

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
 Data File : VN070085.D
 Acq On : 14 Dec 2021 21:22
 Operator : JC/MD
 Sample : M4970-10
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-32

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: VN070085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.260	88	101	113	rBV	335056	538313	6.84%	0.713%
2	2.443	158	169	185	rVB	330623	527680	6.70%	0.699%
3	3.140	411	429	457	rVB	734108	1652953	20.99%	2.189%
4	3.513	556	568	590	rVB3	52636	125820	1.60%	0.167%
5	3.988	723	745	765	rBV4	43542	118786	1.51%	0.157%
6	4.258	820	846	882	rBV6	46025	201925	2.56%	0.267%
7	4.591	947	970	1003	rBV2	94378	318670	4.05%	0.422%
8	5.076	1127	1151	1163	rBV4	104884	364194	4.62%	0.482%
9	5.382	1233	1265	1299	rBV3	211415	766568	9.73%	1.015%
10	5.618	1323	1353	1385	rVB3	308209	1080185	13.72%	1.431%
11	6.498	1648	1681	1708	rBV2	266431	856705	10.88%	1.135%
12	7.147	1899	1923	1948	rBV3	337673	974100	12.37%	1.290%
13	7.327	1973	1990	2016	rVB5	26316	82931	1.05%	0.110%
14	8.024	2226	2250	2260	rBV2	793686	1895332	24.07%	2.510%
15	8.088	2261	2274	2295	rVV2	1703328	4009672	50.91%	5.310%
16	8.177	2296	2307	2332	rVB3	107609	274448	3.48%	0.363%
17	8.300	2335	2353	2363	rBV3	53402	121998	1.55%	0.162%
18	8.359	2364	2375	2386	rVB4	40203	79951	1.02%	0.106%
19	8.456	2387	2411	2430	rBV3	2042761	5823369	73.94%	7.712%
20	8.539	2431	2442	2467	rVV4	211017	616496	7.83%	0.816%
21	8.968	2582	2602	2633	rBV	2446110	5158536	65.50%	6.832%
22	9.429	2754	2774	2776	rBV4	129369	223721	2.84%	0.296%
23	9.639	2842	2852	2869	rVB6	45670	94223	1.20%	0.125%
24	9.880	2933	2942	2961	rVB5	53328	111819	1.42%	0.148%
25	9.974	2961	2977	2984	rBV3	104879	207020	2.63%	0.274%
26	10.017	2986	2993	3011	rVB4	132928	246997	3.14%	0.327%
27	10.202	3047	3062	3072	rBV3	81672	181044	2.30%	0.240%
28	10.443	3133	3152	3173	rBV	3997187	7598234	96.48%	10.063%
29	10.631	3206	3222	3240	rVB10	54828	178497	2.27%	0.236%
30	10.859	3291	3307	3328	rVV7	151315	366949	4.66%	0.486%
31	10.947	3329	3340	3358	rVB3	53928	110846	1.41%	0.147%
32	11.098	3375	3396	3397	rBV3	67001	106253	1.35%	0.141%
33	11.130	3398	3408	3422	rVB	289285	526806	6.69%	0.698%
34	11.744	3619	3637	3665	rBV	4293840	7875378	100.00%	10.430%
35	11.840	3666	3673	3697	rVB	68179	171010	2.17%	0.226%
36	11.956	3704	3716	3724	rBV3	66104	125137	1.59%	0.166%

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37	12.280	3826	3837	3853	rVB5	43010	81919	1.04%	0.108%
38	12.578	3934	3948	3961	rBV	537248	902937	11.47%	1.196%
39	12.634	3962	3969	3988	rVB4	67017	125661	1.60%	0.166%
40	12.731	3988	4005	4028	rBV	3408719	6029279	76.56%	7.985%
41	12.921	4063	4076	4098	rVB	392491	698252	8.87%	0.925%
42	13.222	4175	4188	4201	rBV	94024	159332	2.02%	0.211%
43	13.498	4276	4291	4305	rVB5	47796	111682	1.42%	0.148%
44	13.675	4341	4357	4383	rVV	3871905	6727384	85.42%	8.909%
45	13.771	4383	4393	4404	rVV	67124	112431	1.43%	0.149%
46	13.838	4404	4418	4424	rVV	1297850	2056123	26.11%	2.723%
47	13.876	4425	4432	4442	rVV	1838340	3024173	38.40%	4.005%
48	13.919	4443	4448	4467	rVV2	505040	815159	10.35%	1.080%
49	14.002	4468	4479	4492	rVB2	166749	283138	3.60%	0.375%
50	14.147	4519	4533	4546	rBV2	118628	223326	2.84%	0.296%
51	14.217	4546	4559	4570	rBV	455704	731000	9.28%	0.968%
52	14.278	4571	4582	4589	rVV2	425895	688642	8.74%	0.912%
53	14.327	4590	4600	4617	rVV	1483592	2547627	32.35%	3.374%
54	14.396	4618	4626	4641	rVV8	43020	80724	1.03%	0.107%
55	14.463	4642	4651	4662	rVB2	75320	108782	1.38%	0.144%
56	14.538	4664	4679	4693	rBV	325897	535589	6.80%	0.709%
57	14.619	4698	4709	4716	rBV	92025	144409	1.83%	0.191%
58	14.761	4753	4762	4768	rBV2	65099	94478	1.20%	0.125%
59	14.809	4768	4780	4805	rVB2	898601	1561653	19.83%	2.068%
60	14.930	4806	4825	4839	rBV3	584948	1261204	16.01%	1.670%
61	14.997	4839	4850	4864	rVB7	105179	181995	2.31%	0.241%
62	15.188	4901	4921	4934	rBV4	274588	671042	8.52%	0.889%
63	15.314	4954	4968	4984	rVB2	388263	936013	11.89%	1.240%
64	15.504	5032	5039	5051	rVB	53407	90577	1.15%	0.120%
65	15.614	5069	5080	5095	rBV5	74289	163862	2.08%	0.217%
66	15.804	5136	5151	5168	rBV2	148749	296028	3.76%	0.392%
67	15.981	5196	5217	5238	rBV5	66030	212175	2.69%	0.281%
68	16.183	5282	5292	5310	rVB5	55265	138893	1.76%	0.184%

