

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
 Data File : VN070633.D
 Acq On : 14 Jan 2022 19:28
 Operator : JC/MD
 Sample : N1148-06
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-46

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070633.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.132	404	426	466	rBV	8306818	19552465	5.04%	1.013%
2	3.508	544	566	615	rBV	6202337	15291583	3.94%	0.792%
3	5.077	1123	1151	1154	rBV2	1841991	4514704	1.16%	0.234%
4	5.616	1317	1352	1397	rBV2	4905923	17089967	4.40%	0.885%
5	6.117	1509	1539	1577	rBV	4500951	13849792	3.57%	0.717%
6	6.466	1656	1669	1696	rVB	2217100	6428582	1.66%	0.333%
7	6.605	1697	1721	1741	rBV	1370516	4240957	1.09%	0.220%
8	6.900	1808	1831	1863	rVB2	1996151	5940642	1.53%	0.308%
9	7.147	1899	1923	1946	rBV	14993057	43857040	11.30%	2.271%
10	7.844	2166	2183	2203	rVB	3991448	9810444	2.53%	0.508%
11	8.094	2255	2276	2294	rBV4	9951720	28067113	7.23%	1.453%
12	8.174	2296	2306	2331	rVB3	2418947	6203863	1.60%	0.321%
13	8.295	2331	2351	2366	rBV	3525411	8235668	2.12%	0.426%
14	8.574	2435	2455	2468	rBV5	2953374	8761731	2.26%	0.454%
15	8.708	2494	2505	2526	rVB	2118591	5178959	1.33%	0.268%
16	8.826	2527	2549	2579	rVB3	2380986	6198470	1.60%	0.321%
17	8.965	2579	2601	2615	rBV5	5200601	12956646	3.34%	0.671%
18	9.459	2749	2785	2801	rBV	9974545	26341396	6.79%	1.364%
19	9.971	2962	2976	2987	rBV	4215465	8035688	2.07%	0.416%
20	10.323	3092	3107	3134	rVB	2802415	5751774	1.48%	0.298%
21	10.441	3135	3151	3162	rBV2	4207839	8191255	2.11%	0.424%
22	10.505	3163	3175	3189	rVB	6338478	11537056	2.97%	0.597%
23	11.744	3623	3637	3651	rBV	3013993	5429858	1.40%	0.281%
24	11.846	3657	3675	3696	rBV3	91944157	179237855	46.19%	9.282%
25	11.959	3697	3717	3755	rVB7	165962080	388008614	100.00%	20.093%
26	12.283	3812	3838	3877	rVB3	95108951	182729378	47.09%	9.463%
27	12.578	3933	3948	3967	rVB	10727041	17763451	4.58%	0.920%
28	12.731	3991	4005	4024	rVB	2679540	4558593	1.17%	0.236%
29	12.919	4059	4075	4087	rBV2	22641290	37976127	9.79%	1.967%
30	12.983	4087	4099	4106	rBV2	56923832	98155749	25.30%	5.083%
31	13.058	4120	4127	4151	rVB2	27817174	44384765	11.44%	2.298%
32	13.222	4171	4188	4209	rBV2	41589206	72419075	18.66%	3.750%
33	13.369	4224	4243	4259	rBV3	117022664	214993811	55.41%	11.133%
34	13.704	4345	4368	4403	rVB2	44335656	80648742	20.79%	4.176%
35	13.839	4404	4418	4420	rBV	5082170	6377840	1.64%	0.330%
36	13.876	4421	4432	4468	rVB4	44655658	96443341	24.86%	4.994%

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37	14.061	4487	4501	4515	rVB2	7237107	13515522	3.48%	0.700%
38	14.131	4515	4527	4532	rBV	7840728	12429231	3.20%	0.644%
39	14.217	4548	4559	4571	rVB	11443376	17899643	4.61%	0.927%
40	14.278	4571	4582	4590	rVV	2881123	4638594	1.20%	0.240%
41	14.327	4590	4600	4620	rVB2	10034572	17155639	4.42%	0.888%
42	14.458	4637	4649	4662	rVB	3440541	5438185	1.40%	0.282%
43	14.539	4663	4679	4686	rBV	6406504	10373965	2.67%	0.537%
44	14.579	4686	4694	4705	rVB	8441981	13014879	3.35%	0.674%
45	14.809	4768	4780	4792	rBV	9067265	14442079	3.72%	0.748%
46	14.930	4806	4825	4838	rBV3	15079849	30122026	7.76%	1.560%
47	14.995	4838	4849	4865	rVB3	2462476	4505961	1.16%	0.233%
48	15.083	4868	4882	4899	rBV	3665387	6587131	1.70%	0.341%
49	15.196	4900	4924	4935	rBV6	2690195	6794108	1.75%	0.352%
50	15.311	4951	4967	4988	rVB3	1783345	4323484	1.11%	0.224%
51	15.504	5022	5039	5059	rVB2	27725962	53312503	13.74%	2.761%
52	16.617	5437	5454	5485	rVB	5031551	11372183	2.93%	0.589%

