

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
 Data File : VN070281.D
 Acq On : 21 Dec 2021 20:57
 Operator : JC/MD
 Sample : M5039-04
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-16

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: VN070281.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.143	416	430	453	rVB	276004	627788	13.68%	1.654%
2	3.518	556	570	588	rVB3	31600	74757	1.63%	0.197%
3	4.264	821	848	849	rBV6	35987	76609	1.67%	0.202%
4	5.082	1125	1153	1163	rBV2	152161	517624	11.28%	1.364%
5	5.621	1324	1354	1387	rBV4	250500	877994	19.14%	2.313%
6	6.466	1656	1669	1696	rVB8	17332	55943	1.22%	0.147%
7	7.048	1863	1886	1901	rBV4	31361	90184	1.97%	0.238%
8	7.147	1902	1923	1948	rVV3	244518	703892	15.34%	1.854%
9	7.332	1975	1992	2022	rVB5	13888	50522	1.10%	0.133%
10	8.021	2227	2249	2260	rBV	590022	1434017	31.26%	3.778%
11	8.086	2261	2273	2293	rVV2	1178041	2759780	60.15%	7.270%
12	8.174	2294	2306	2329	rVB3	113332	303397	6.61%	0.799%
13	8.295	2334	2351	2365	rBV4	39547	92084	2.01%	0.243%
14	8.440	2384	2405	2430	rBV	775997	1901796	41.45%	5.010%
15	8.574	2442	2455	2458	rBV7	65311	106535	2.32%	0.281%
16	8.968	2583	2602	2628	rBV	1664642	3524073	76.81%	9.284%
17	9.429	2754	2774	2775	rBV5	81890	135753	2.96%	0.358%
18	9.636	2826	2851	2867	rVB5	51129	138977	3.03%	0.366%
19	9.880	2932	2942	2962	rVB2	85313	174306	3.80%	0.459%
20	9.974	2962	2977	2980	rBV4	40046	60329	1.31%	0.159%
21	10.014	2981	2992	3009	rVB3	166341	346097	7.54%	0.912%
22	10.199	3046	3061	3092	rBV2	104228	295360	6.44%	0.778%
23	10.330	3095	3110	3134	rBV3	83103	192631	4.20%	0.507%
24	10.440	3134	3151	3169	rBV	2461801	4587994	100.00%	12.087%
25	10.859	3296	3307	3326	rVB5	53828	119473	2.60%	0.315%
26	10.947	3326	3340	3359	rVB3	39263	84857	1.85%	0.224%
27	11.092	3369	3394	3403	rBV2	100467	209961	4.58%	0.553%
28	11.492	3535	3543	3562	rVB3	29490	50845	1.11%	0.134%
29	11.744	3619	3637	3661	rBV	2186385	4006577	87.33%	10.555%
30	11.843	3661	3674	3695	rVV	494197	913719	19.92%	2.407%
31	11.953	3698	3715	3740	rVB2	164570	357371	7.79%	0.941%
32	12.280	3824	3837	3854	rVB3	48214	86947	1.90%	0.229%
33	12.578	3934	3948	3962	rBV	141090	236733	5.16%	0.624%
34	12.731	3987	4005	4030	rBV	1549200	2751445	59.97%	7.248%
35	12.921	4060	4076	4092	rVB	393996	681258	14.85%	1.795%
36	13.015	4102	4111	4119	rBV	46303	72606	1.58%	0.191%

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37	13.055	4120	4126	4141	rVB2	43106	73389	1.60%	0.193%
38	13.219	4171	4187	4202	rBV	128620	226353	4.93%	0.596%
39	13.366	4230	4242	4259	rVB	142585	241807	5.27%	0.637%
40	13.498	4273	4291	4307	rBV4	71446	173352	3.78%	0.457%
41	13.675	4340	4357	4381	rBV	1564105	2973976	64.82%	7.835%
42	13.839	4403	4418	4425	rBV	554103	921644	20.09%	2.428%
43	13.876	4426	4432	4441	rVV	452530	717809	15.65%	1.891%
44	13.919	4442	4448	4467	rVV5	189919	350821	7.65%	0.924%
45	14.002	4468	4479	4492	rVV2	92306	148955	3.25%	0.392%
46	14.131	4517	4527	4544	rBV7	25480	56518	1.23%	0.149%
47	14.217	4544	4559	4572	rBV	832837	1361579	29.68%	3.587%
48	14.278	4573	4582	4589	rVV2	72484	119417	2.60%	0.315%
49	14.327	4589	4600	4615	rVB3	281273	502150	10.94%	1.323%
50	14.539	4660	4679	4690	rBV	344061	584449	12.74%	1.540%
51	14.809	4768	4780	4791	rBV	167426	277314	6.04%	0.731%
52	14.930	4809	4825	4837	rBV4	52211	110275	2.40%	0.291%
53	14.994	4837	4849	4863	rVB4	25020	53647	1.17%	0.141%
54	15.083	4870	4882	4896	rBV5	39349	69776	1.52%	0.184%
55	15.193	4903	4923	4934	rBV7	46847	105472	2.30%	0.278%
56	15.308	4950	4966	4985	rVB5	52469	126854	2.76%	0.334%
57	15.504	5027	5039	5054	rVB3	32574	63547	1.39%	0.167%