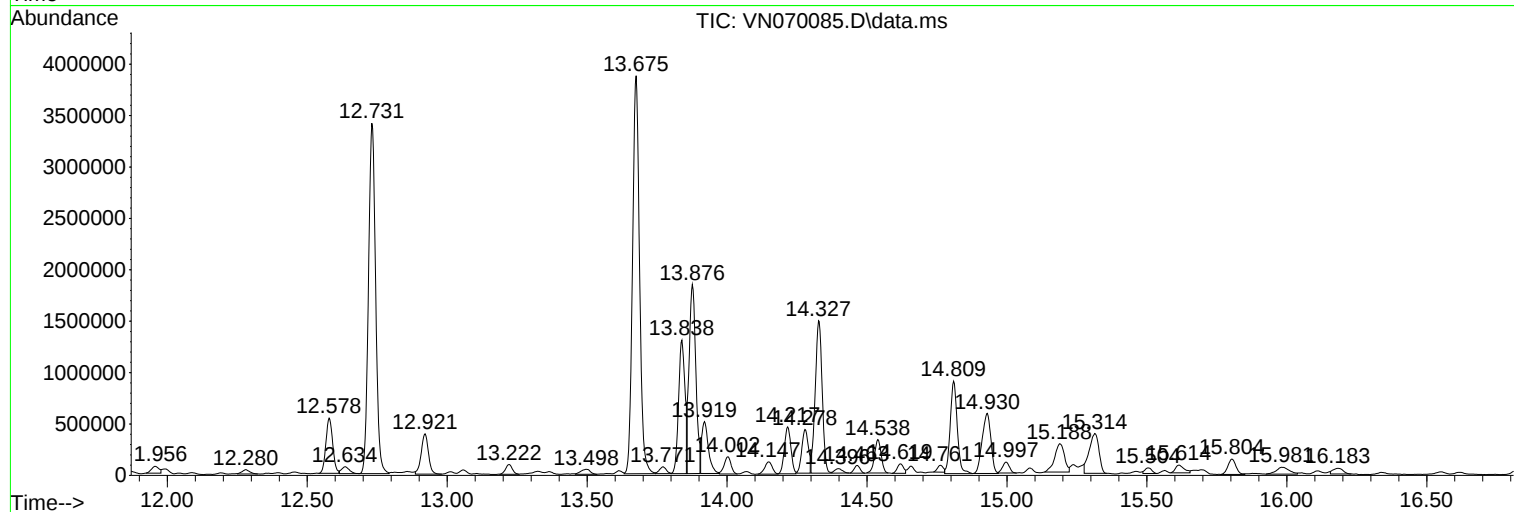
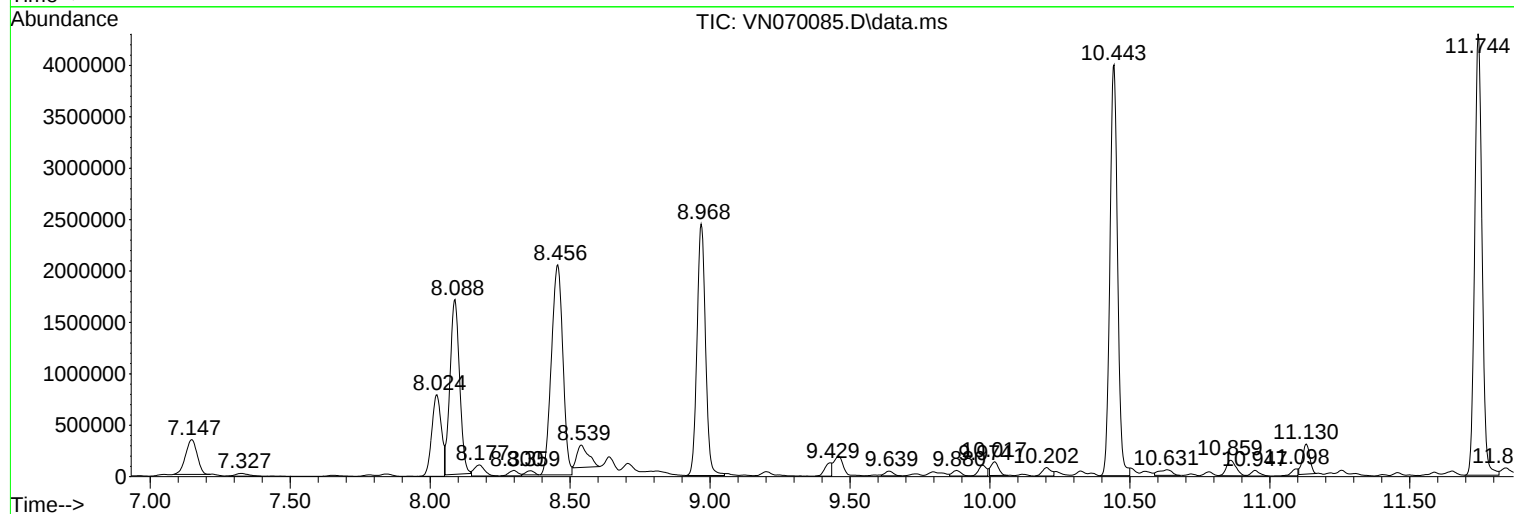
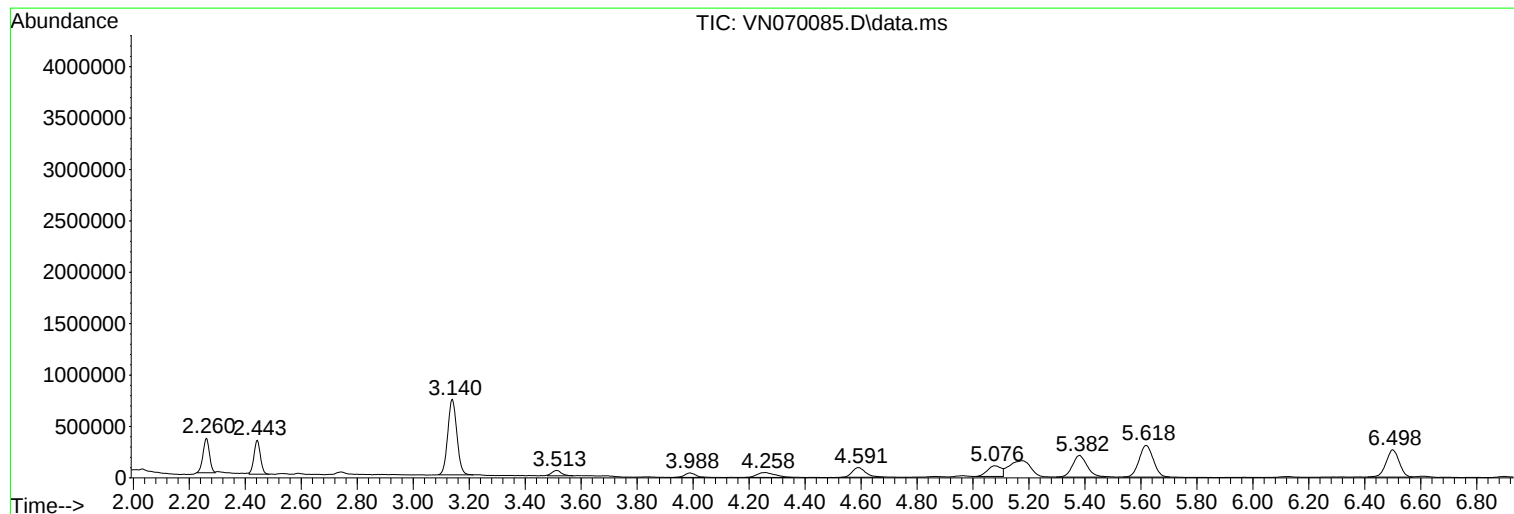
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-32