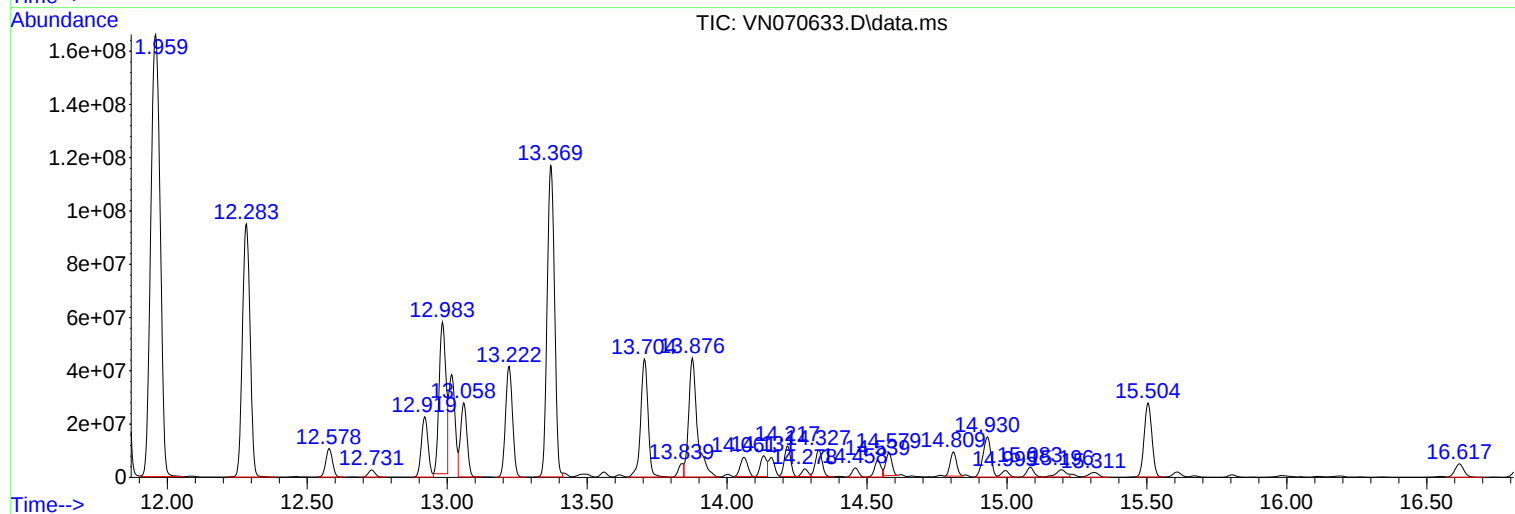
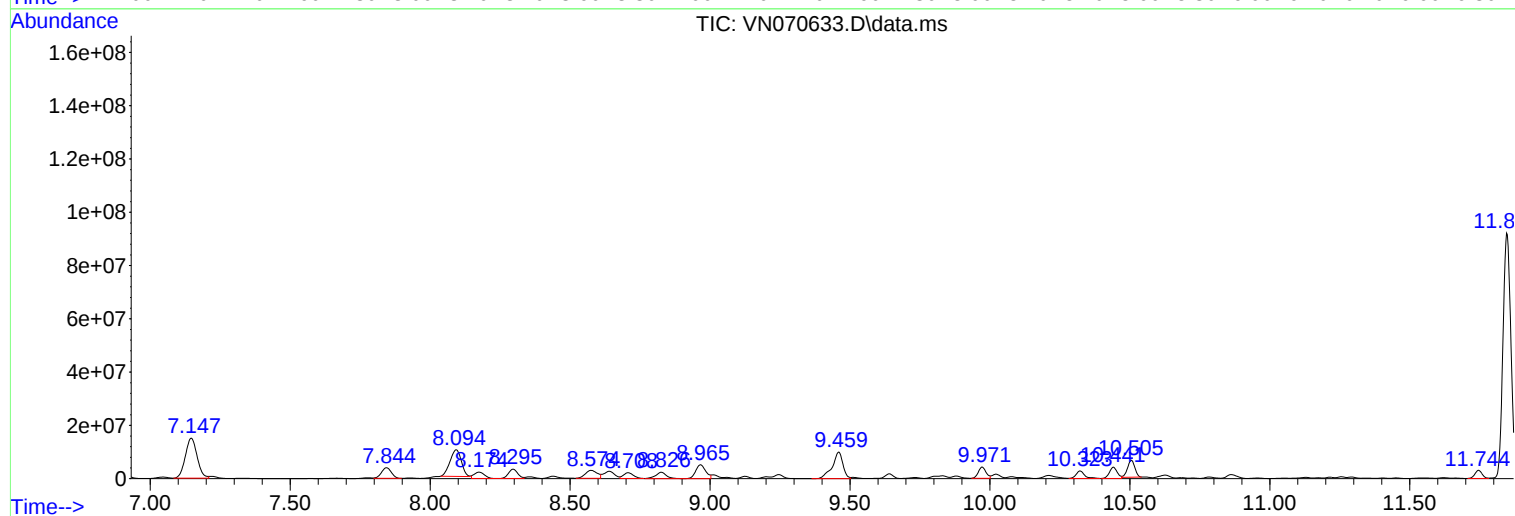
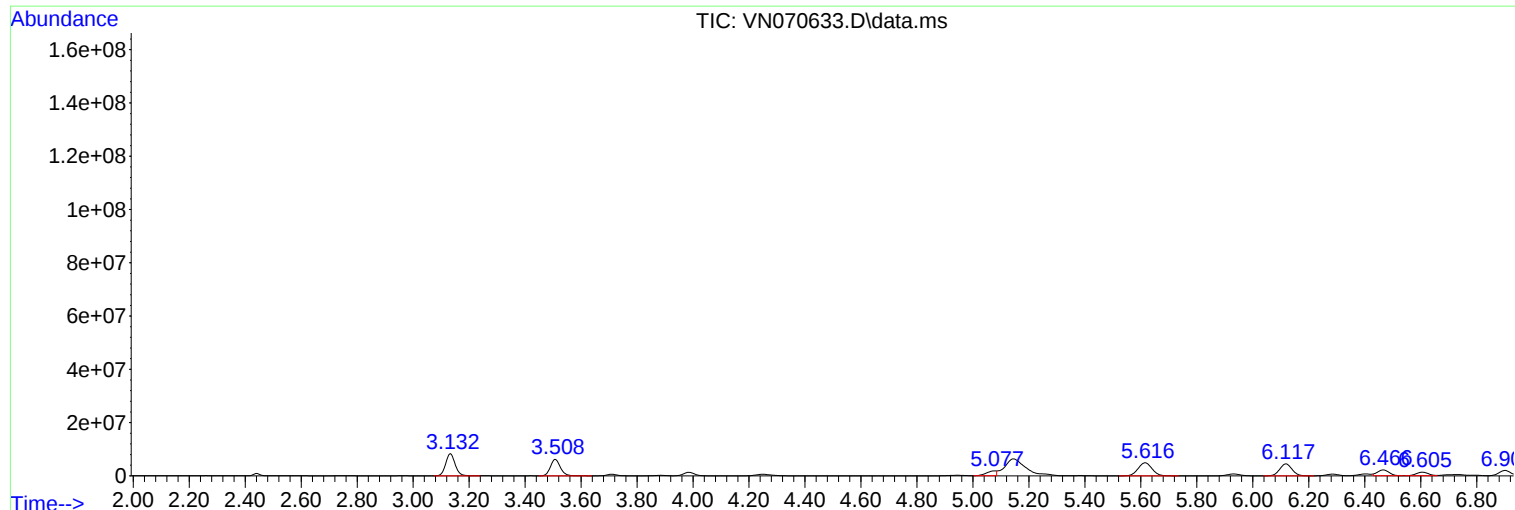
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Quant Title : SW846 8260