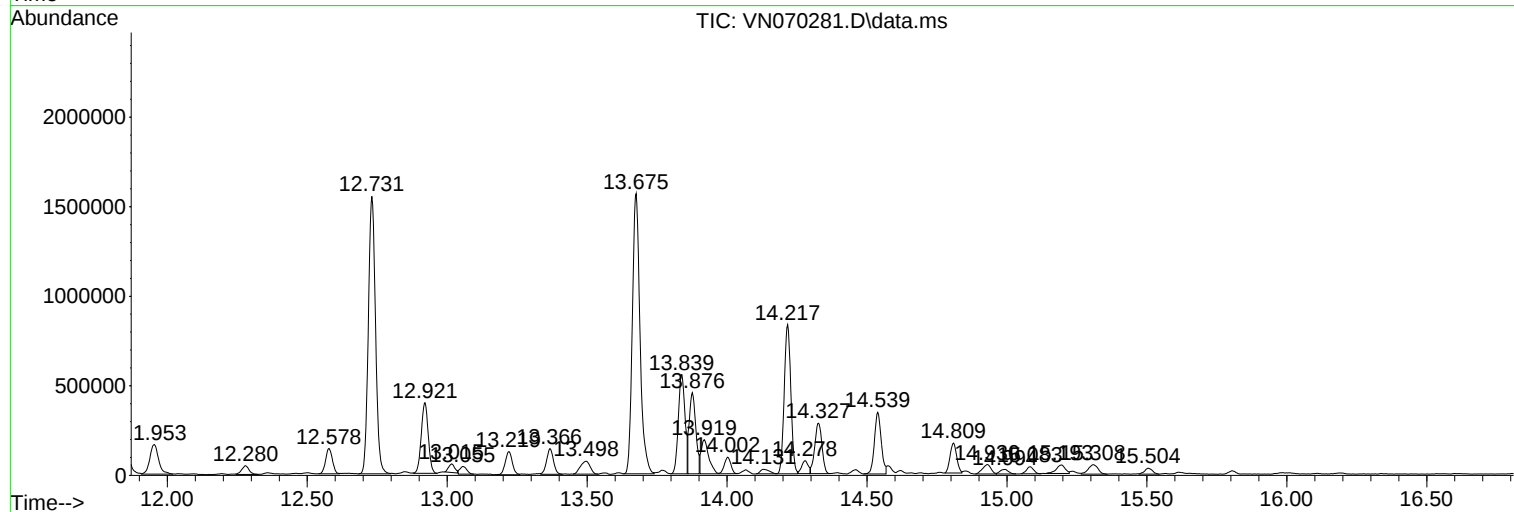
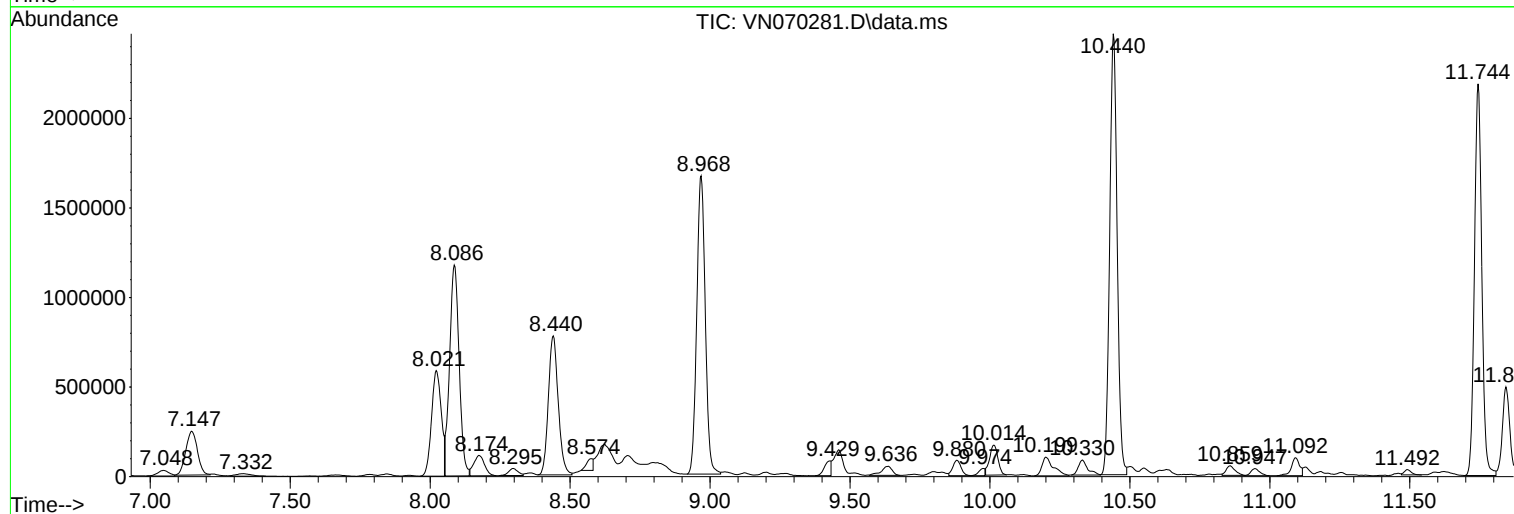
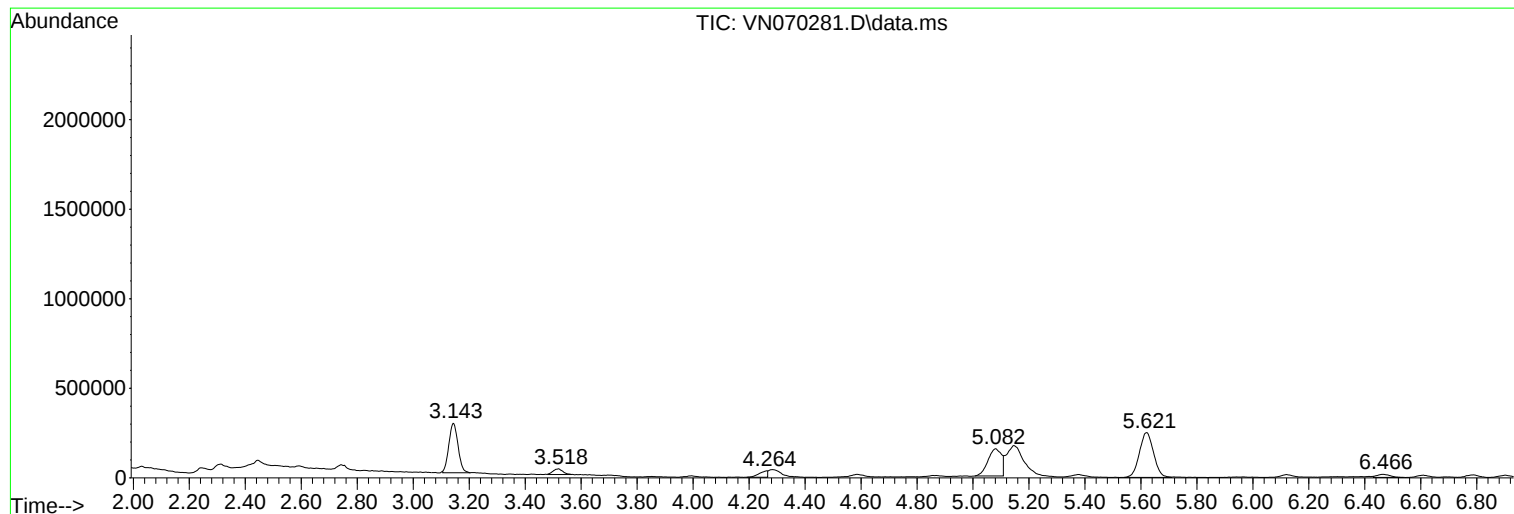
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Quant Title : SW846 8260