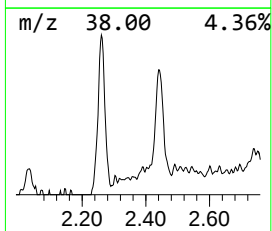
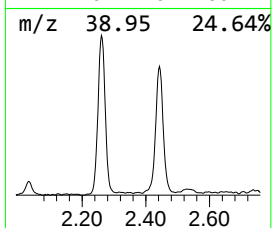
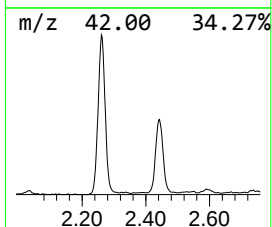
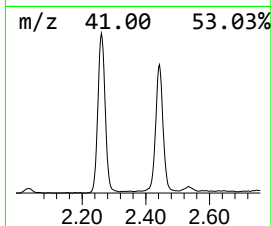
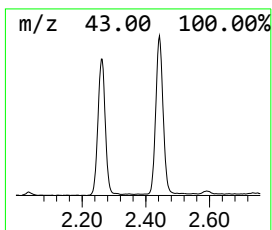
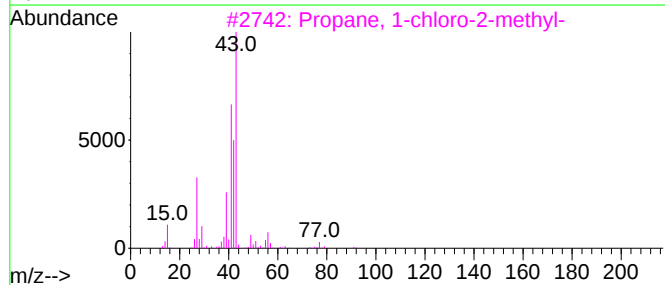
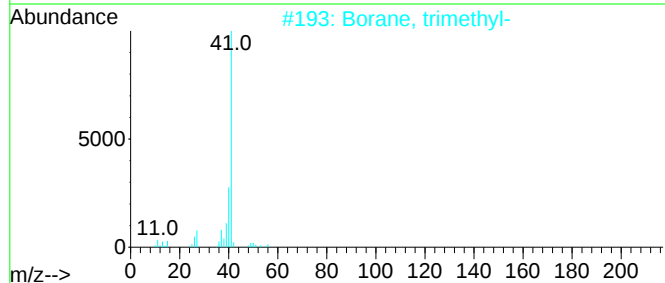
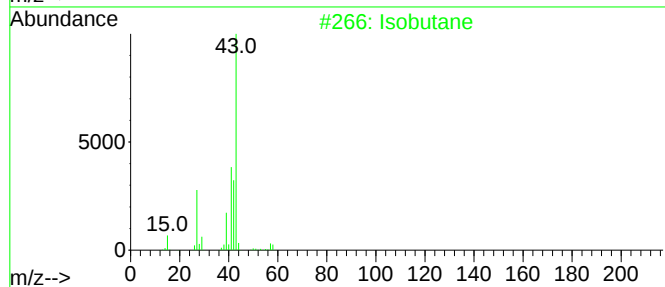
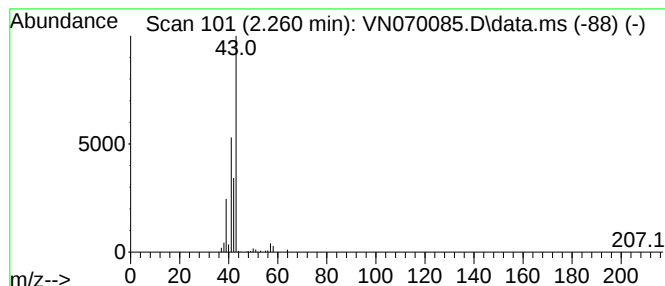
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Isobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.260	6.71 ug/l	538313	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	64
2			Borane, trimethyl-	56	C3H9B	000593-90-8	9
3			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	9
4			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
5			Propene	42	C3H6	000115-07-1	4



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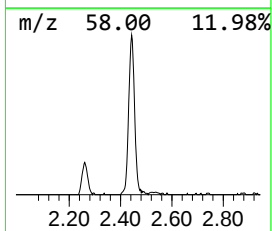
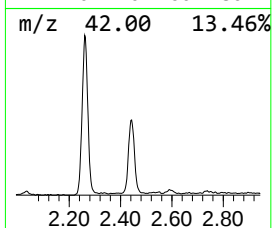
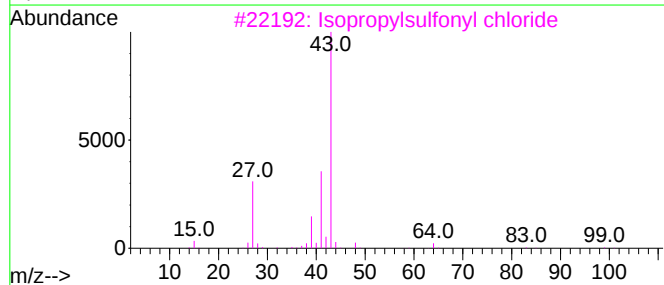
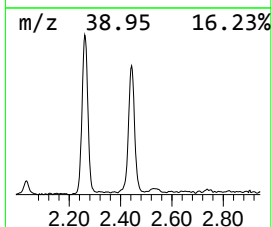
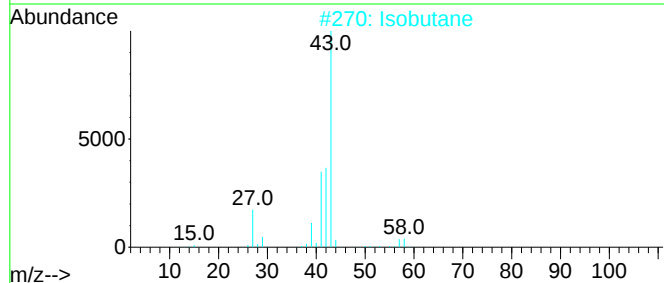
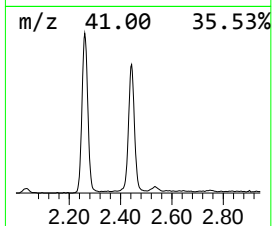
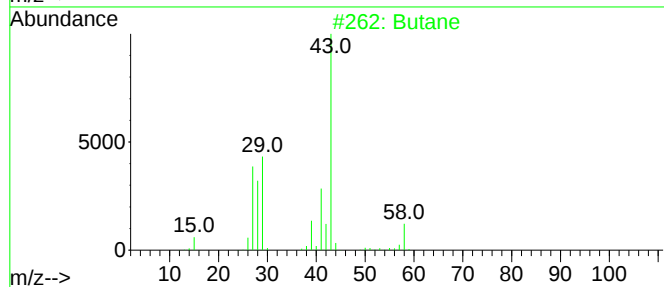
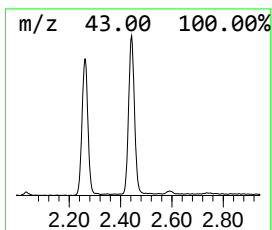
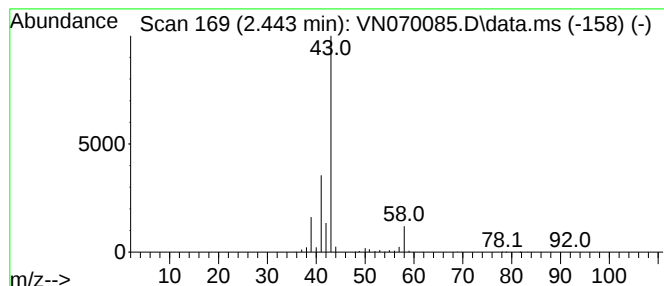
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.443	6.58 ug/l	527680	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	64
2			Isobutane	58	C4H10	000075-28-5	9
3			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	4