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



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ClientSampleId :
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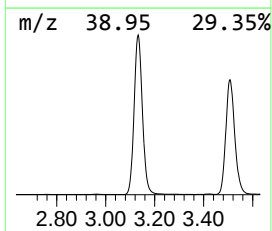
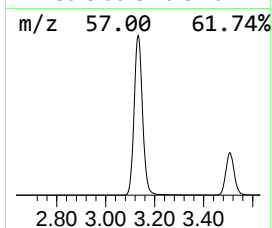
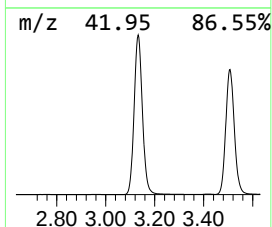
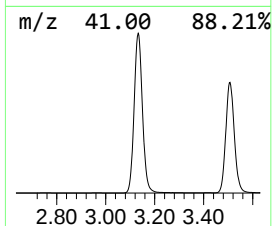
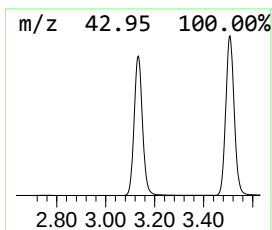
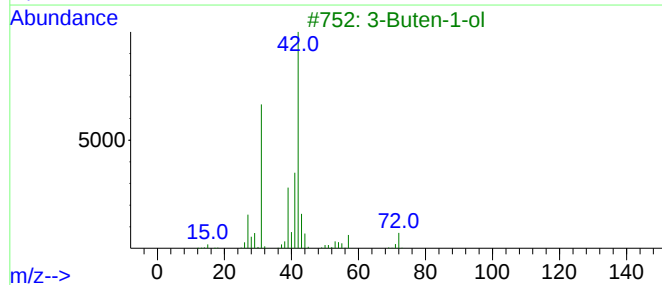
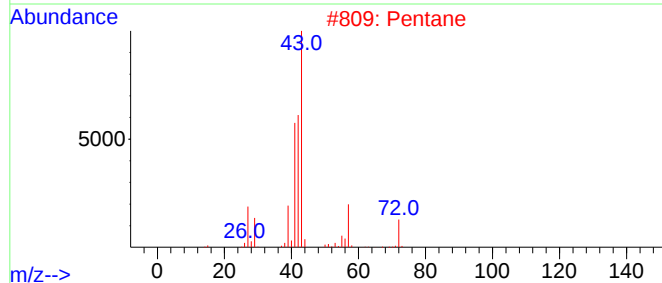
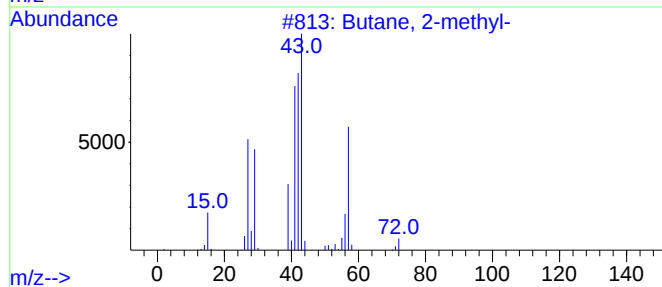
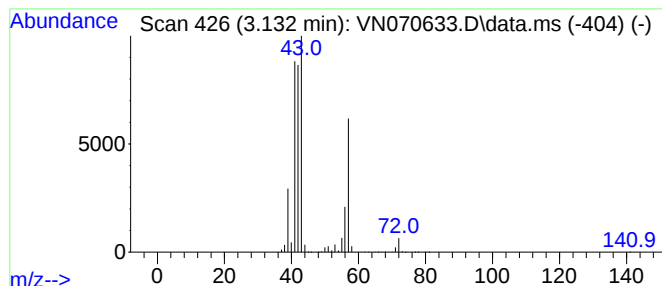
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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.
3.132	34.83 ug/l	19552500	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	33
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			Methane, isocyanato-	57	C2H3NO	000624-83-9	9
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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Instrument :
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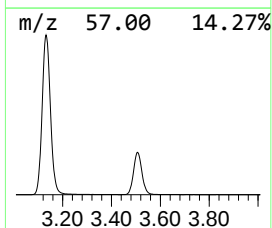
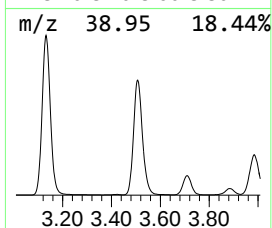
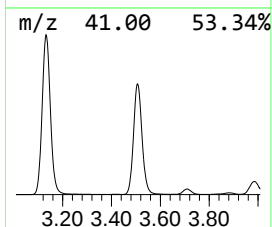
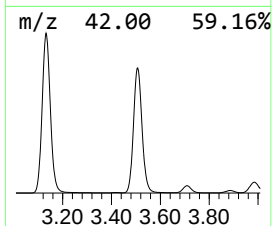
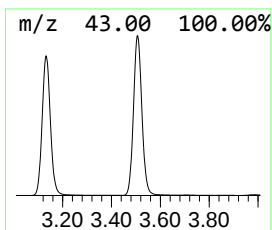
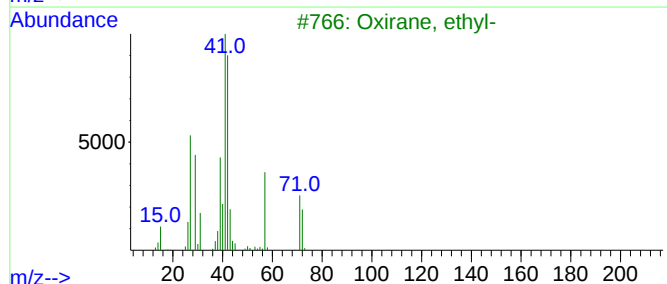
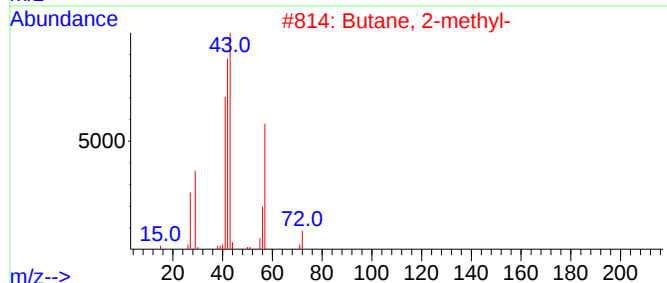
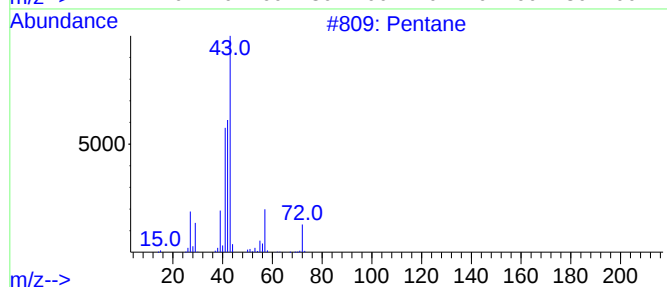
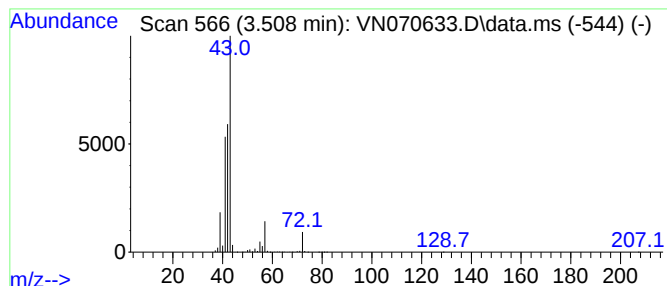
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.508	27.24 ug/l	15291600	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	91
2			Butane, 2-methyl-	72	C5H12	000078-78-4	50
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	9
4			Butanenitrile, 2-hydroxy-3-methyl-	99	C5H9NO	010021-64-4	9
5			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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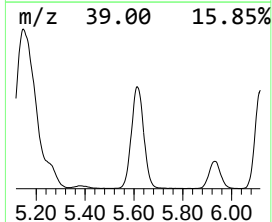
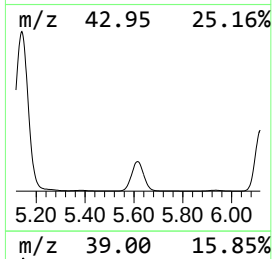
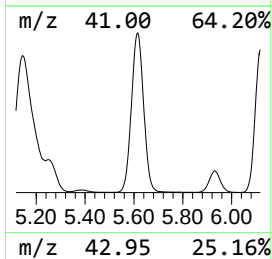
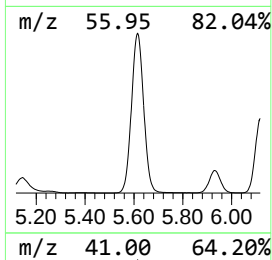
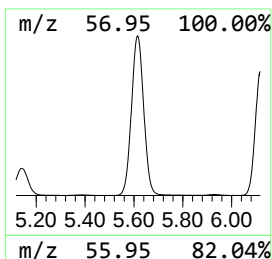
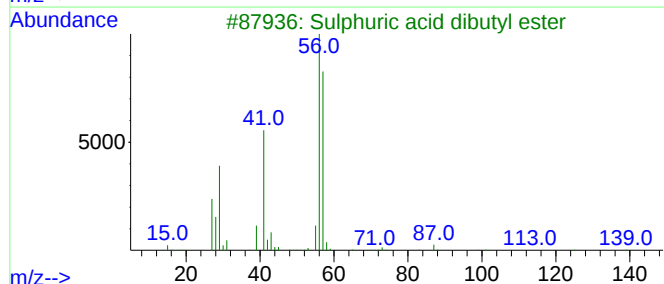
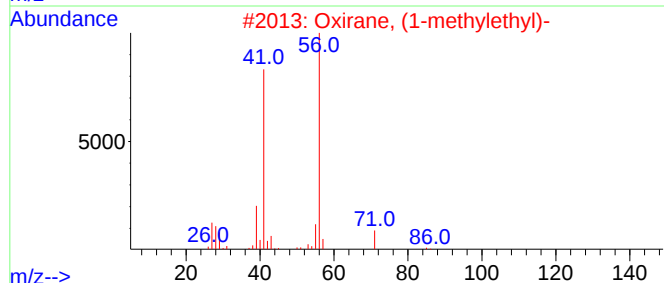
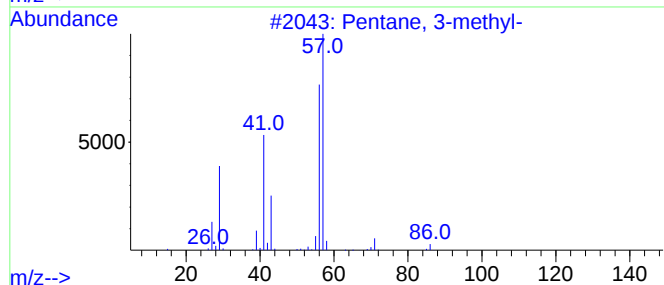
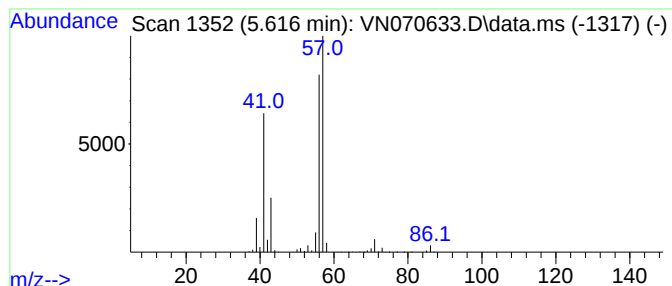
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Quant Title : SW846 8260

