098-83-9	43
3			2(1H)-Quinoxalinone	146	C8H6N2O	001196-57-2	38
4			1H-Tetrazole, 5-phenyl-	146	C7H6N4	018039-42-4	38
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065626.D
Acq On : 27 Jan 2021 13:46
Operator : JC/MD
Sample : M1190-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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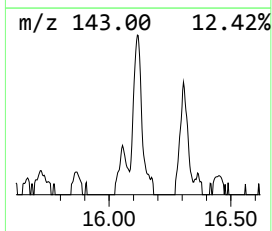
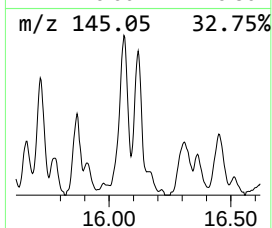
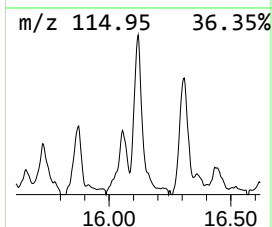
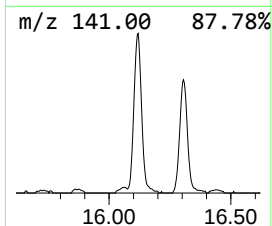
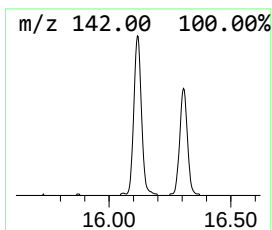
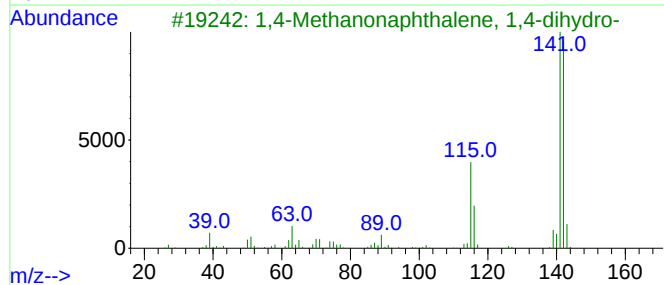
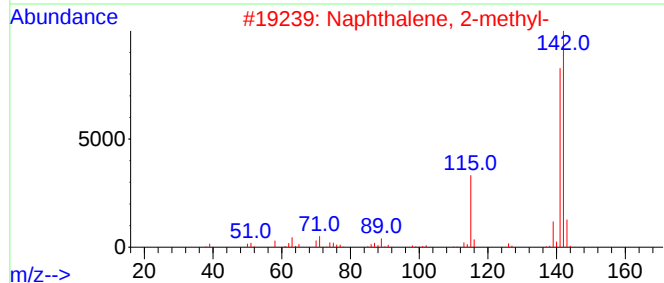
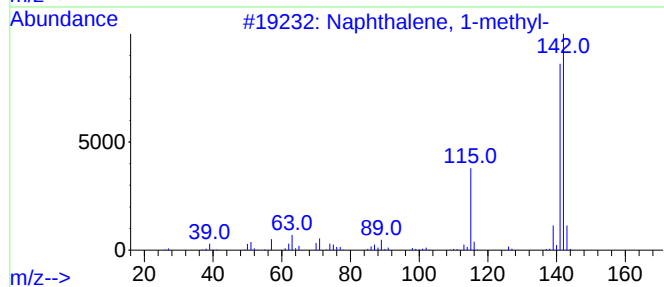
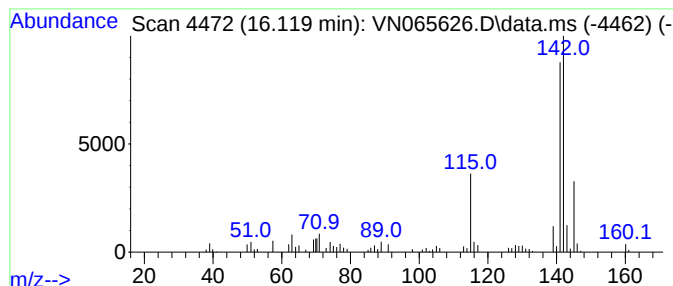
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.119	11.48 ug/l	189463	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	87
5			Benzocycloheptatriene	142	C11H10	000264-09-5	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
Data File : VN065626.D
Acq On : 27 Jan 2021 13:46
Operator : JC/MD
Sample : M1190-05
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41053

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
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Benzene, 1-ethy...	12.624	30.3	ug/l	500226	4	13.315	825044	50.0
Benzene, 1-ethy...	12.862	17.6	ug/l	290461	4	13.315	825044	50.0
Indane	13.511	28.9	ug/l	476352	4	13.315	825044	50.0
Benzene, 1-meth...	13.859	8.7	ug/l	142765	4	13.315	825044	50.0
Benzene, 1,2,3,...	14.219	10.6	ug/l	174717	4	13.315	825044	50.0
1H-Indene, 2,3-...	14.444	9.4	ug/l	155963	4	13.315	825044	50.0
Indan, 1-methyl-	14.563	27.7	ug/l	457376	4	13.315	825044	50.0
Benzene, (1-met...	15.572	9.6	ug/l	159079	4	13.315	825044	50.0
Naphthalene, 1-...	16.119	11.5	ug/l	189463	4	13.315	825044	50.0