

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
 Data File : VN069922.D
 Acq On : 9 Dec 2021 19:44
 Operator : JC/MD
 Sample : M4969-07
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-28D

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN069922.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.445	157	170	193	rVB	1292725	2104511	2.68%	0.497%
2	3.145	411	431	464	rBV	4993861	11424322	14.54%	2.698%
3	3.521	549	571	605	rBV4	1870745	5495671	6.99%	1.298%
4	3.996	725	748	784	rVB	2867448	7762736	9.88%	1.833%
5	4.964	1076	1109	1130	rBV2	590640	2036898	2.59%	0.481%
6	5.082	1132	1153	1164	rBV2	654865	2145499	2.73%	0.507%
7	5.374	1239	1262	1317	rVB	2490479	8861637	11.27%	2.093%
8	5.621	1326	1354	1400	rVB	2078905	7323658	9.32%	1.730%
9	5.935	1446	1471	1502	rVB2	381398	1225565	1.56%	0.289%
10	6.471	1642	1671	1700	rBV2	2094727	6758669	8.60%	1.596%
11	6.611	1701	1723	1741	rVV2	1339127	4241337	5.40%	1.002%
12	6.699	1743	1756	1776	rVV	670983	2019935	2.57%	0.477%
13	6.801	1778	1794	1811	rVV2	372310	1116151	1.42%	0.264%
14	6.906	1812	1833	1870	rVB2	1581421	4722959	6.01%	1.115%
15	7.150	1899	1924	1942	rBV	5640085	16651381	21.19%	3.932%
16	7.844	2167	2183	2207	rVB	2552207	6290311	8.00%	1.486%
17	8.021	2225	2249	2260	rBV2	987893	2543468	3.24%	0.601%
18	8.094	2260	2276	2295	rVB2	4110151	10292129	13.09%	2.431%
19	8.461	2388	2413	2433	rBV2	32521425	78597186	100.00%	18.562%
20	8.587	2450	2460	2474	rVB2	1790673	3609369	4.59%	0.852%
21	8.705	2496	2504	2526	rVB5	451915	1046346	1.33%	0.247%
22	8.802	2528	2540	2580	rVB5	244623	786616	1.00%	0.186%
23	8.968	2580	2602	2616	rBV4	4303692	10005676	12.73%	2.363%
24	9.199	2674	2688	2696	rVV	668484	1360589	1.73%	0.321%
25	9.244	2697	2705	2726	rVB	902091	1801435	2.29%	0.425%
26	9.459	2752	2785	2803	rBV2	1653494	4800133	6.11%	1.134%
27	9.802	2897	2913	2917	rBV3	632411	1153625	1.47%	0.272%
28	9.971	2959	2976	2988	rBV	2113384	4090372	5.20%	0.966%
29	10.202	3046	3062	3068	rBV2	1002277	1958877	2.49%	0.463%
30	10.322	3093	3107	3121	rBV	1668502	2987982	3.80%	0.706%
31	10.440	3135	3151	3164	rBV	4680907	8735905	11.11%	2.063%
32	10.505	3165	3175	3184	rVV	1529300	2837359	3.61%	0.670%
33	10.550	3185	3192	3207	rVB	861601	1484749	1.89%	0.351%
34	10.856	3293	3306	3327	rVB2	731074	1483421	1.89%	0.350%
35	11.130	3397	3408	3421	rVB	1873944	3159866	4.02%	0.746%
36	11.612	3560	3588	3616	rBV4	466398	1685177	2.14%	0.398%

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37	11.744	3619	3637	3663	rBV	5651007	11097020	14.12%	2.621%
38	11.846	3664	3675	3695	rVB2	982398	2154441	2.74%	0.509%
39	11.948	3696	3713	3739	rBV	14273687	27592963	35.11%	6.516%
40	12.087	3755	3765	3790	rVB6	489238	998630	1.27%	0.236%
41	12.280	3825	3837	3852	rVB	846035	1508725	1.92%	0.356%
42	12.578	3934	3948	3963	rVB	5462621	9082866	11.56%	2.145%
43	12.731	3989	4005	4030	rVB	4377338	7936591	10.10%	1.874%
44	12.919	4061	4075	4093	rVB	12629191	20856000	26.54%	4.925%
45	13.058	4119	4127	4144	rVB	786824	1330110	1.69%	0.314%
46	13.219	4172	4187	4213	rBV	2677819	4643863	5.91%	1.097%
47	13.498	4275	4291	4304	rVB2	455696	1064016	1.35%	0.251%
48	13.672	4342	4356	4364	rBV	4639619	8451443	10.75%	1.996%
49	13.838	4405	4418	4420	rBV	2141660	2726212	3.47%	0.644%
50	13.876	4421	4432	4467	rVV	21941834	39235665	49.92%	9.266%
51	14.069	4491	4504	4517	rVB	823180	1361249	1.73%	0.321%
52	14.214	4544	4558	4571	rBV	4526166	7205742	9.17%	1.702%
53	14.278	4571	4582	4589	rVV	1347637	2216325	2.82%	0.523%
54	14.327	4589	4600	4620	rVB	5375321	9021935	11.48%	2.131%
55	14.538	4663	4679	4690	rBV	2266957	3839586	4.89%	0.907%
56	14.807	4767	4779	4793	rBV	3219804	5115811	6.51%	1.208%
57	14.927	4806	4824	4838	rBV3	3709218	7572914	9.64%	1.788%
58	15.083	4869	4882	4898	rBV	745246	1330336	1.69%	0.314%
59	15.193	4901	4923	4934	rBV5	517058	1248470	1.59%	0.295%
60	15.311	4952	4967	4984	rVB3	487269	1185213	1.51%	0.280%
61	15.504	5022	5039	5057	rBV	5324758	10058727	12.80%	2.375%