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

Peak Number 3 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.616	30.44 ug/l	17090000	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
3			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	43
4			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	40
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	40



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Instrument :
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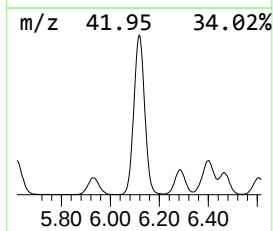
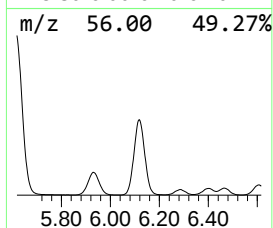
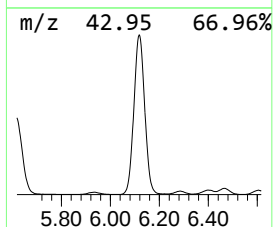
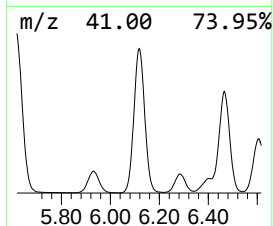
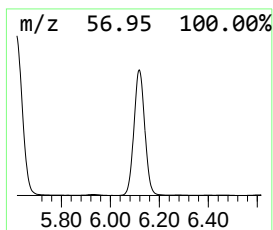
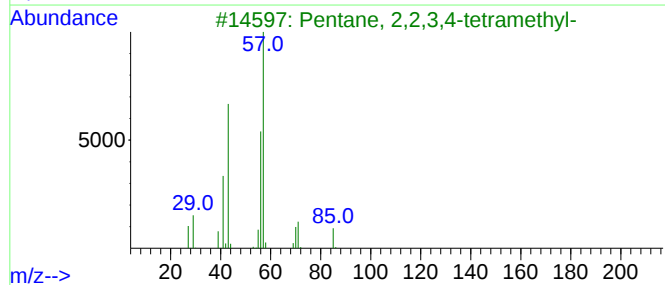
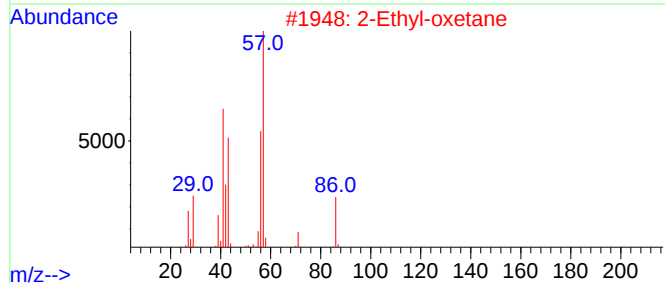
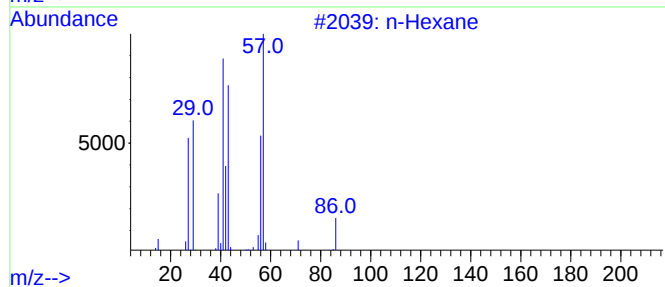
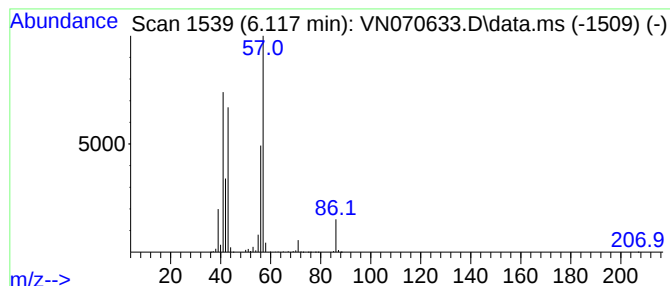
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 4 n-Hexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.117	24.67 ug/l	13849800	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	91
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	53
3			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
4			Butanal, 2-methyl-	86	C5H10O	000096-17-3	38
5			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38