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Instrument :
MSVOA_N
ClientSampleId :
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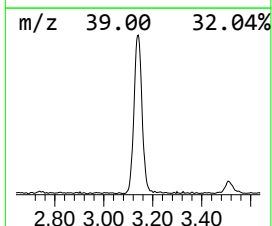
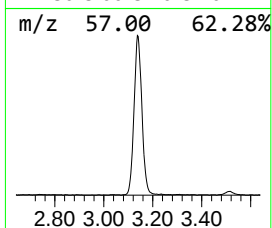
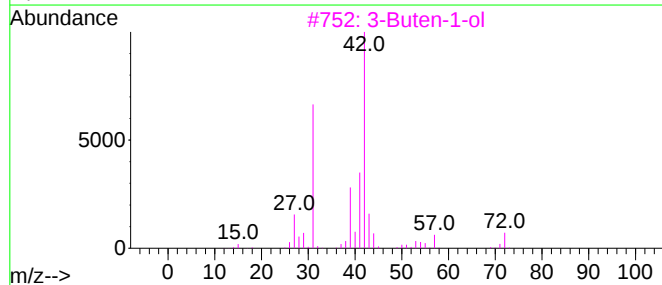
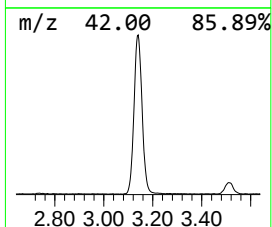
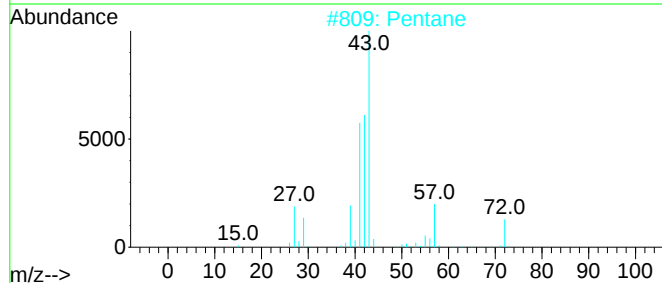
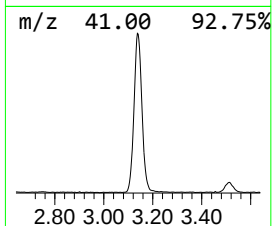
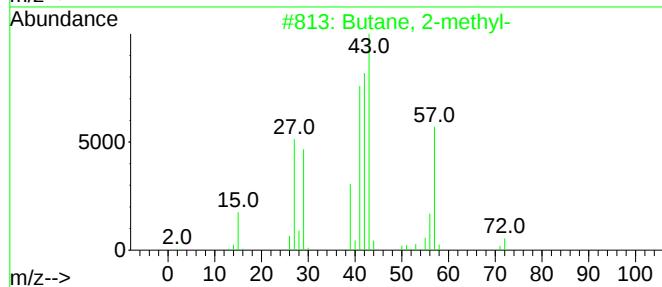
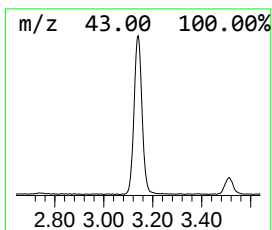
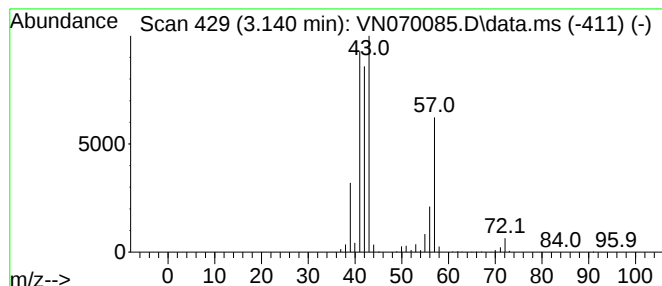
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Peak Number 3 Butane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	20.61 ug/l	1652950	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			Pentane	72	C5H12	000109-66-0	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Butene	56	C4H8	000106-98-9	9
5			Azetidine	57	C3H7N	000503-29-7	9