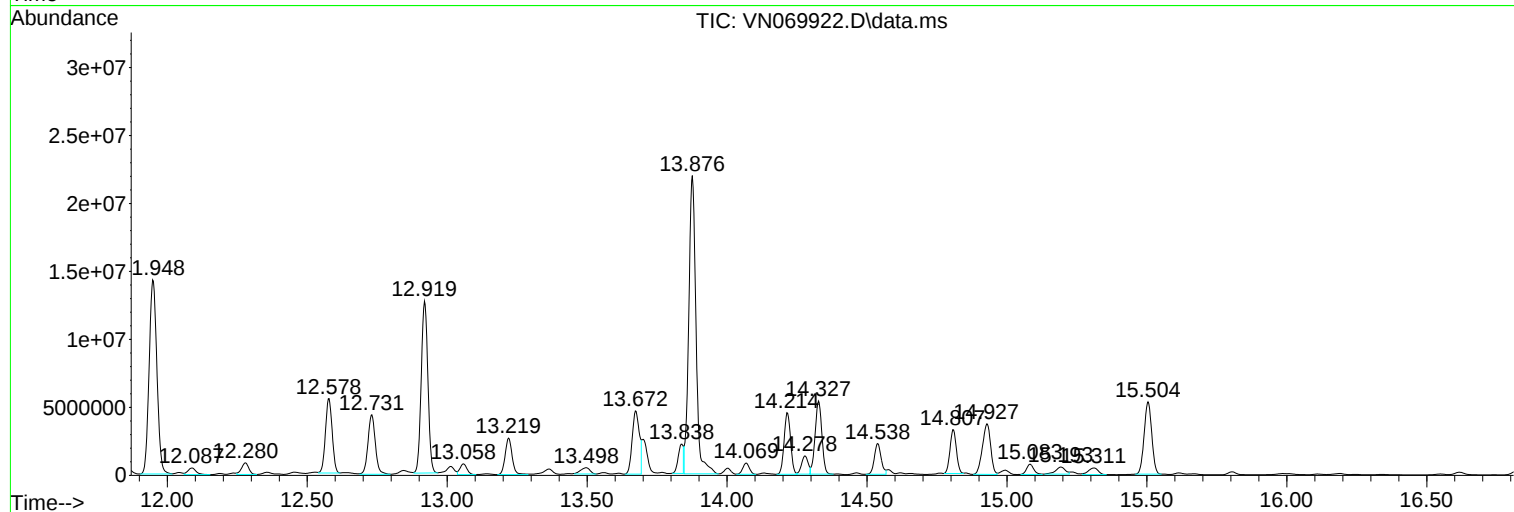
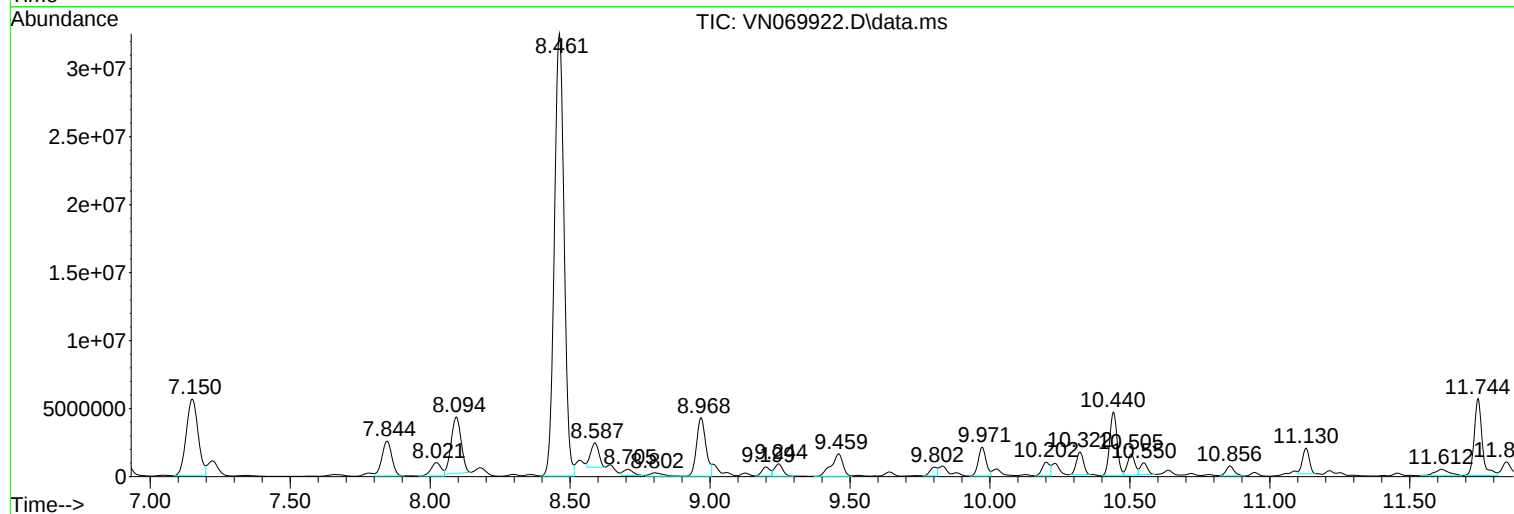
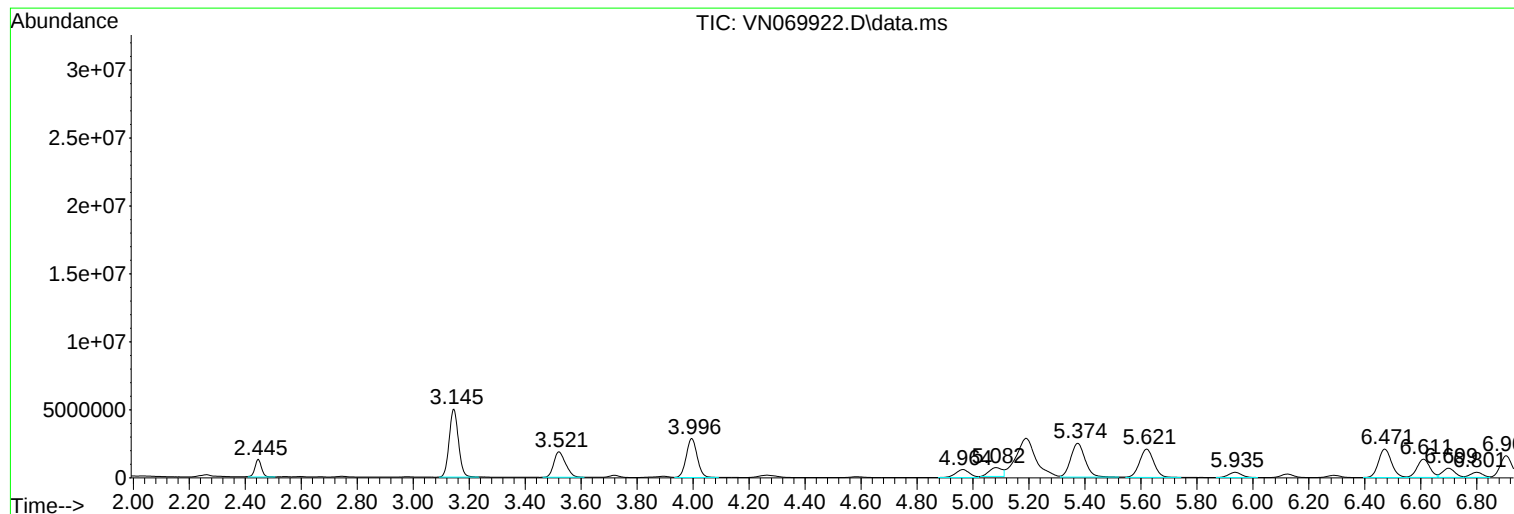
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28D