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MW-46

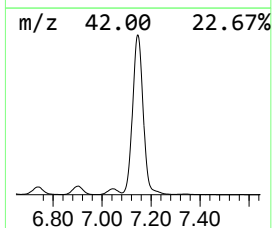
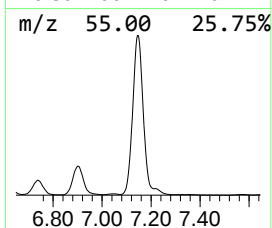
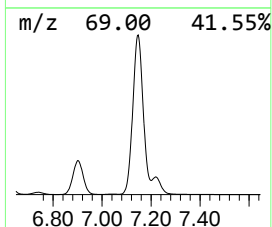
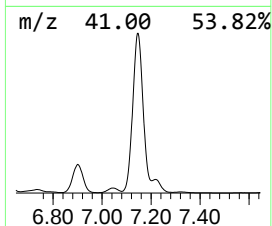
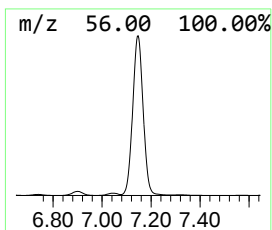
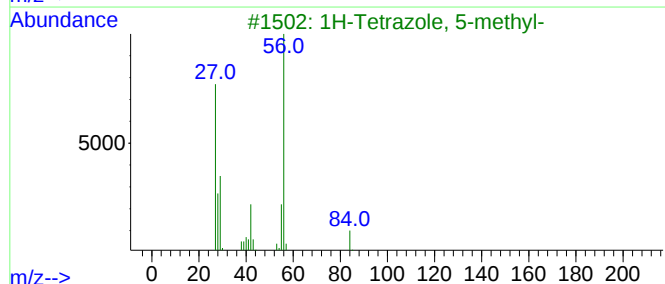
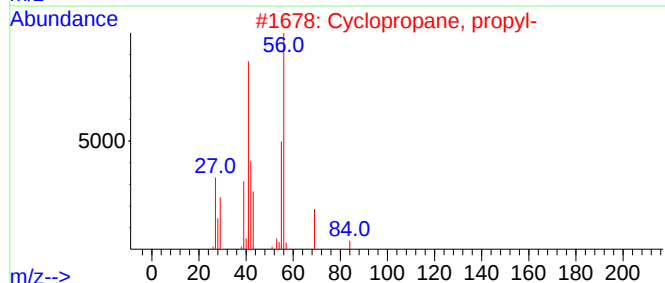
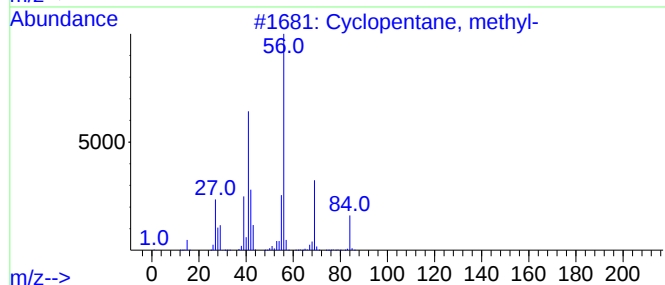
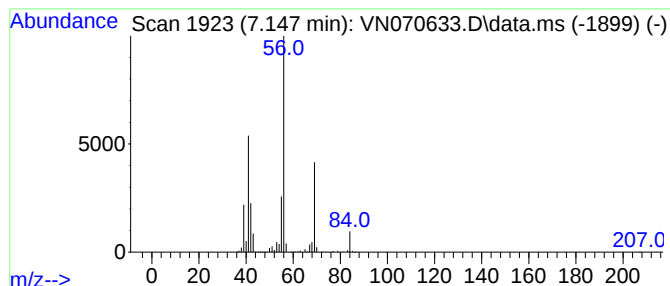
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.147	78.13 ug/l	43857000	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopropane, propyl-	84	C6H12	002415-72-7	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070633.D
Acq On : 14 Jan 2022 19:28
Operator : JC/MD
Sample : N1148-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-46