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



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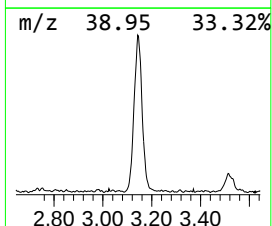
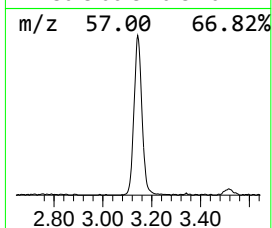
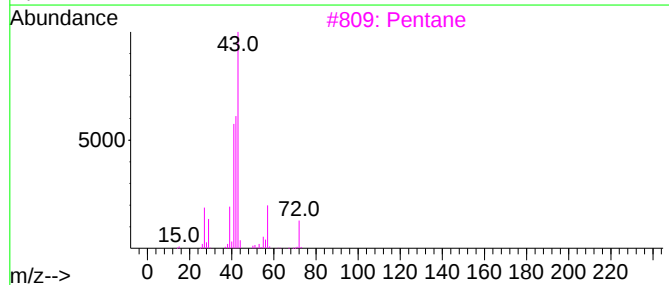
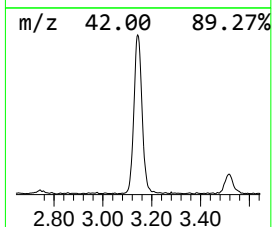
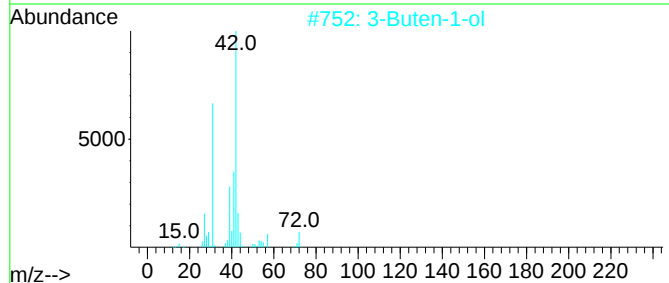
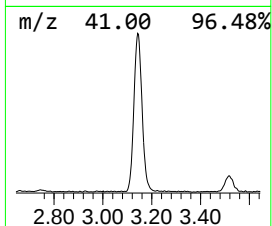
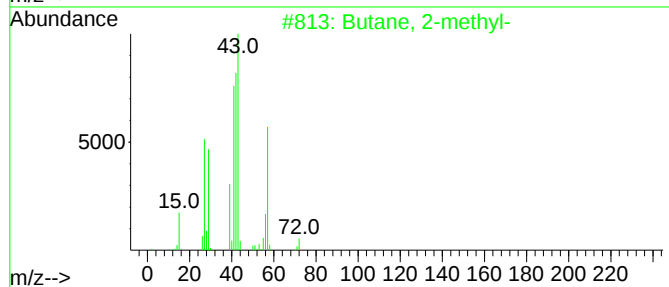
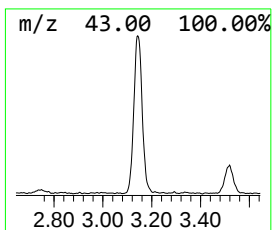
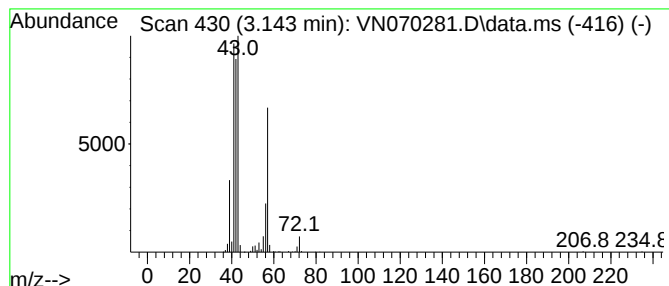
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.143	11.37 ug/l	627788	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	12
5			Butane, 1-isocyano-	83	C5H9N	002769-64-4	12