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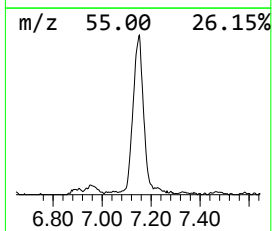
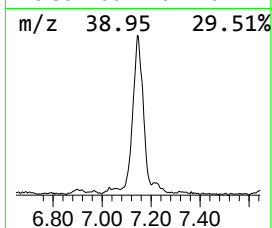
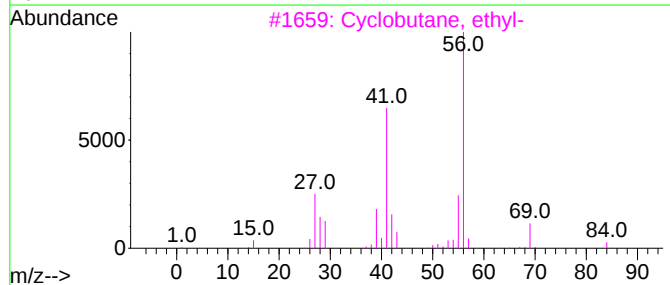
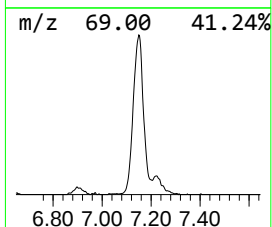
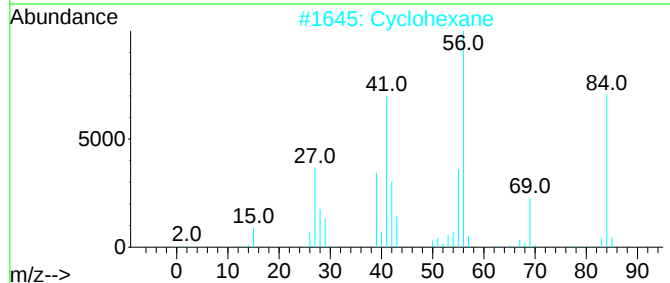
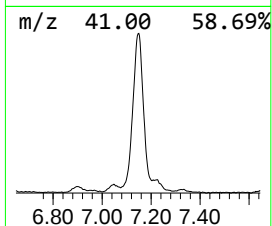
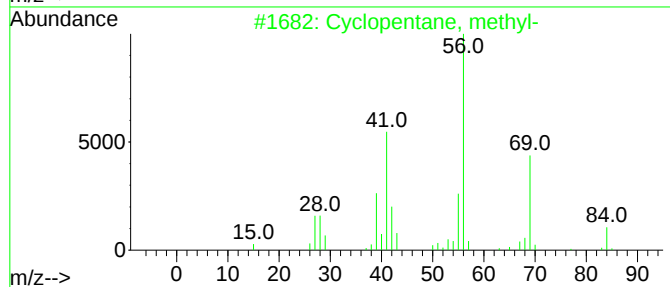
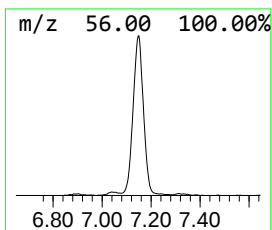
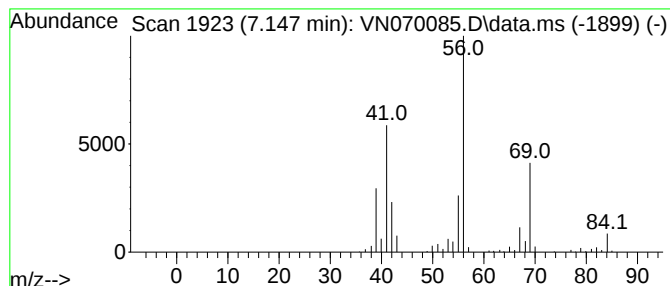
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	12.15 ug/l	974100	Pentafluorobenzene	8.086

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	86
2		Cyclohexane	84	C6H12	000110-82-7	78
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070085.D
Acq On : 14 Dec 2021 21:22
Operator : JC/MD
Sample : M4970-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-32

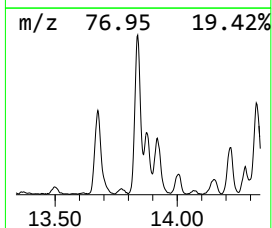
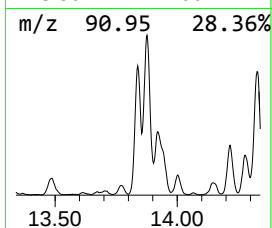
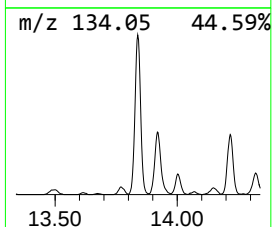
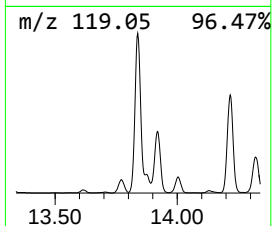
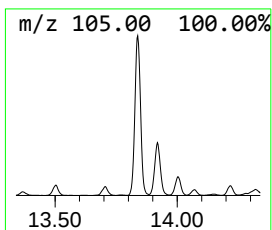
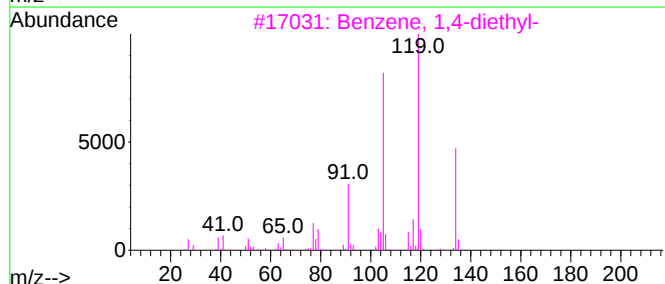
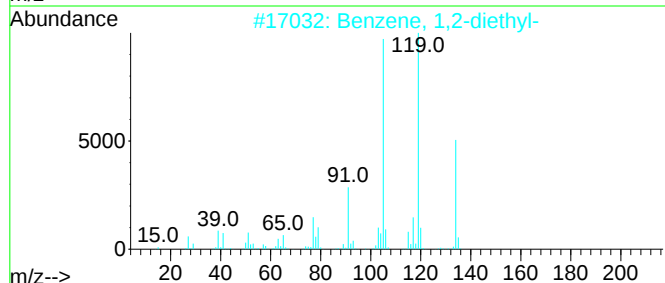
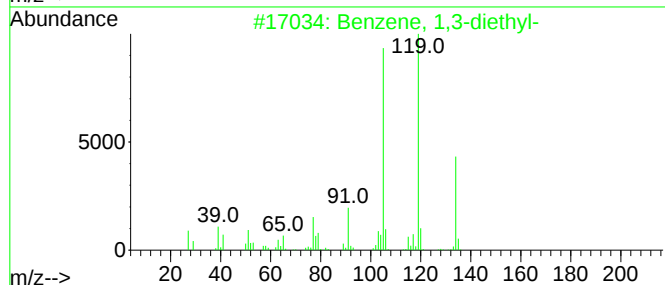
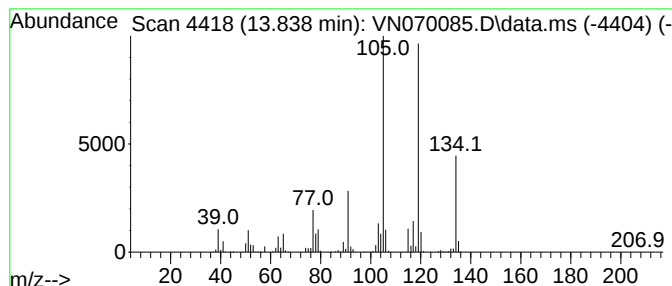
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,3-diethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	15.28 ug/l	2056120	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
2			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	96
3			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
4			o-Cymene	134	C10H14	000527-84-4	81
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070085.D
Acq On : 14 Dec 2021 21:22
Operator : JC/MD
Sample : M4970-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-32