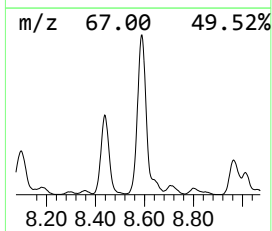
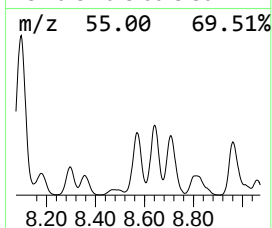
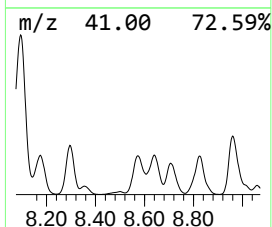
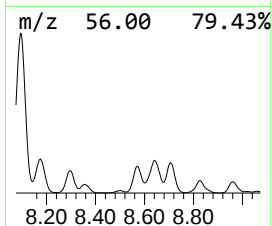
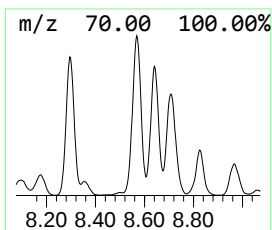
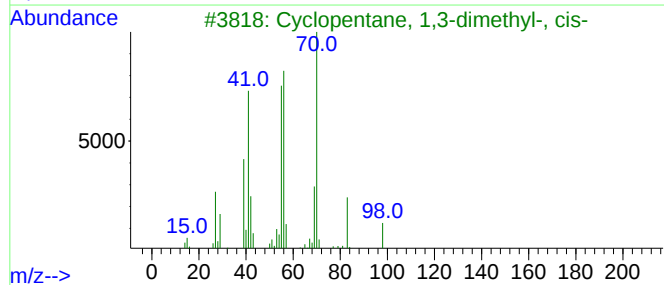
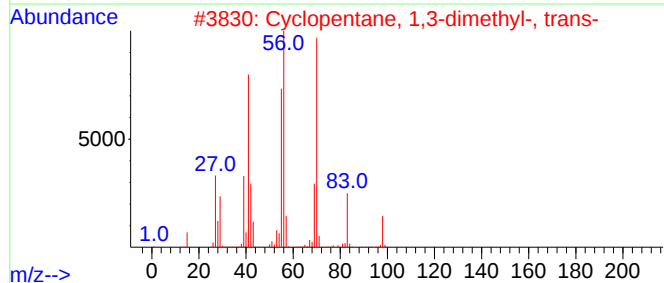
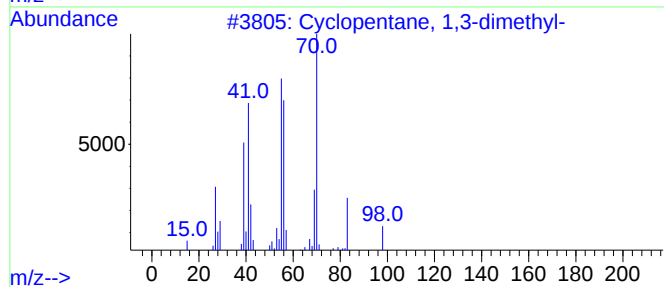
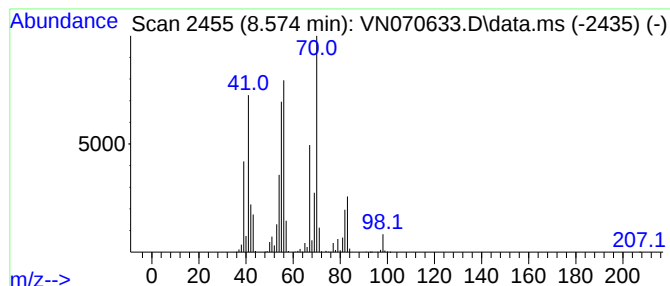
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, 1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.574	33.81 ug/l	8761730	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	76
2			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	64
3			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	64
4			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	60
5			Isopropylcyclobutane	98	C7H14	000872-56-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070633.D
Acq On : 14 Jan 2022 19:28
Operator : JC/MD
Sample : N1148-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-46

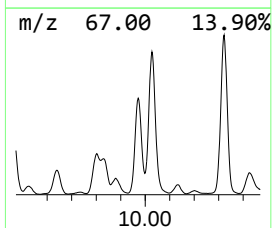
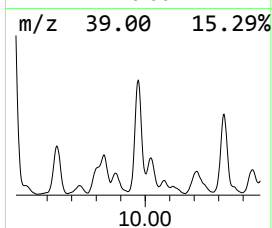
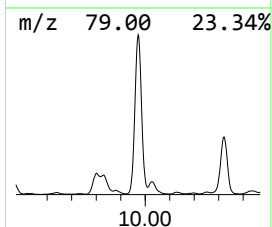
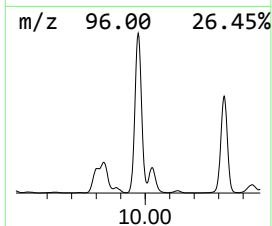
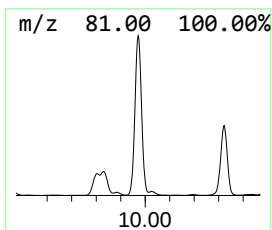
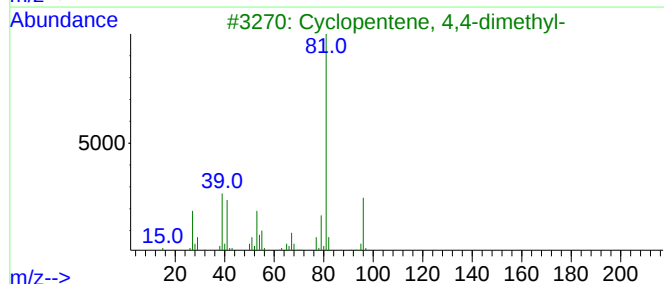
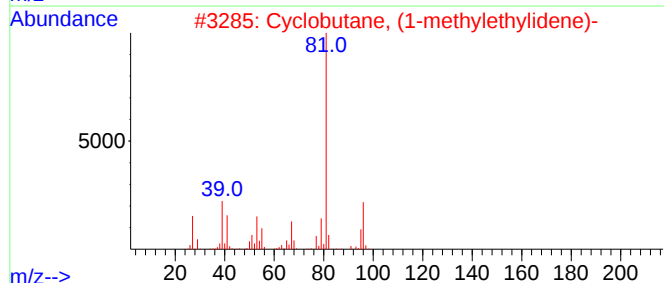
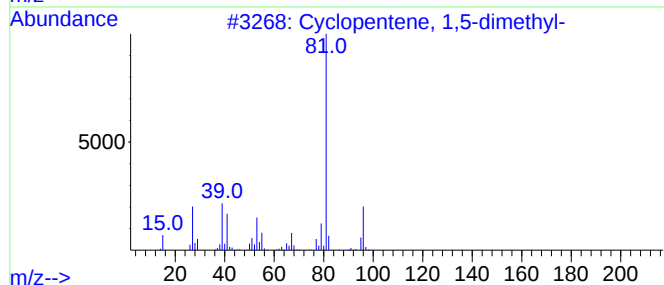
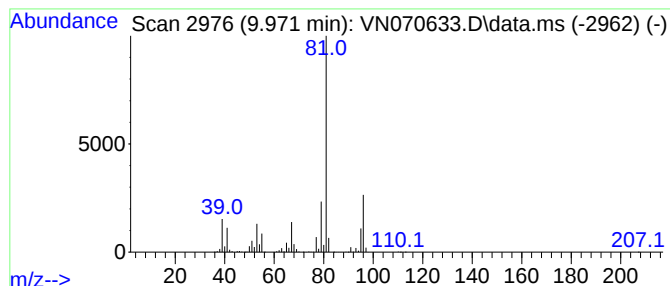
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Quant Title : SW846 8260