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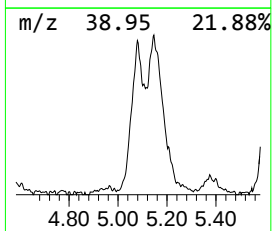
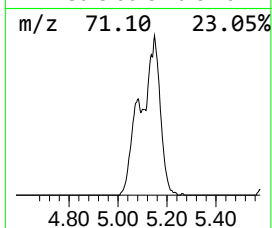
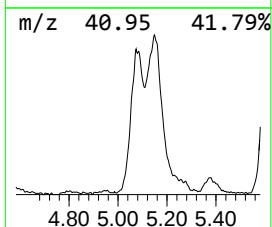
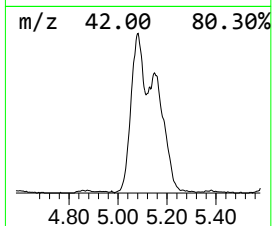
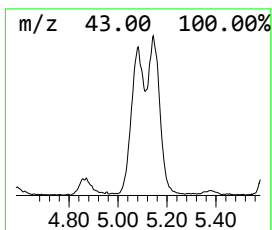
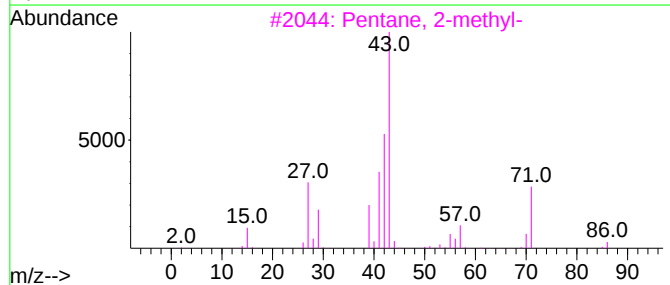
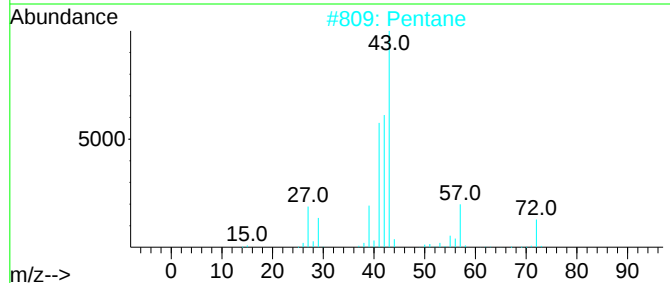
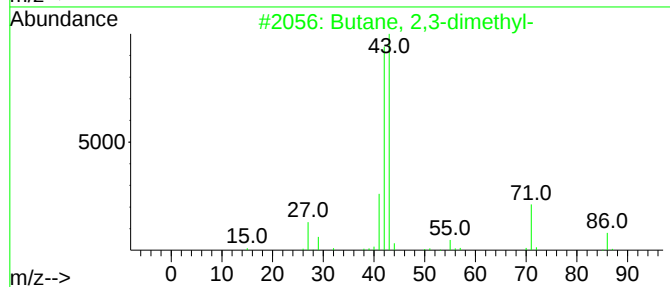
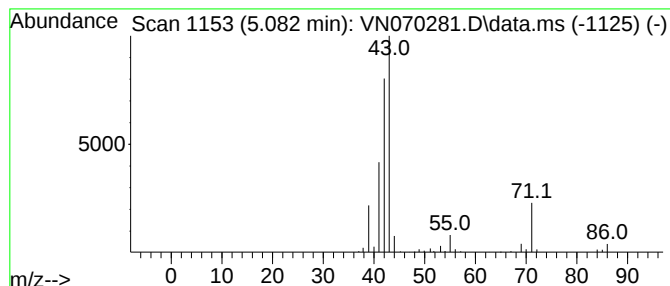
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.082	9.38 ug/l	517624	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2			Pentane	72	C5H12	000109-66-0	42
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	38
4			1-Pentene	70	C5H10	000109-67-1	25
5			Pyrrolidine	71	C4H9N	000123-75-1	9



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ALS Vial : 26 Sample Multiplier: 1

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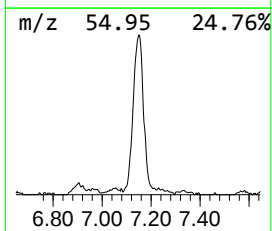
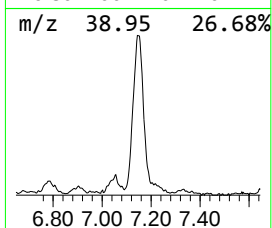
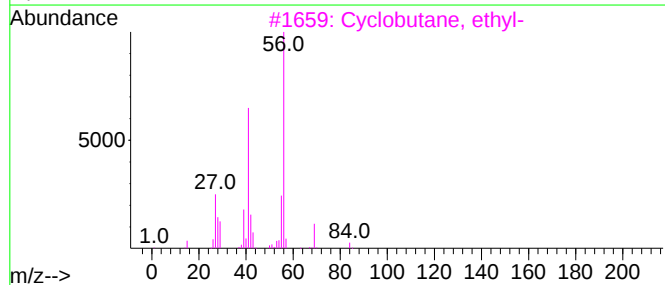
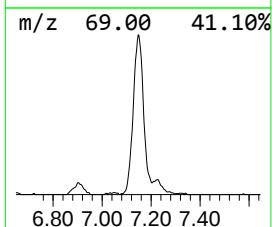
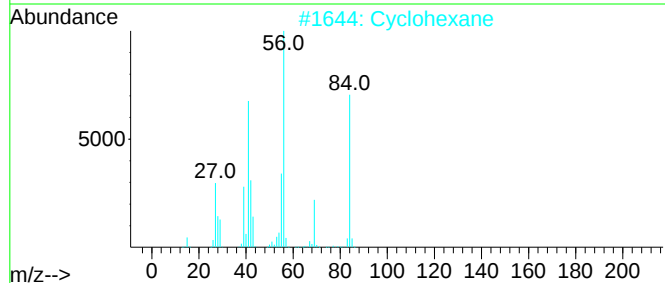
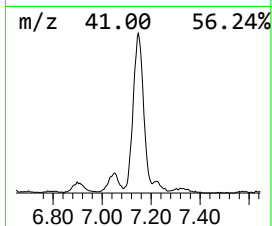
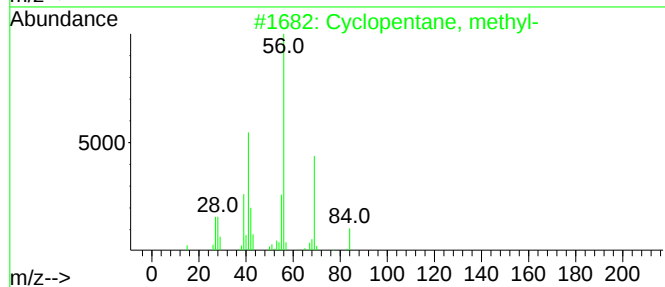
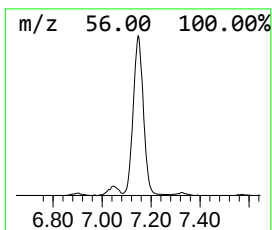
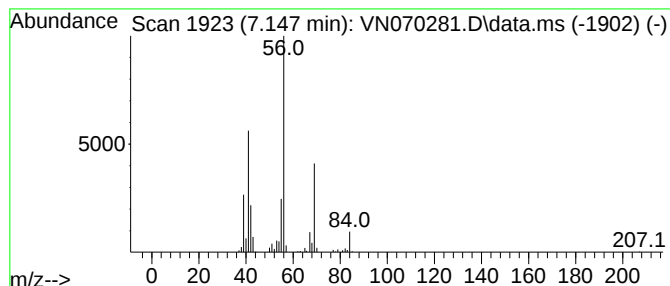
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	12.75 ug/l	703892	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2			Cyclohexane	84	C6H12	000110-82-7	72
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			Cyclobutane	56	C4H8	000287-23-0	50
5			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50