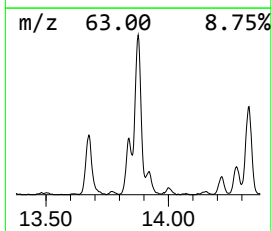
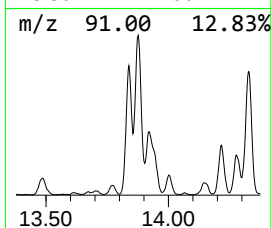
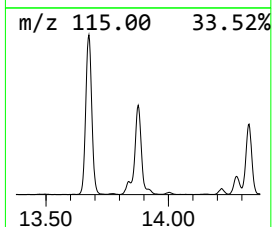
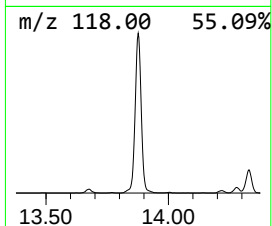
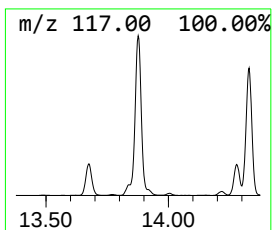
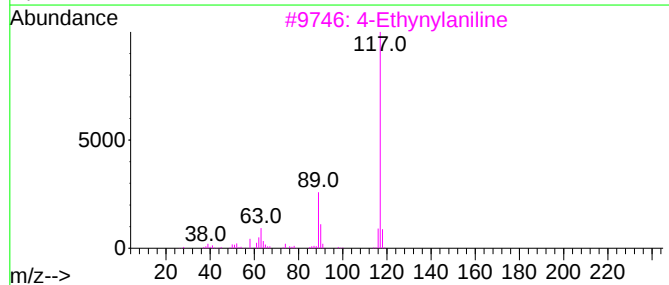
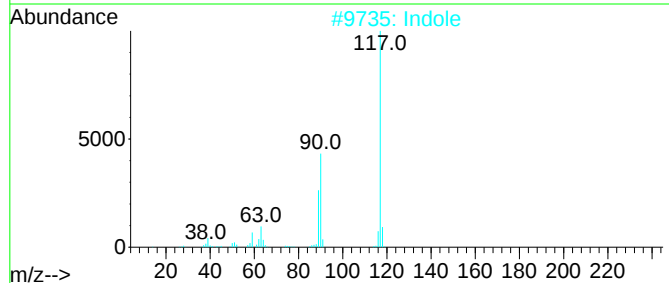
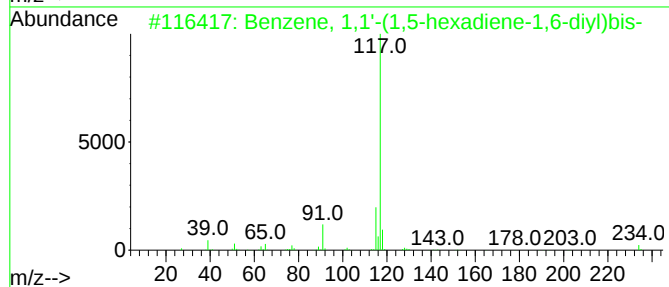
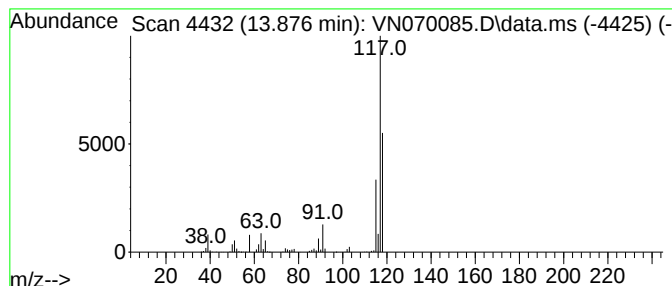
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	22.48 ug/l	3024170	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
2			Indole	117	C8H7N	000120-72-9	46
3			4-Ethynylaniline	117	C8H7N	014235-81-5	43
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	42
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070085.D
Acq On : 14 Dec 2021 21:22
Operator : JC/MD
Sample : M4970-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-32

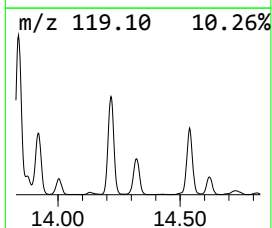
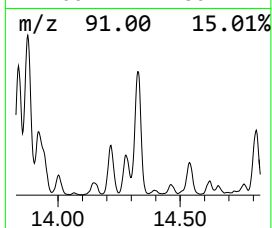
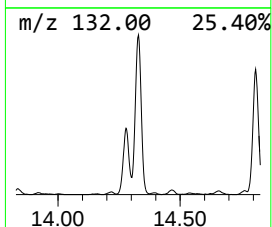
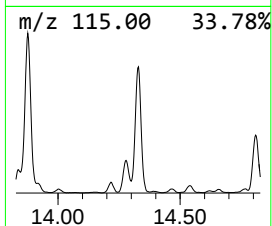
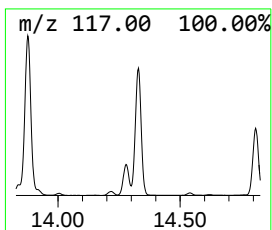
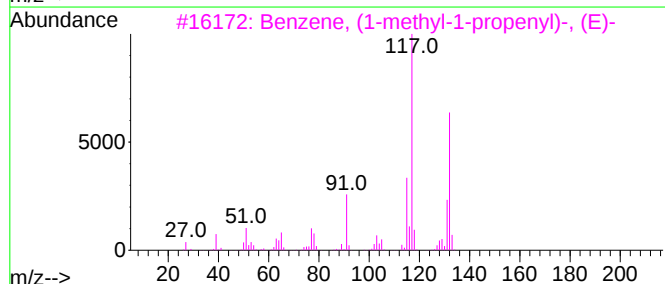
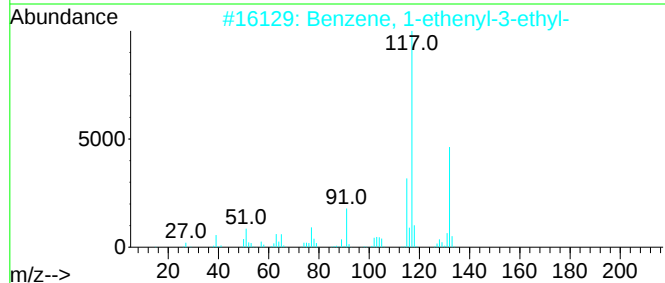
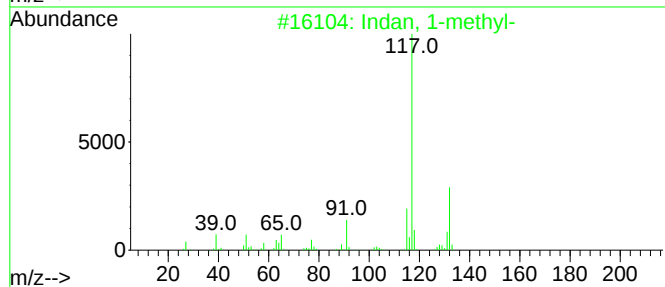
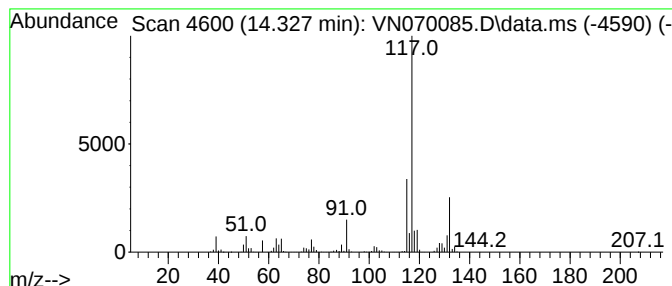
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Quant Title : SW846 8260