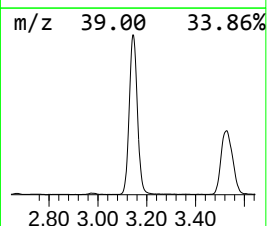
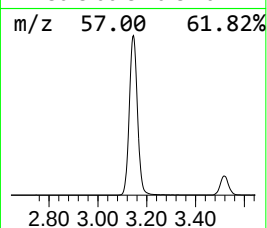
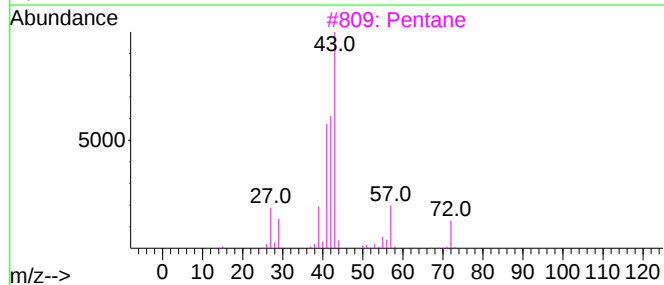
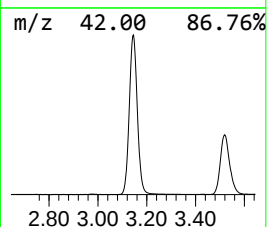
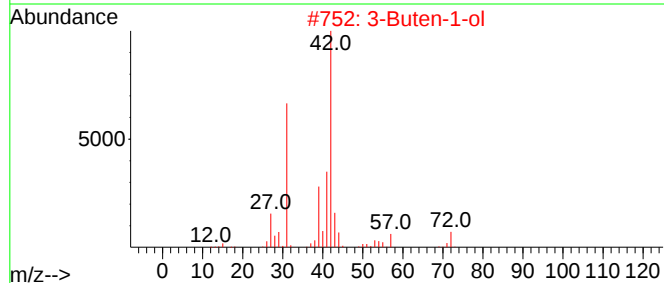
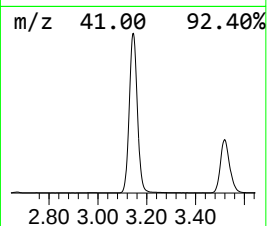
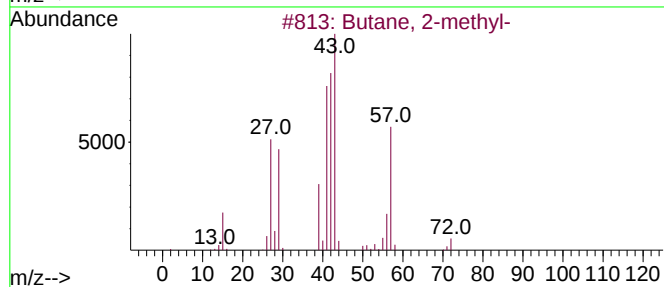
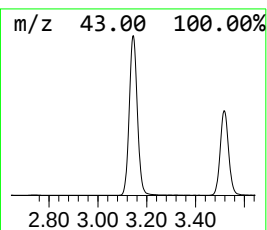
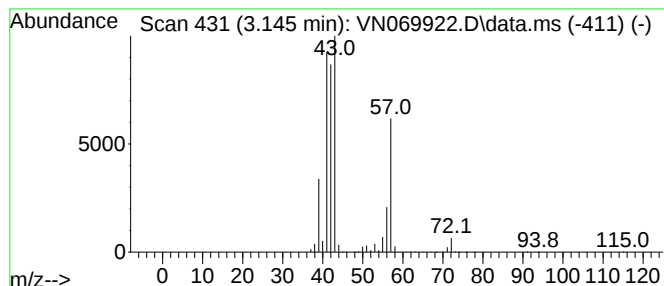
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.145	55.50 ug/l	11424300	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			Azetidine	57	C3H7N	000503-29-7	9
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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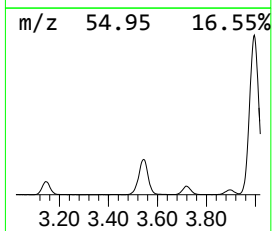
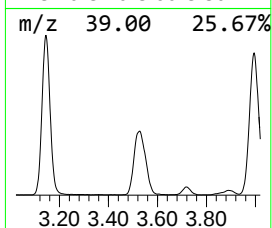
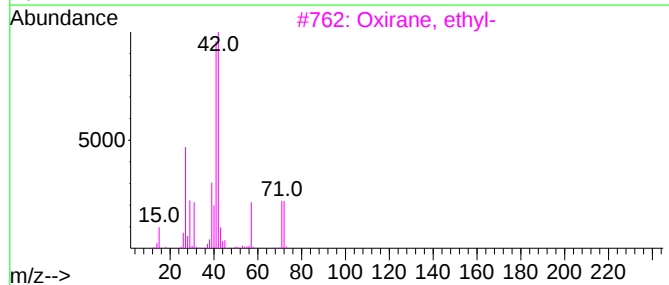
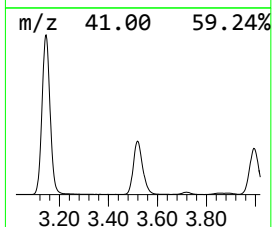
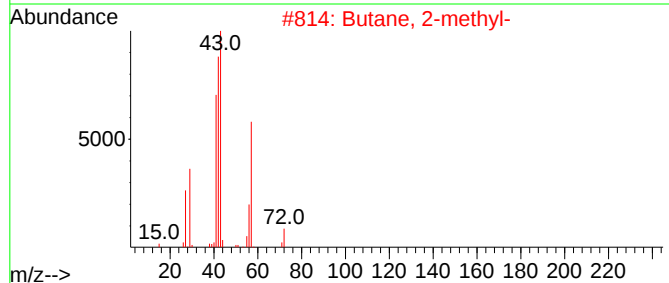
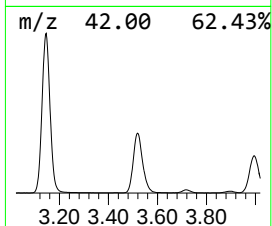
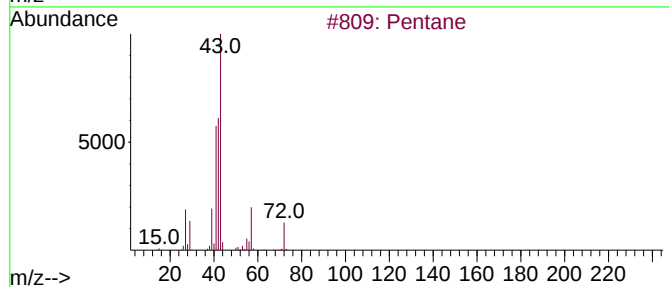
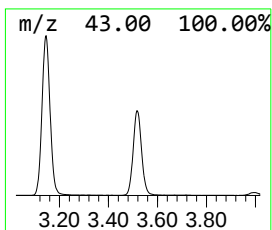
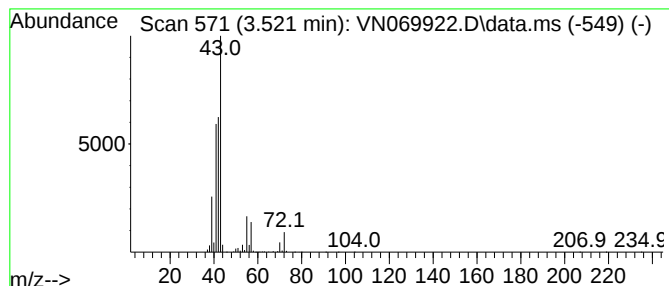
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.521	26.70 ug/l	5495670	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Butane, 2-methyl-	72	C5H12	000078-78-4	45
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	40
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	32
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	17