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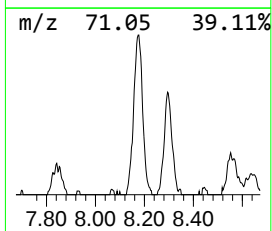
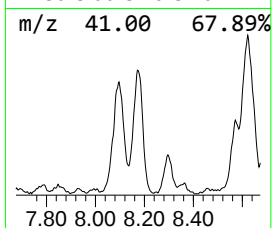
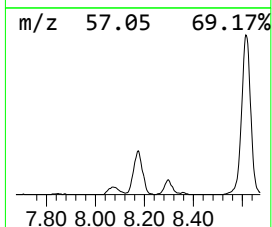
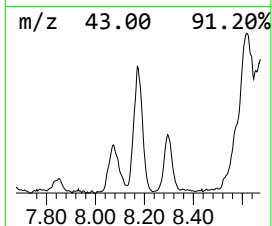
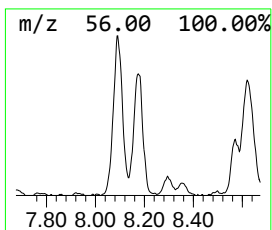
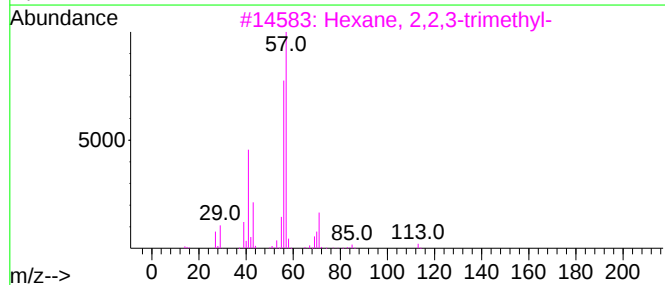
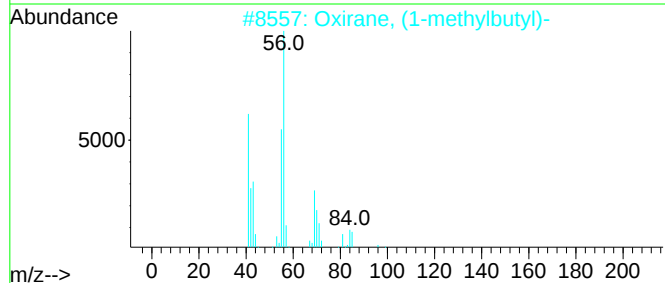
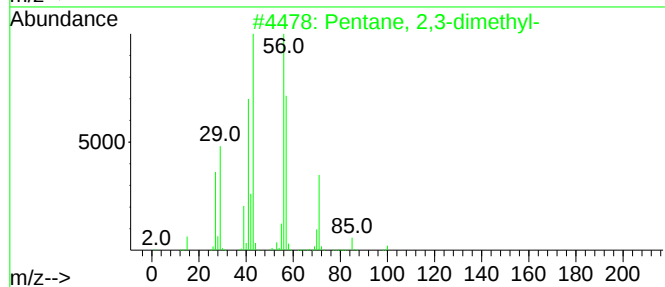
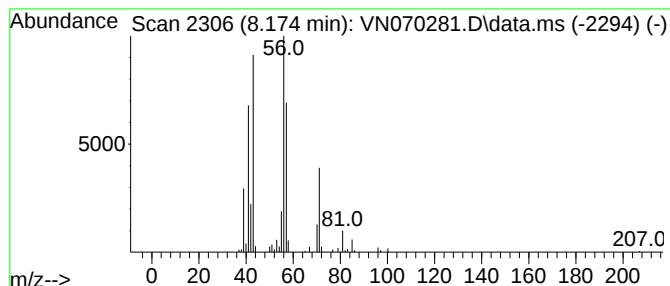
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	5.50 ug/l	303397	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2			Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	47
3			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	47
4			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
5			cis-4,6-Dimethylcyclohexane-1,3-...	140	C8H12O2	069841-15-2	37



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MW-16

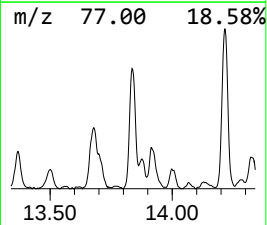
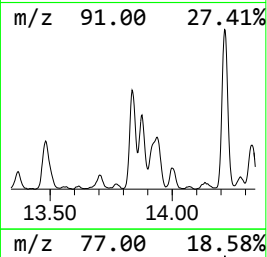
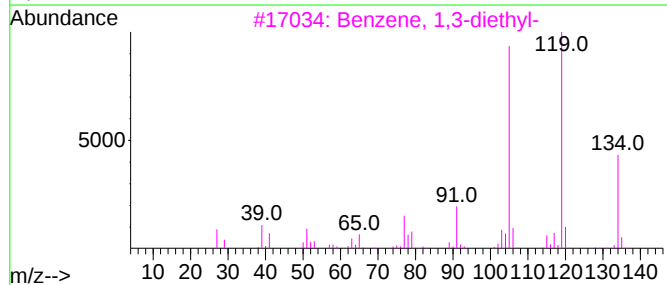
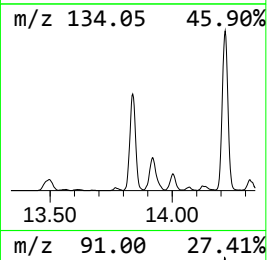
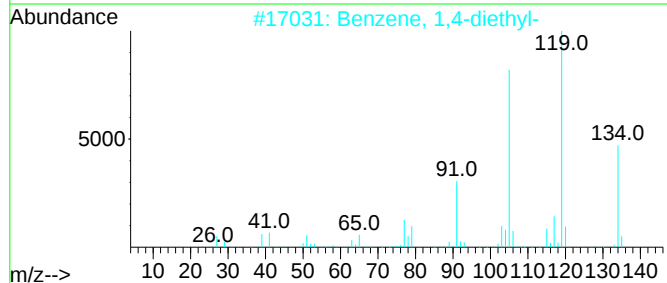
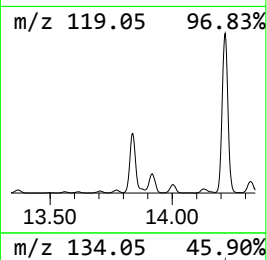
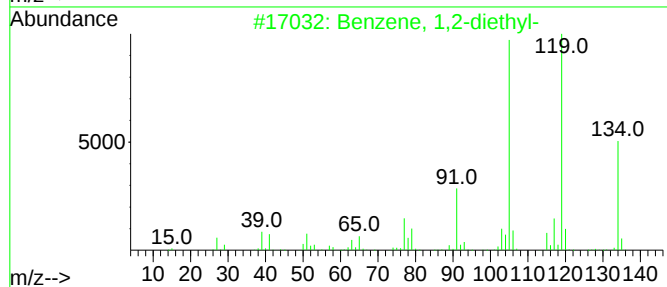
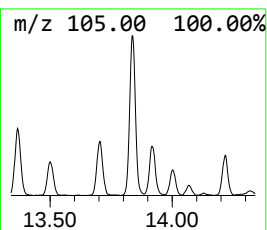
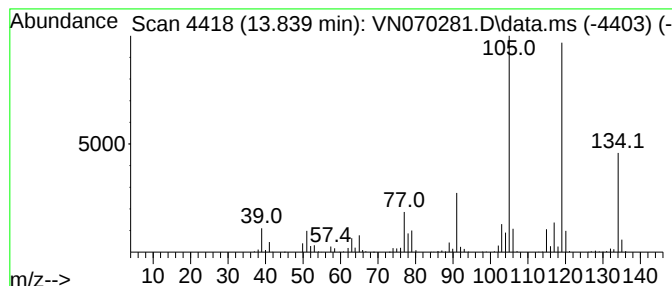
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1,2-diethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	15.50 ug/l	921644	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	97
2			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
3			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	96
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070281.D
Acq On : 21 Dec 2021 20:57
Operator : JC/MD
Sample : M5039-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