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

Peak Number 7 Indan, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	18.93 ug/l	2547630	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indan, 1-methyl-	132	C10H12	000767-58-8	87
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	80
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	74
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070085.D
Acq On : 14 Dec 2021 21:22
Operator : JC/MD
Sample : M4970-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-32

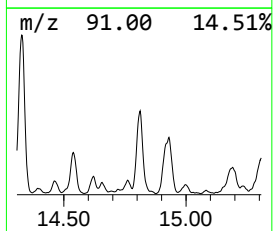
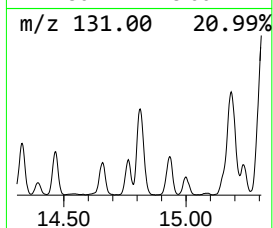
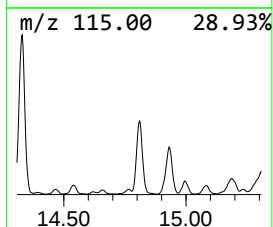
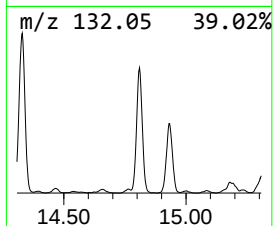
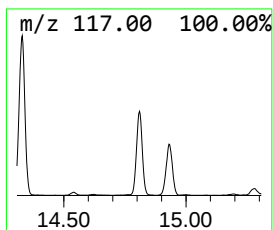
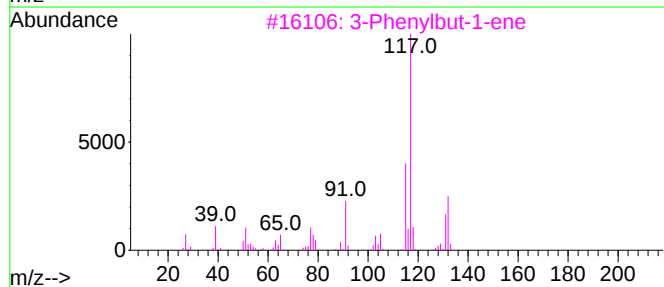
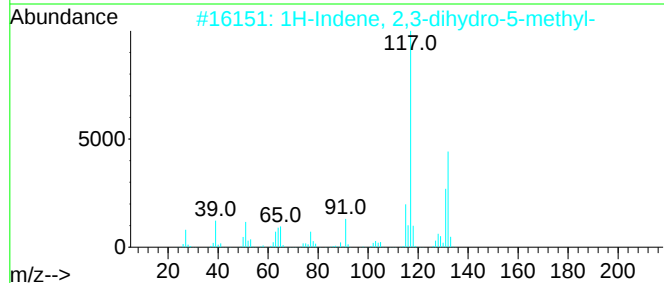
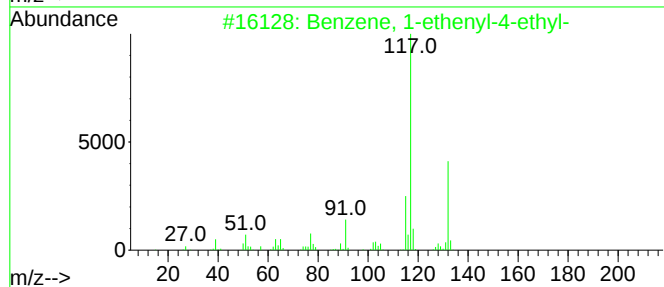
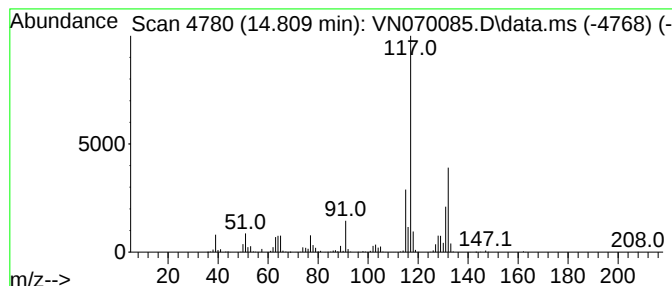
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.809	11.61 ug/l	1561650	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
2			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070085.D
Acq On : 14 Dec 2021 21:22
Operator : JC/MD
Sample : M4970-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-32

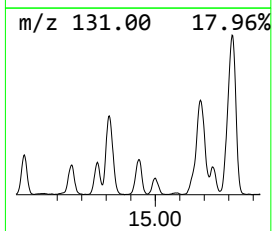
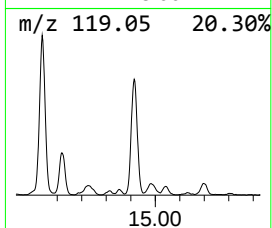
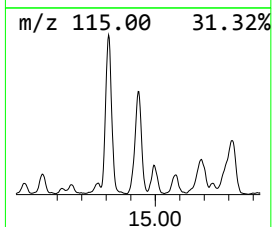
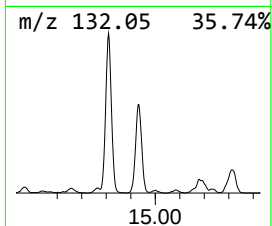
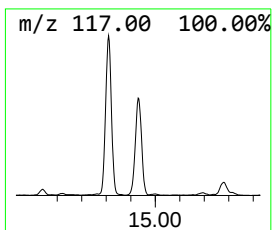
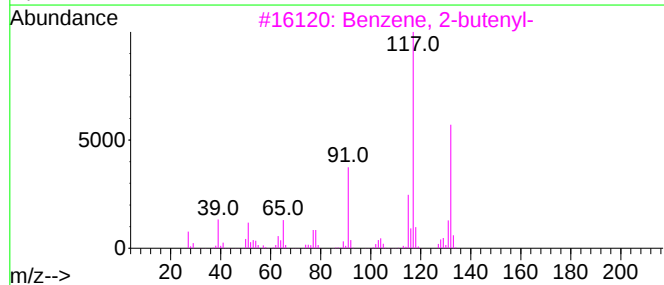
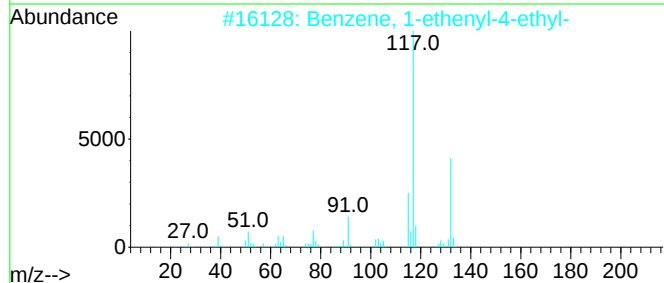
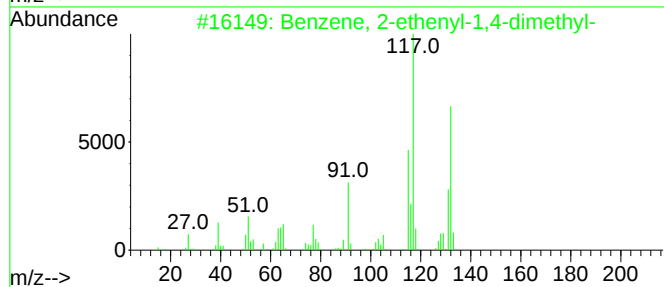
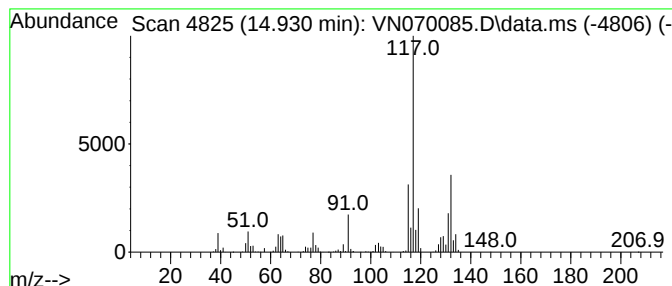
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	9.37 ug/l	1261200	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070085.D
Acq On : 14 Dec 2021 21:22
Operator : JC/MD
Sample : M4970-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-32