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28D

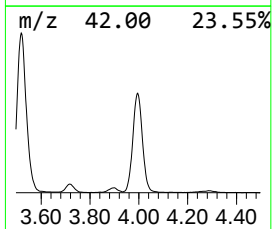
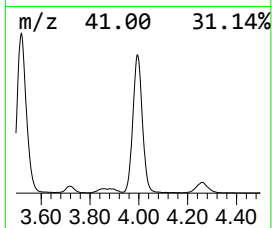
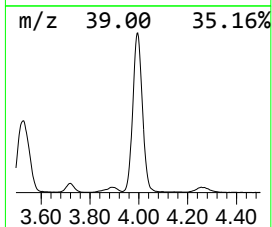
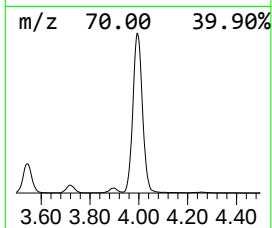
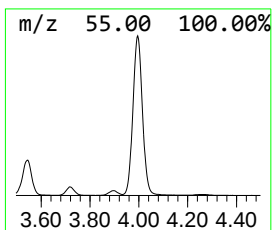
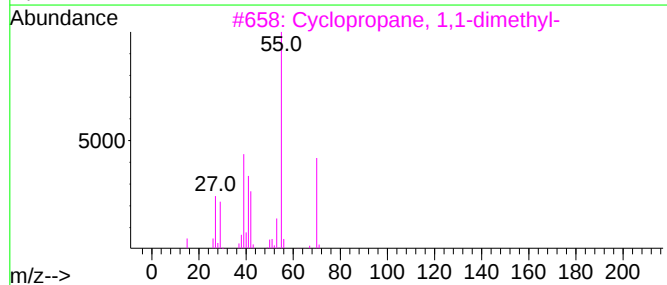
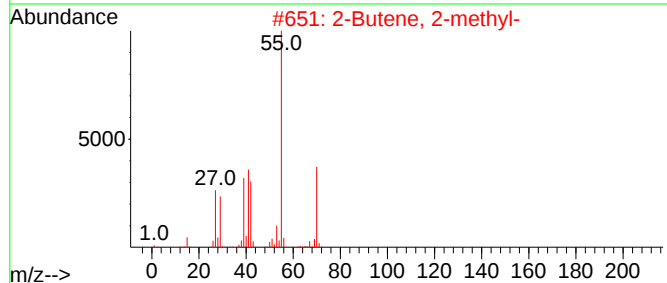
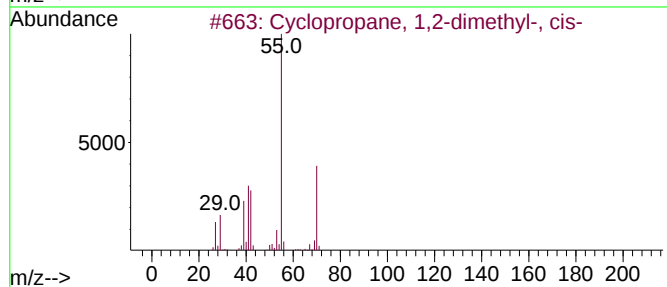
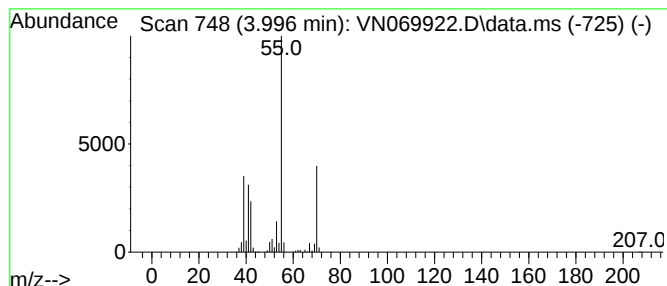
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.996	37.71 ug/l	7762740	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
4			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	86
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	81