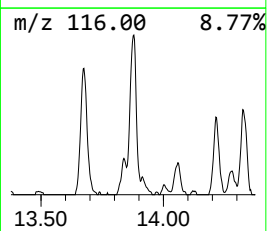
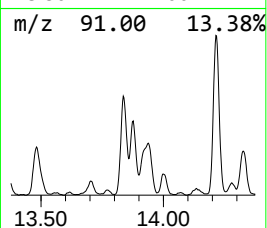
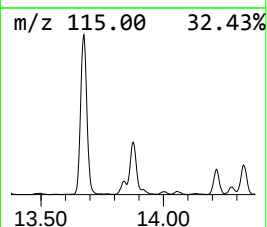
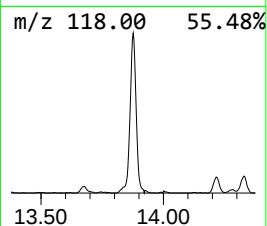
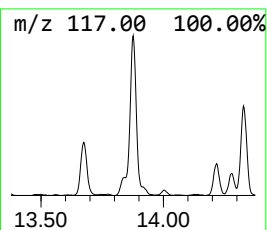
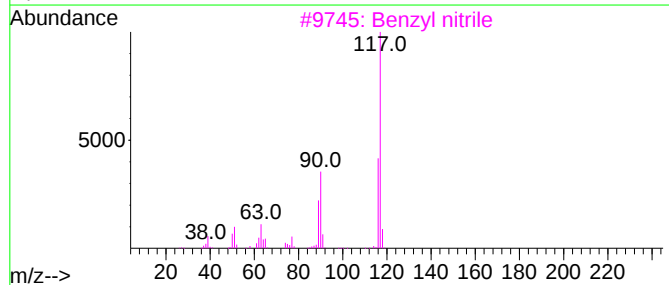
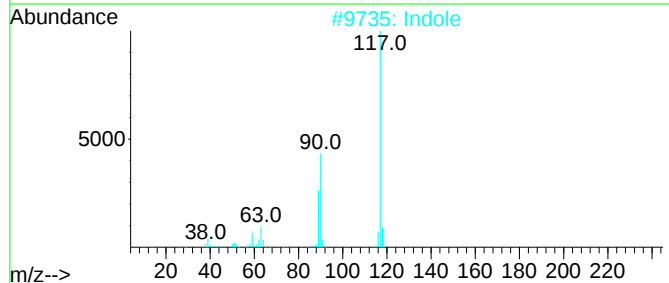
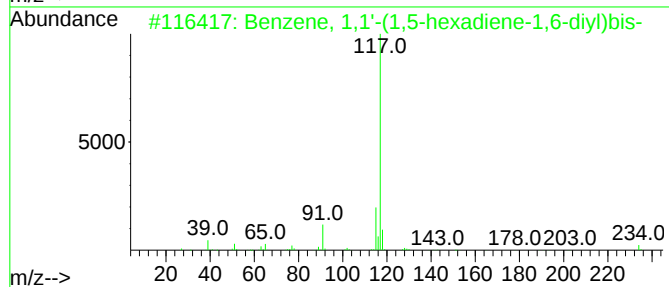
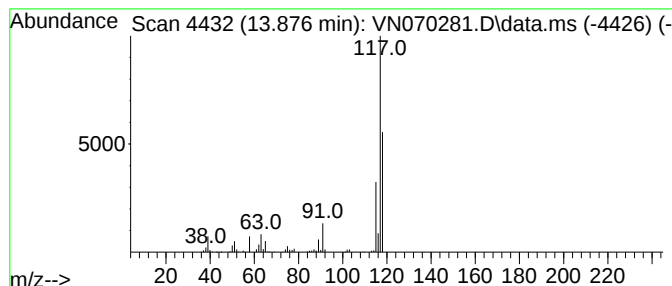
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1,1'-(1,5-hexadien... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	12.07 ug/l	717809	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			Benzyl nitrile	117	C8H7N	000140-29-4	43
4			4-Ethynylaniline	117	C8H7N	014235-81-5	43
5			5H-1-Pyridine	117	C8H7N	000270-91-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070281.D
Acq On : 21 Dec 2021 20:57
Operator : JC/MD
Sample : M5039-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