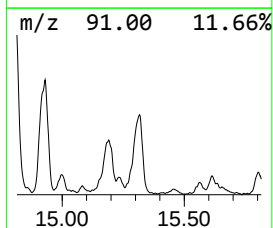
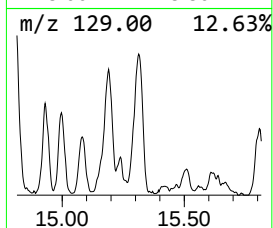
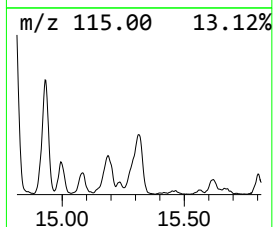
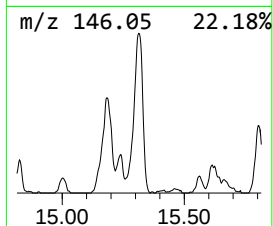
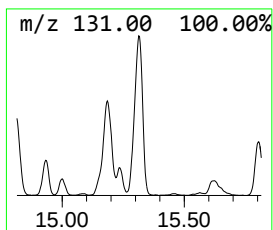
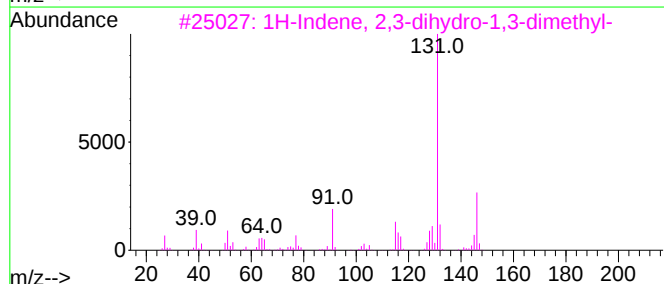
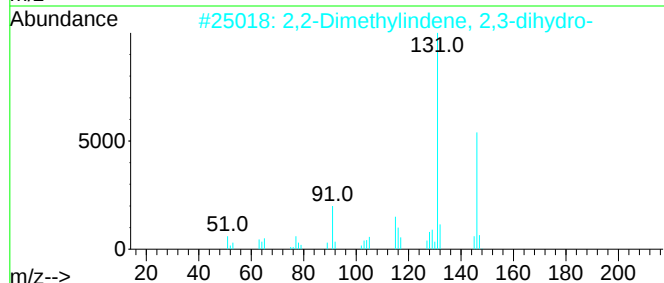
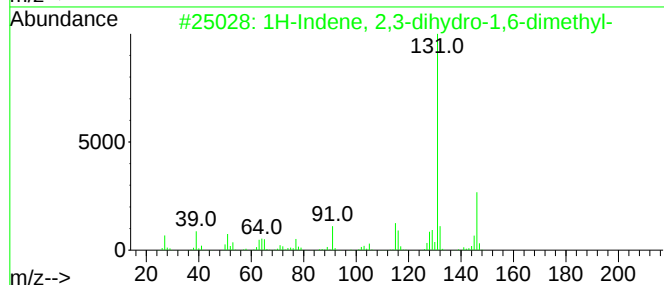
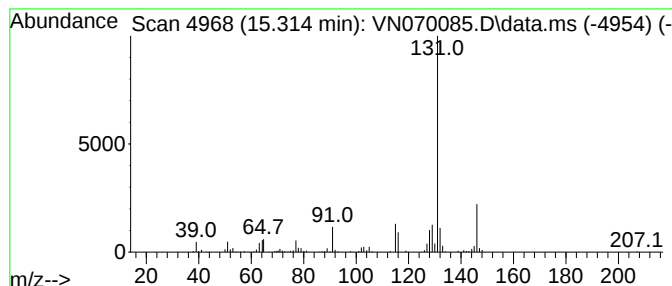
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.314	6.96 ug/l	936013	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	94		
2	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	91		
3	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	91		
4	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	91		
5	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	91		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121421\
Data File : VN070085.D
Acq On : 14 Dec 2021 21:22
Operator : JC/MD
Sample : M4970-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-32

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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Butane	2.443	6.6	ug/l	527680	1	8.086	4009670	50.0
Butane, 2-methyl-	3.140	20.6	ug/l	1652950	1	8.086	4009670	50.0
Cyclopentane, m...	7.147	12.2	ug/l	974100	1	8.086	4009670	50.0
Benzene, 1,3-di...	13.839	15.3	ug/l	2056120	4	13.675	6727380	50.0
Benzene, 1,1'-(...	13.876	22.5	ug/l	3024170	4	13.675	6727380	50.0
Indan, 1-methyl-	14.327	18.9	ug/l	2547630	4	13.675	6727380	50.0
Benzene, 1-ethe...	14.809	11.6	ug/l	1561650	4	13.675	6727380	50.0
Benzene, 2-ethe...	14.930	9.4	ug/l	1261200	4	13.675	6727380	50.0
1H-Indene, 2,3-...	15.314	7.0	ug/l	936013	4	13.675	6727380	50.0