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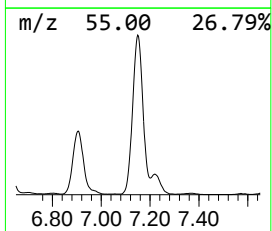
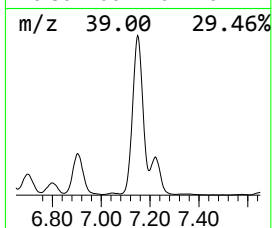
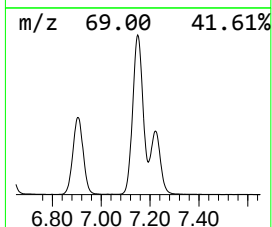
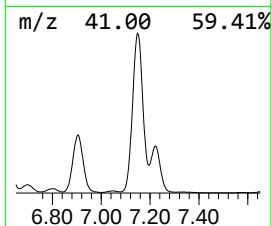
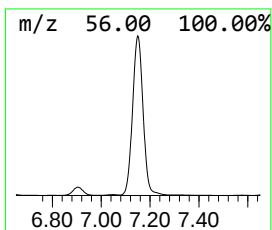
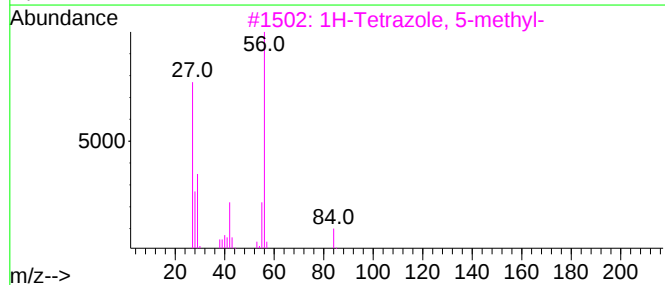
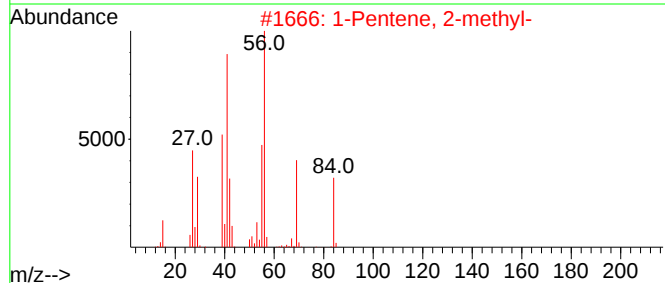
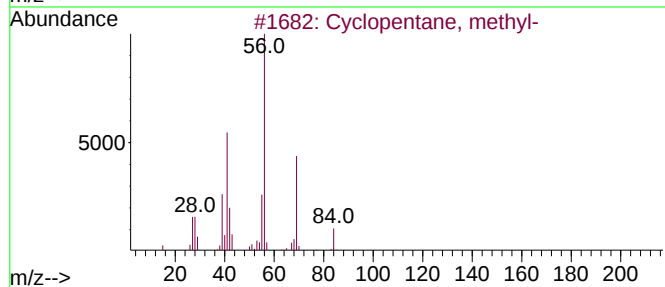
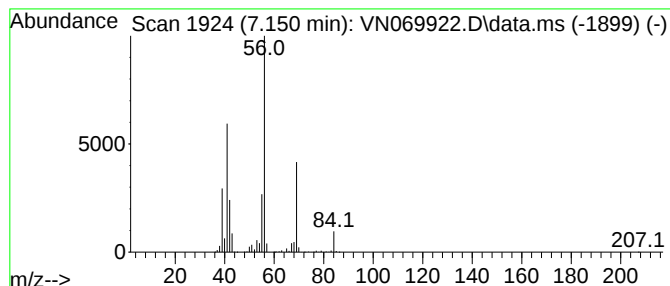
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.150	80.89 ug/l	16651400	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5			Cyclohexane	84	C6H12	000110-82-7	56



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Operator : JC/MD
Sample : M4969-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28D

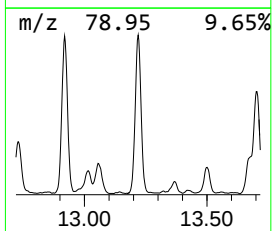
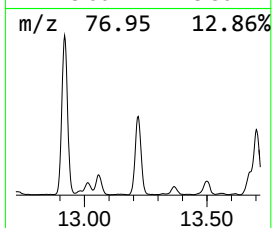
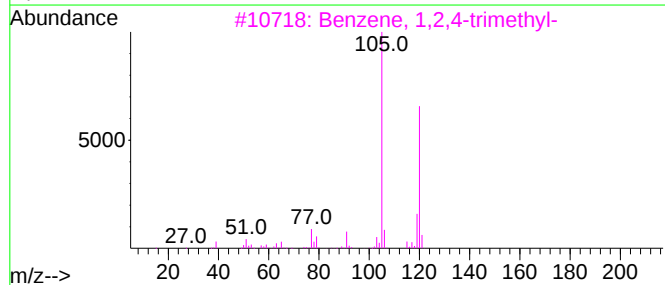
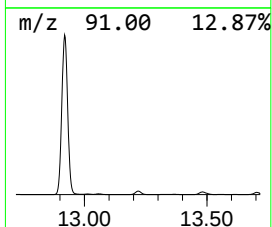
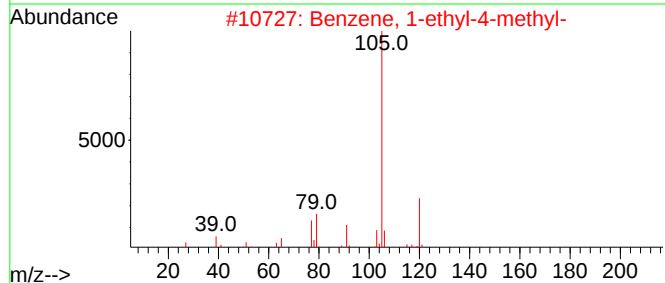
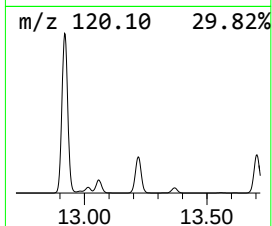
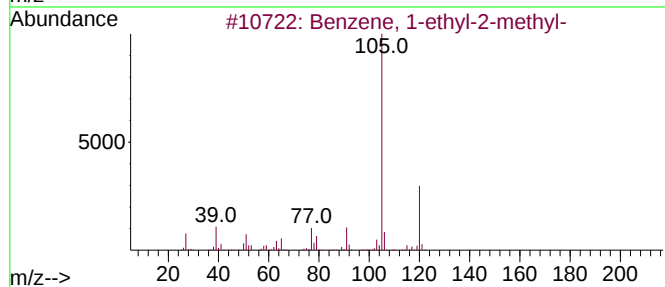
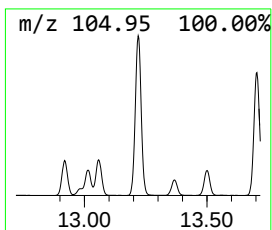
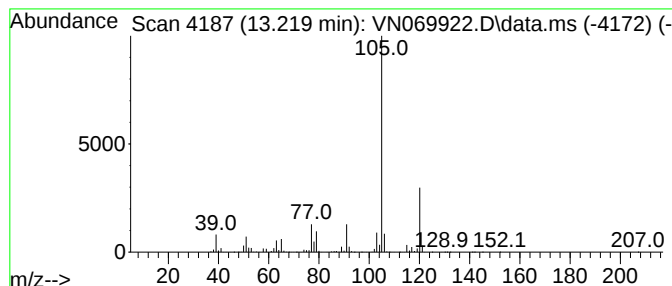
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	27.47 ug/l	4643860	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069922.D
Acq On : 9 Dec 2021 19:44
Operator : JC/MD
Sample : M4969-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28D