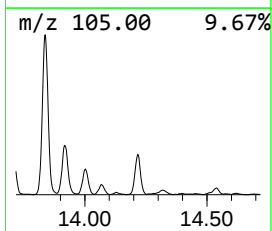
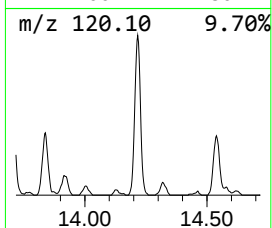
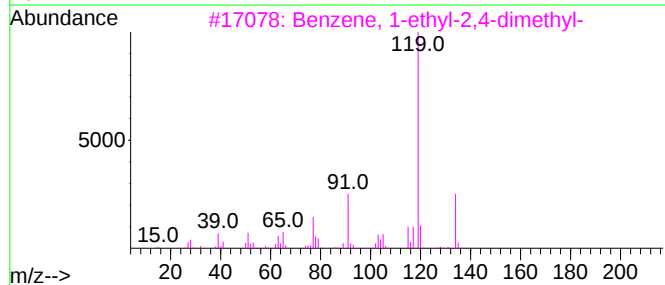
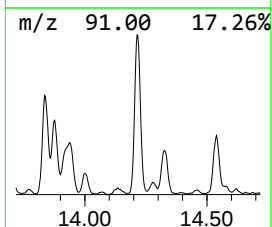
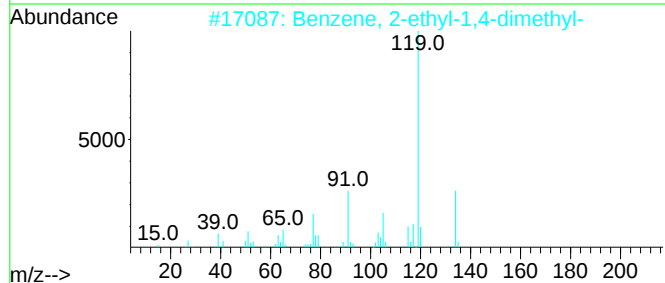
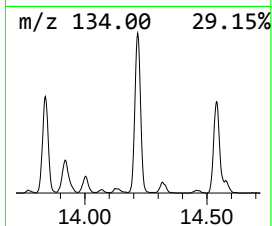
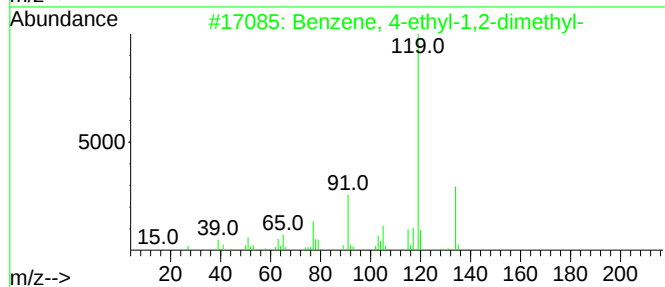
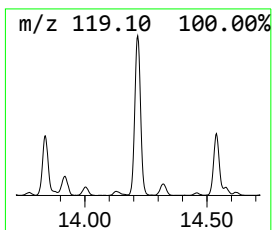
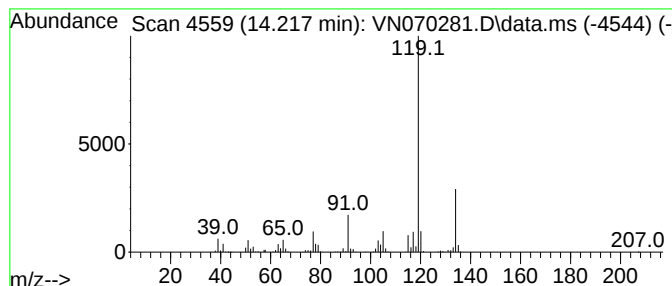
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	22.89 ug/l	1361580	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	97
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
4			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5			o-Cymene	134	C10H14	000527-84-4	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070281.D
Acq On : 21 Dec 2021 20:57
Operator : JC/MD
Sample : M5039-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

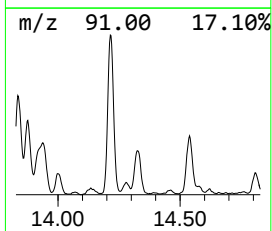
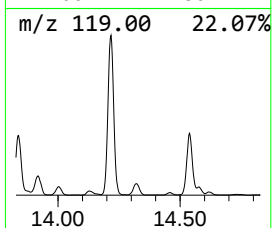
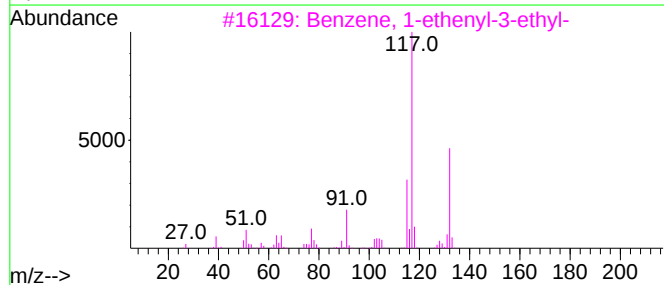
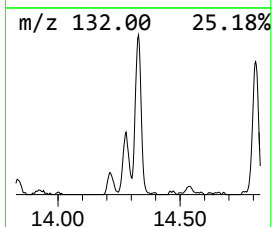
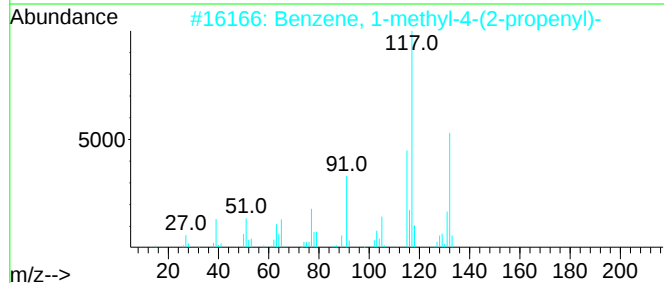
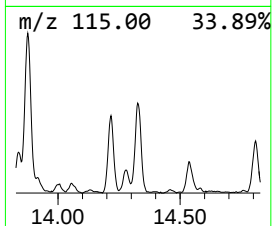
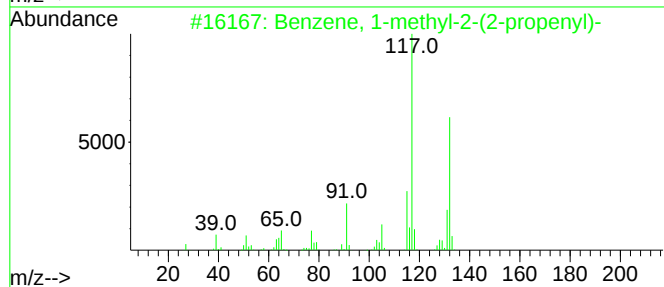
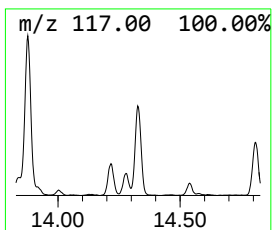
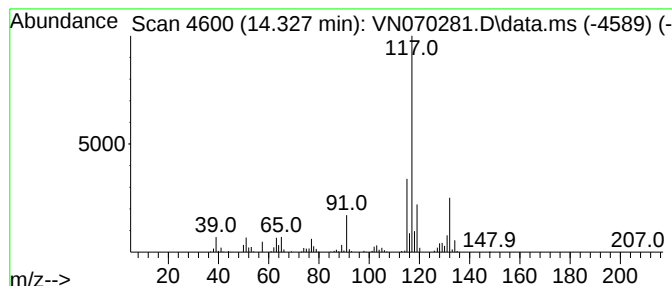
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-methyl-2-(2-prop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.327	8.44 ug/l	502150	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	72
2			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	72
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	72
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	72
5			Indan, 1-methyl-	132	C10H12	000767-58-8	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070281.D
Acq On : 21 Dec 2021 20:57
Operator : JC/MD
Sample : M5039-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