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

Peak Number 7 Cyclopentene, 1,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.971	31.01 ug/l	8035690	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	90
2			Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
3			Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	87
4			Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	86
5			3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070633.D
Acq On : 14 Jan 2022 19:28
Operator : JC/MD
Sample : N1148-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-46

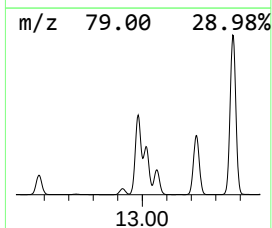
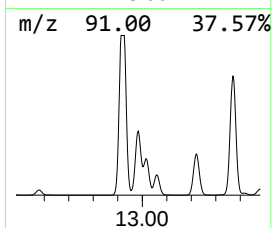
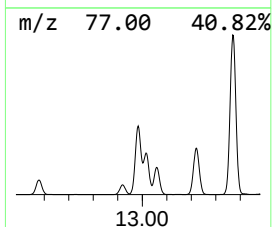
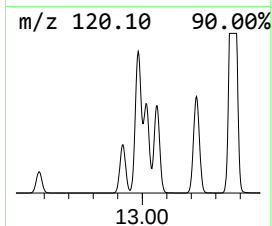
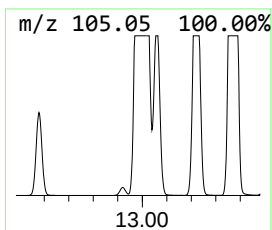
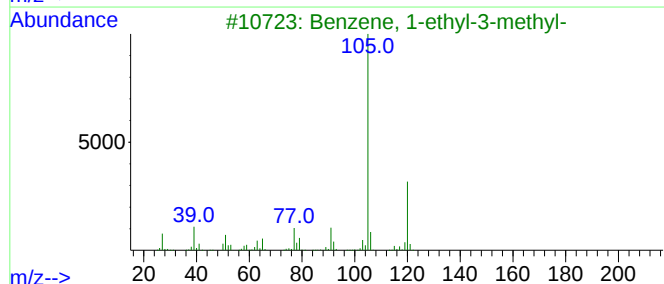
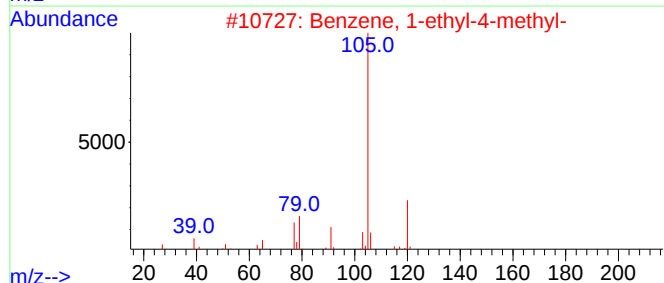
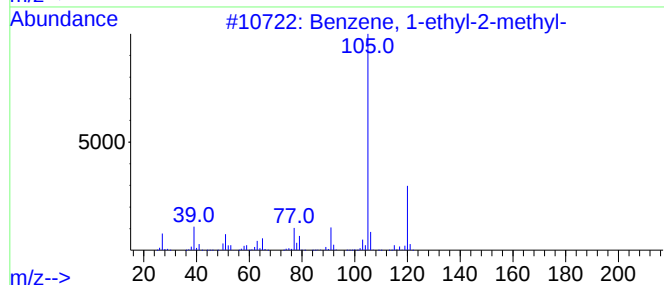
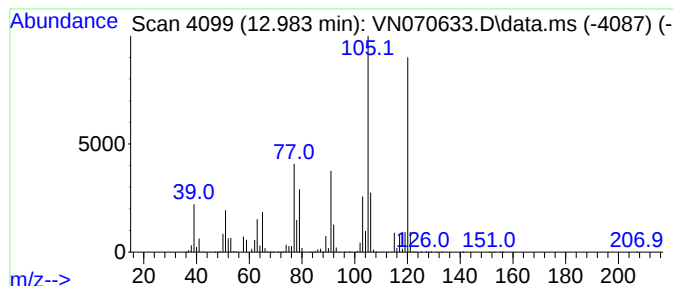
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	60.85 ug/l	98155700	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	81
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	81
4			1,3-Cyclopentadiene, 5-(1-methyl...	120	C9H12	003141-02-4	80
5			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070633.D
Acq On : 14 Jan 2022 19:28
Operator : JC/MD
Sample : N1148-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-46

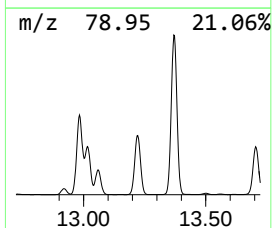
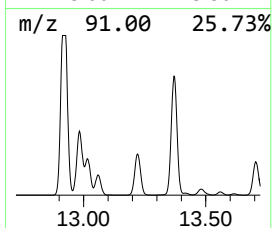
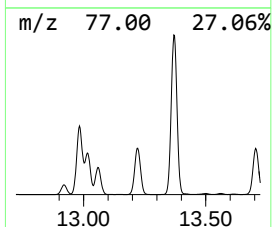
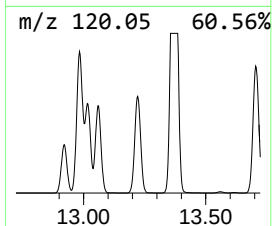
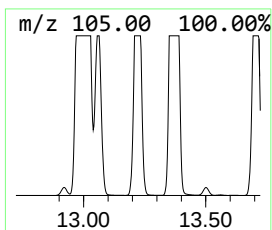
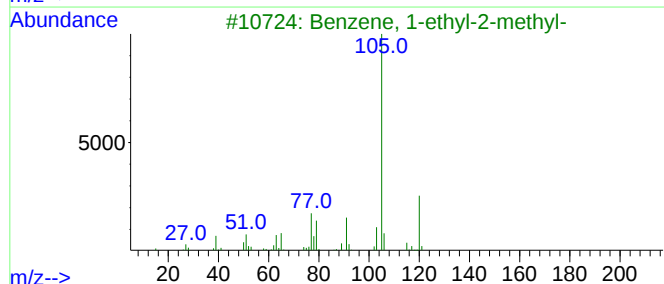
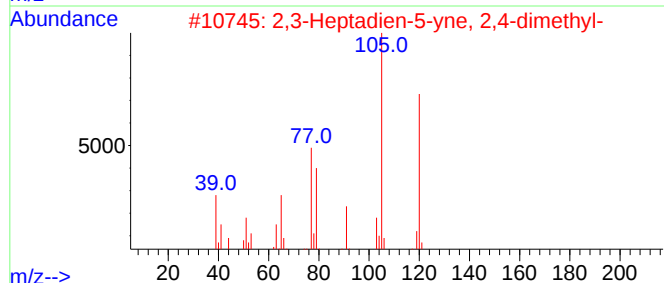
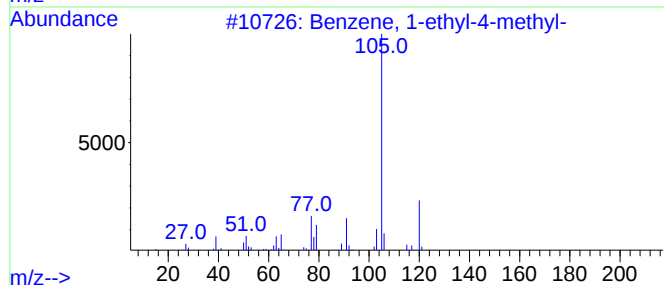
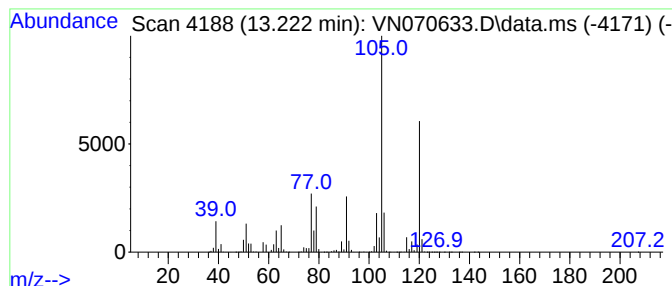
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1-ethyl-4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	44.90 ug/l	72419100	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	87
2			2,3-Heptadien-5-yne, 2,4-dimethyl-	120	C9H12	041898-89-9	87
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	83
5			1,3-Cyclopentadiene, 5-(1-methyl...	120	C9H12	003141-02-4	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070633.D
Acq On : 14 Jan 2022 19:28
Operator : JC/MD
Sample : N1148-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-46