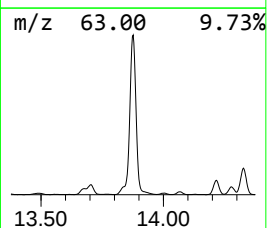
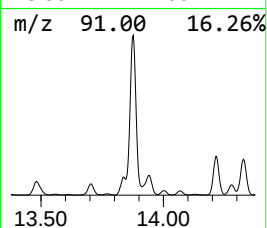
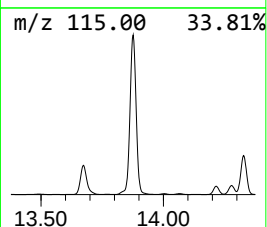
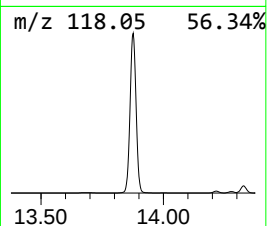
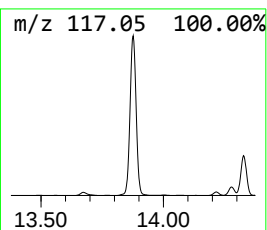
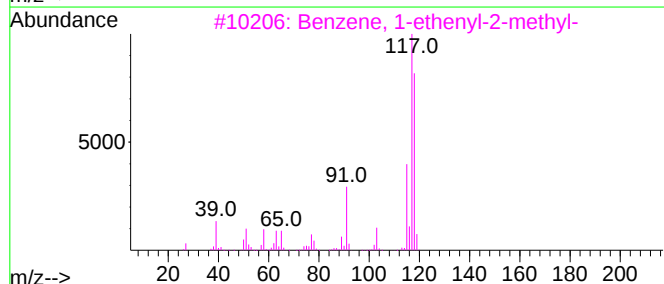
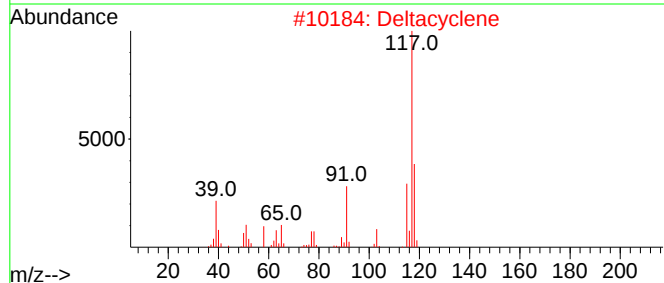
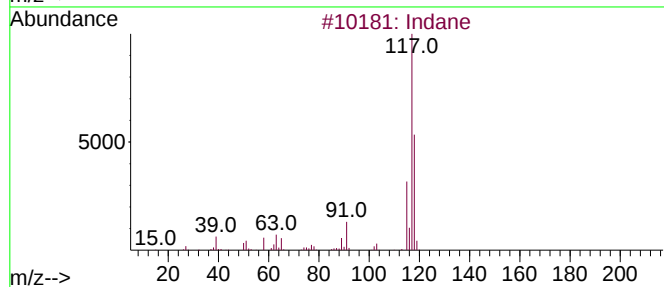
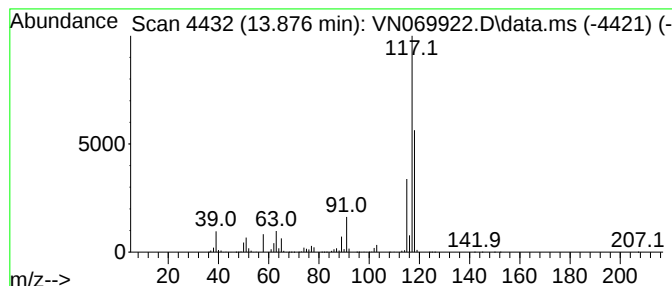
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	232.12 ug/l	39235700	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Deltacyclene	118	C9H10	007785-10-6	64
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
5			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069922.D
Acq On : 9 Dec 2021 19:44
Operator : JC/MD
Sample : M4969-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28D