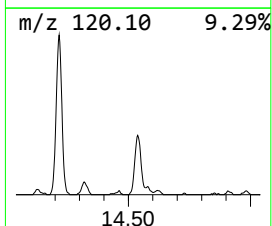
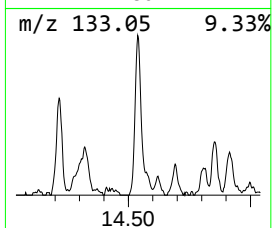
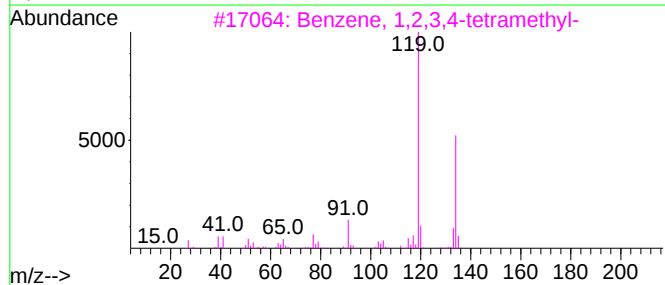
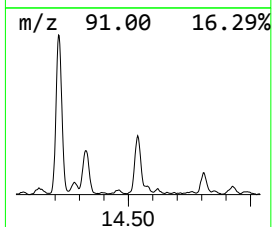
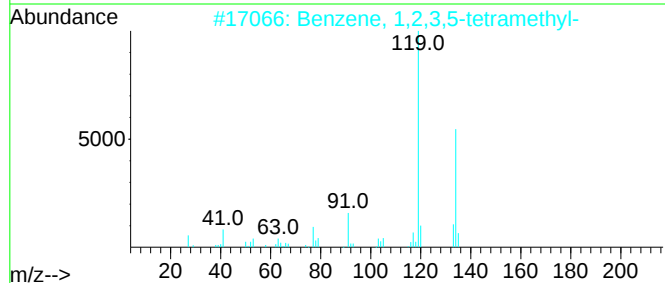
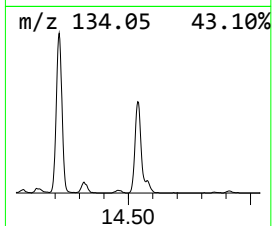
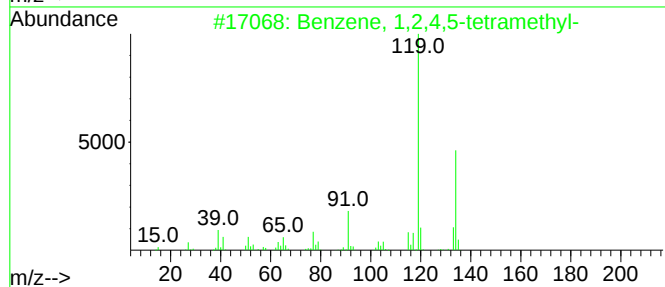
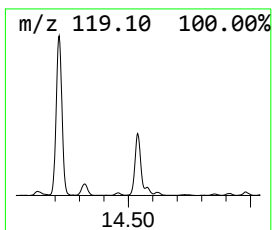
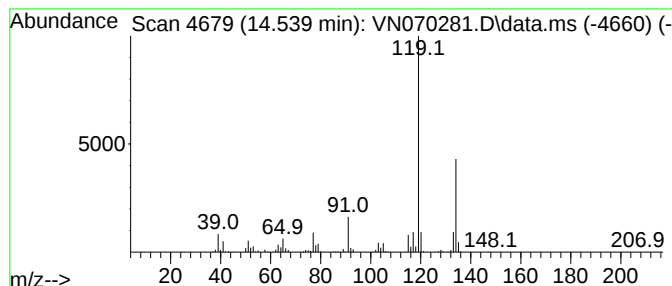
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.539	9.83 ug/l	584449	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			o-Cymene	134	C10H14	000527-84-4	93
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122121\
Data File : VN070281.D
Acq On : 21 Dec 2021 20:57
Operator : JC/MD
Sample : M5039-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-16

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, 2,3-dim...	5.082	9.4	ug/l	517624	1	8.086	2759780	50.0
Cyclopentane, m...	7.147	12.8	ug/l	703892	1	8.086	2759780	50.0
Pentane, 2,3-di...	8.174	5.5	ug/l	303397	1	8.086	2759780	50.0
Benzene, 1,2-di...	13.839	15.5	ug/l	921644	4	13.675	2973980	50.0
Benzene, 1,1'-(...	13.876	12.1	ug/l	717809	4	13.675	2973980	50.0
Benzene, 4-ethy...	14.217	22.9	ug/l	1361580	4	13.675	2973980	50.0
Benzene, 1-meth...	14.327	8.4	ug/l	502150	4	13.675	2973980	50.0
Benzene, 1,2,4,...	14.539	9.8	ug/l	584449	4	13.675	2973980	50.0