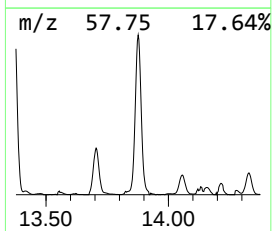
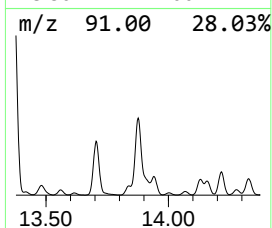
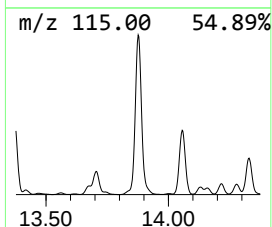
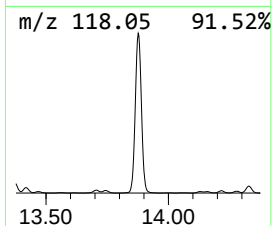
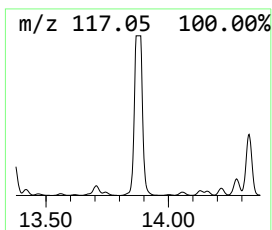
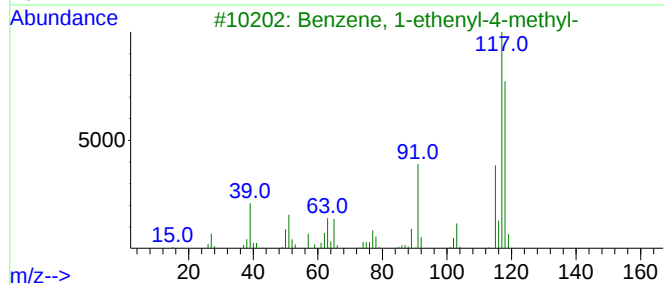
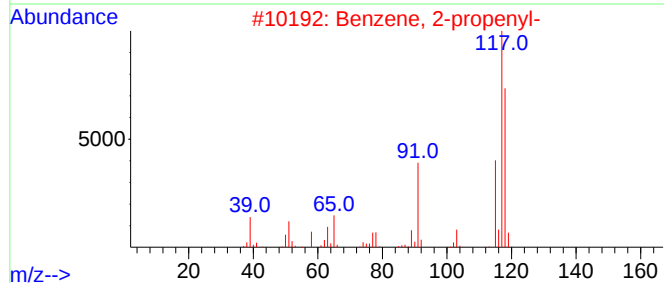
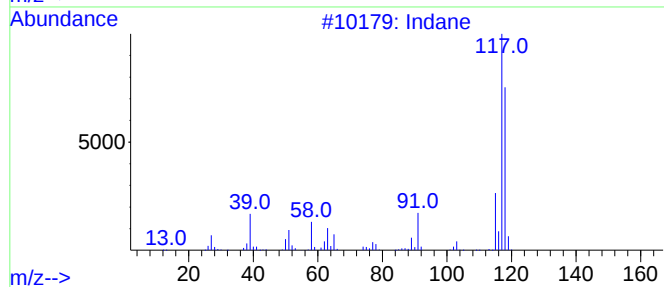
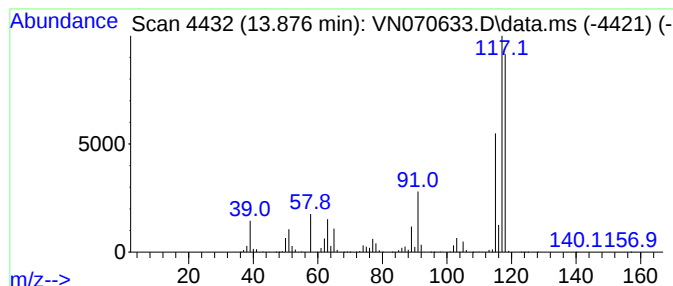
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	59.79 ug/l	96443300	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
Data File : VN070633.D
Acq On : 14 Jan 2022 19:28
Operator : JC/MD
Sample : N1148-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-46

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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					#	RT	Resp	Conc
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Pentane	3.508	27.2	ug/l	15291600	1	8.086	28067100	50.0
Pentane, 3-methyl-	5.616	30.4	ug/l	17090000	1	8.086	28067100	50.0
n-Hexane	6.117	24.7	ug/l	13849800	1	8.086	28067100	50.0
Cyclopentane, m...	7.147	78.1	ug/l	43857000	1	8.086	28067100	50.0
Cyclopentane, 1...	8.574	33.8	ug/l	8761730	2	8.968	12956600	50.0
Cyclopentene, 1...	9.971	31.0	ug/l	8035690	2	8.968	12956600	50.0
Benzene, 1-ethy...	12.983	60.9	ug/l	98155700	4	13.675	80648700	50.0
Benzene, 1-ethy...	13.222	44.9	ug/l	72419100	4	13.675	80648700	50.0
Indane	13.876	59.8	ug/l	96443300	4	13.675	80648700	50.0