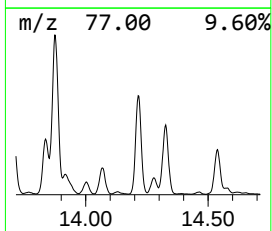
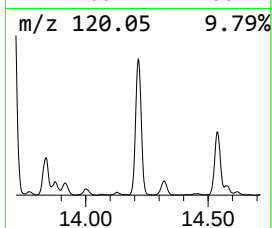
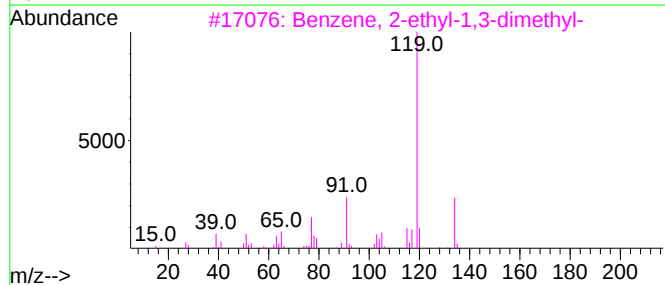
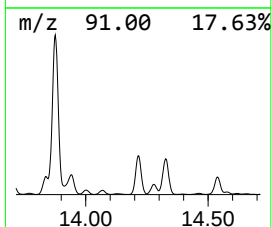
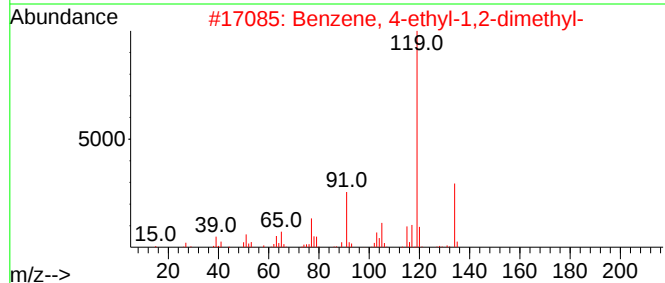
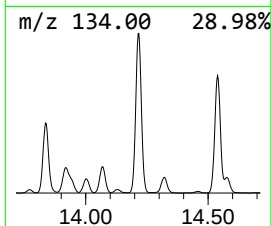
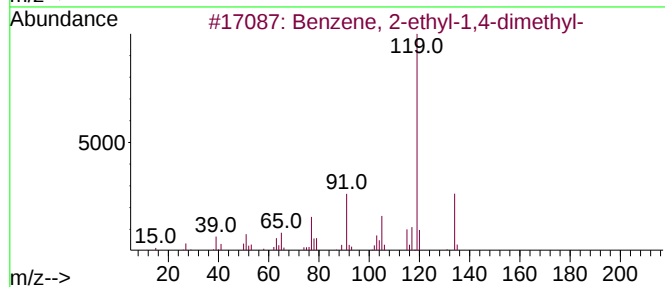
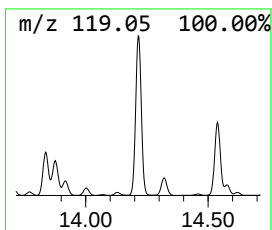
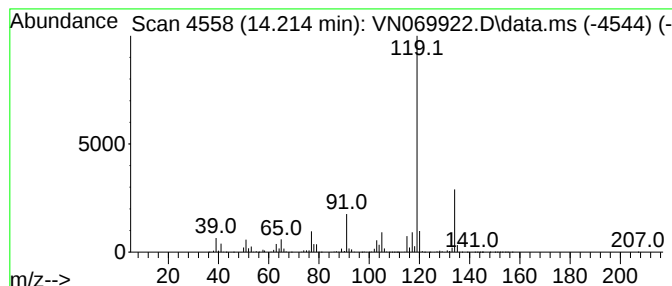
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	42.63 ug/l	7205740	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
2			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069922.D
Acq On : 9 Dec 2021 19:44
Operator : JC/MD
Sample : M4969-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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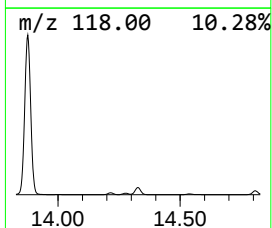
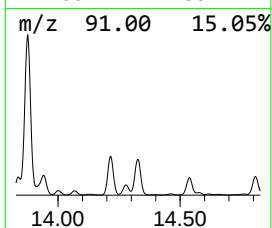
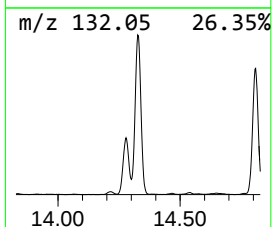
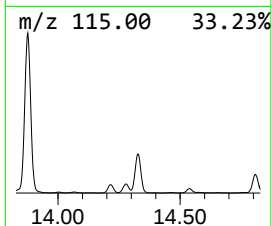
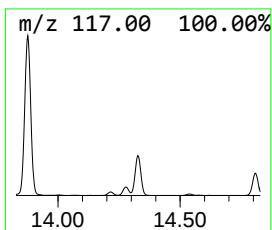
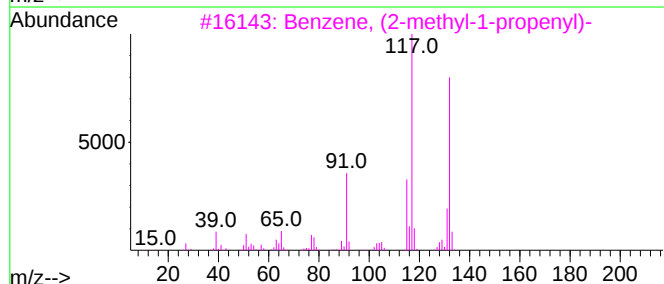
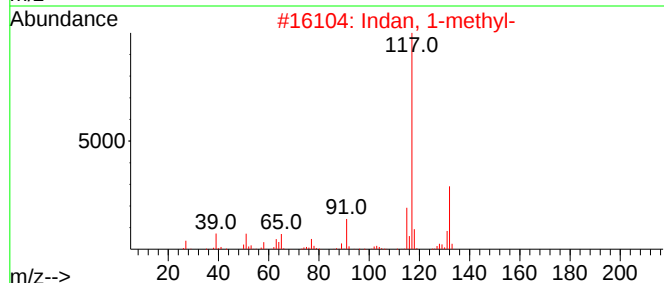
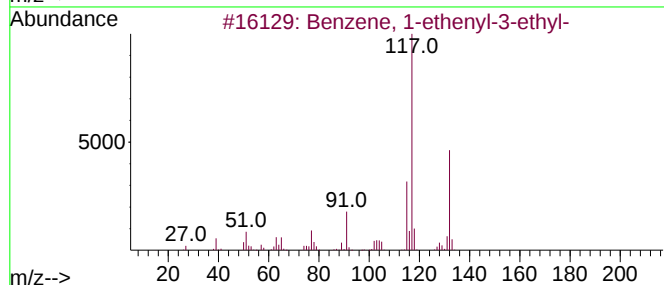
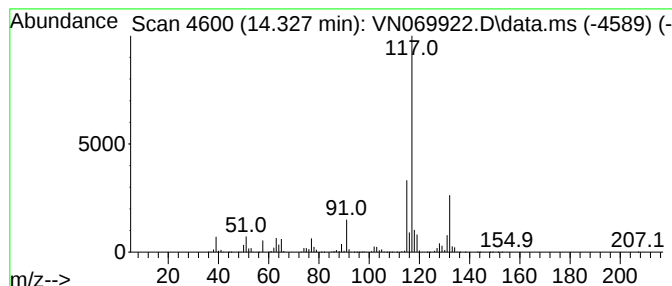
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	53.38 ug/l	9021940	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Indan, 1-methyl-	132	C10H12	000767-58-8	87
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
4			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069922.D
Acq On : 9 Dec 2021 19:44
Operator : JC/MD
Sample : M4969-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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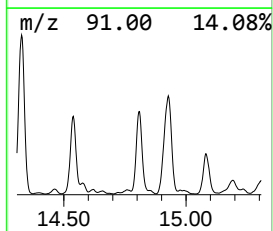
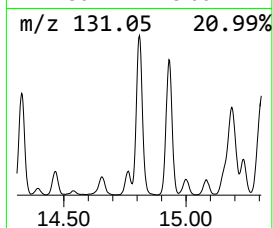
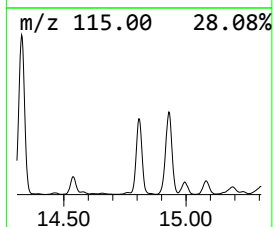
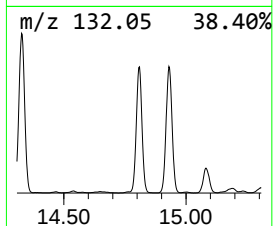
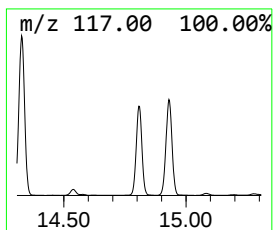
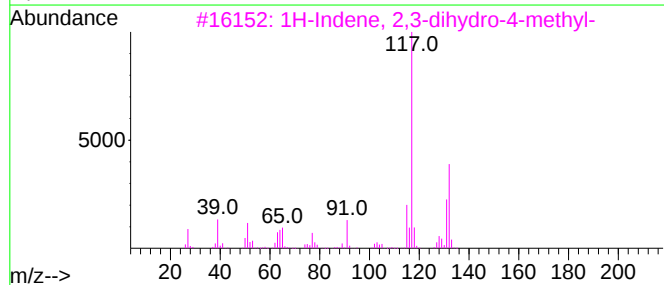
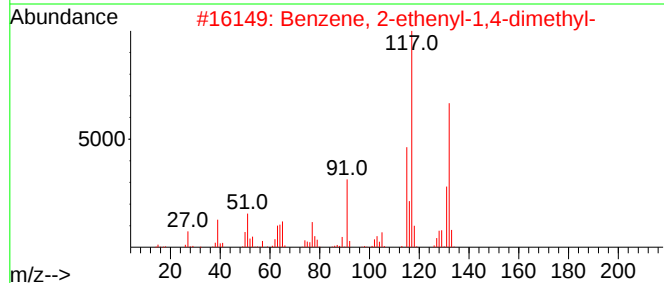
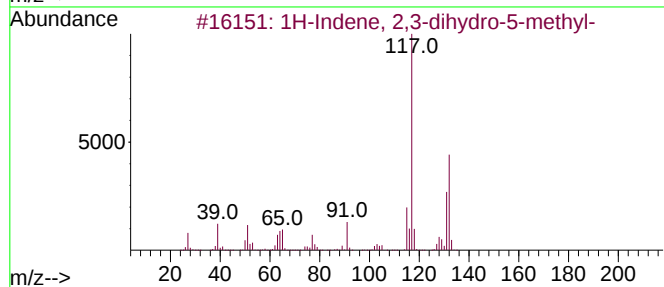
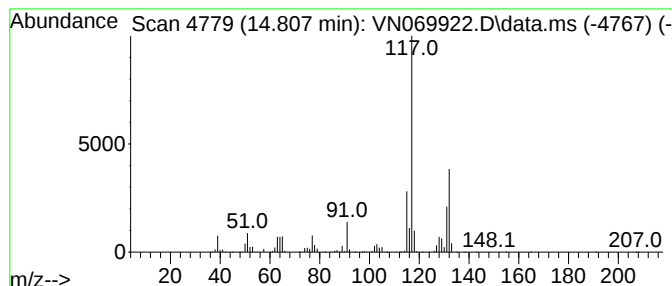
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.807	30.27 ug/l	5115810	1,4-Dichlorobenzene-d4	13.672

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	96
2		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
3		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	95
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
5		3-Phenylbut-1-ene	132	C10H12	000934-10-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069922.D
Acq On : 9 Dec 2021 19:44
Operator : JC/MD
Sample : M4969-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28D

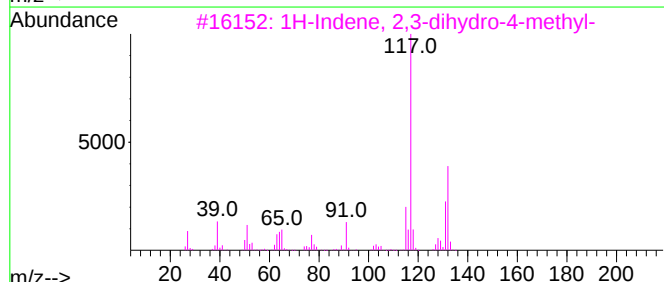
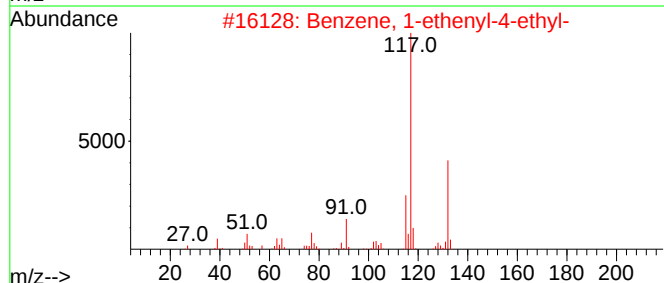
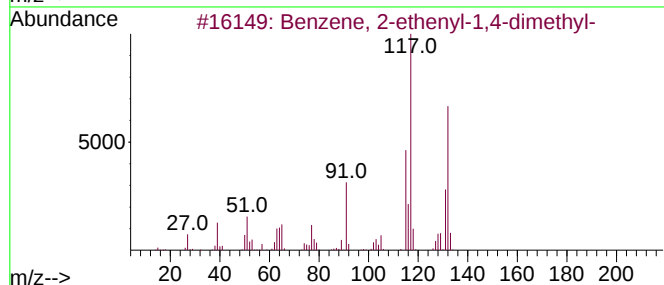
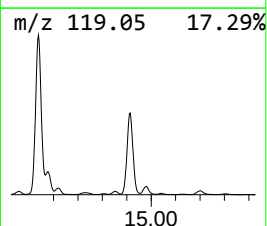
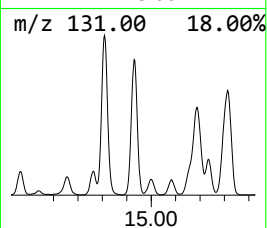
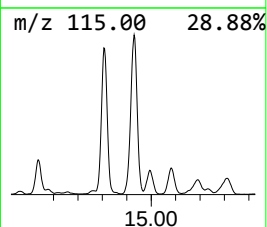
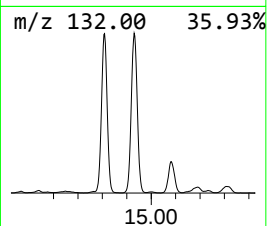
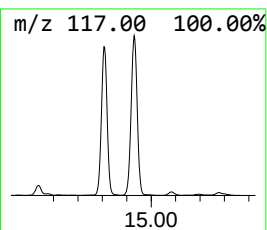
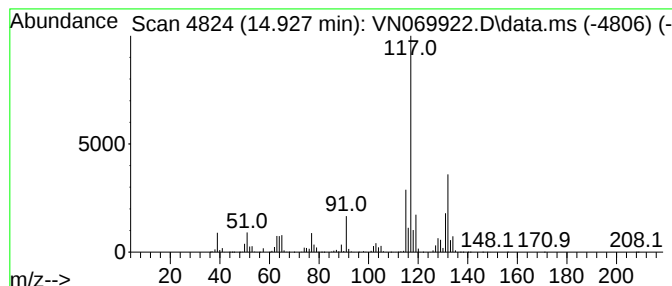
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	44.80 ug/l	7572910	1,4-Dichlorobenzene-d4	13.672

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
4		1-Phenyl-1-butene	132	C10H12	000824-90-8	91
5		Indan, 1-methyl-	132	C10H12	000767-58-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120921\
Data File : VN069922.D
Acq On : 9 Dec 2021 19:44
Operator : JC/MD
Sample : M4969-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-28D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Pentane	3.521	26.7	ug/l	5495670	1	8.086	10292100	50.0
Cyclopropane, 1...	3.996	37.7	ug/l	7762740	1	8.086	10292100	50.0
Cyclopentane, m...	7.150	80.9	ug/l	16651400	1	8.086	10292100	50.0
Benzene, 1-ethy...	13.219	27.5	ug/l	4643860	4	13.672	8451440	50.0
Indane	13.876	232.1	ug/l	39235700	4	13.672	8451440	50.0
Benzene, 2-ethy...	14.214	42.6	ug/l	7205740	4	13.672	8451440	50.0
Benzene, 1-ethe...	14.327	53.4	ug/l	9021940	4	13.672	8451440	50.0
1H-Indene, 2,3-...	14.807	30.3	ug/l	5115810	4	13.672	8451440	50.0
Benzene, 2-ethe...	14.927	44.8	ug/l	7572910	4	13.672	8451440	50.0