

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011722\
 Data File : VN070649.D
 Acq On : 17 Jan 2022 16:54
 Operator : JC/MD
 Sample : N1141-04 10X
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41861

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: VN070649.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.021	2224	2249	2257	rBV	682935	1633159	10.40%	2.785%
2	8.080	2259	2271	2291	rVV3	1698451	4360762	27.78%	7.437%
3	8.171	2292	2305	2329	rVB2	217075	532032	3.39%	0.907%
4	8.295	2329	2351	2384	rBV	832965	1959575	12.48%	3.342%
5	8.437	2385	2404	2429	rBV	862403	1962059	12.50%	3.346%
6	8.557	2432	2449	2465	rBV4	116748	293935	1.87%	0.501%
7	8.826	2531	2549	2575	rVB	764093	1562497	9.95%	2.665%
8	8.965	2581	2601	2627	rBV	2078777	4333667	27.61%	7.391%
9	9.456	2756	2784	2797	rBV2	171210	441209	2.81%	0.752%
10	10.440	3133	3151	3162	rBV	3090098	5775708	36.80%	9.851%
11	10.505	3162	3175	3203	rVB	8409466	15696436	100.00%	26.771%
12	11.526	3538	3556	3581	rVB4	177668	460662	2.93%	0.786%
13	11.628	3581	3594	3610	rBV	145116	249618	1.59%	0.426%
14	11.744	3619	3637	3658	rBV	2830181	5160885	32.88%	8.802%
15	11.956	3697	3716	3738	rBV4	1213224	2468354	15.73%	4.210%
16	12.277	3811	3836	3853	rBV3	273461	872847	5.56%	1.489%
17	12.366	3861	3869	3881	rVB	106451	171596	1.09%	0.293%
18	12.731	3993	4005	4030	rVB	2251550	4125565	26.28%	7.036%
19	12.980	4086	4098	4107	rBV	223452	409071	2.61%	0.698%
20	13.047	4113	4123	4138	rVB3	796901	1444497	9.20%	2.464%
21	13.221	4171	4188	4203	rBV4	69939	219674	1.40%	0.375%
22	13.369	4230	4243	4255	rBV	382664	637048	4.06%	1.086%
23	13.675	4342	4357	4377	rVB	2050876	3704479	23.60%	6.318%
24	13.994	4466	4476	4487	rBV4	102724	157752	1.01%	0.269%

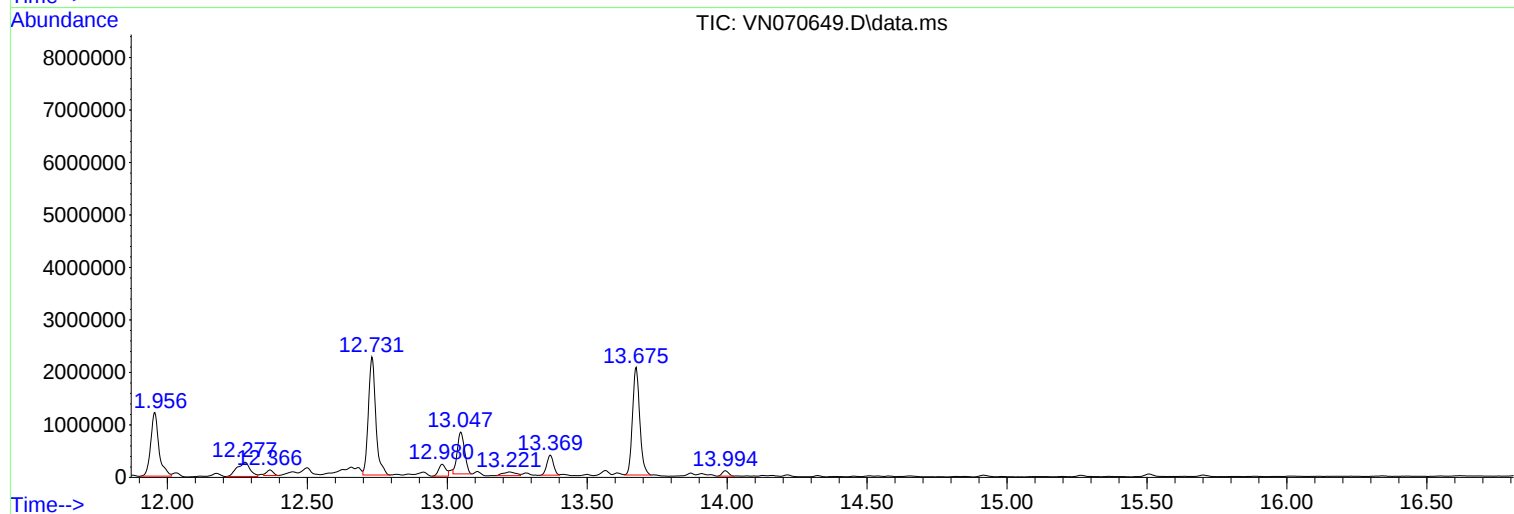
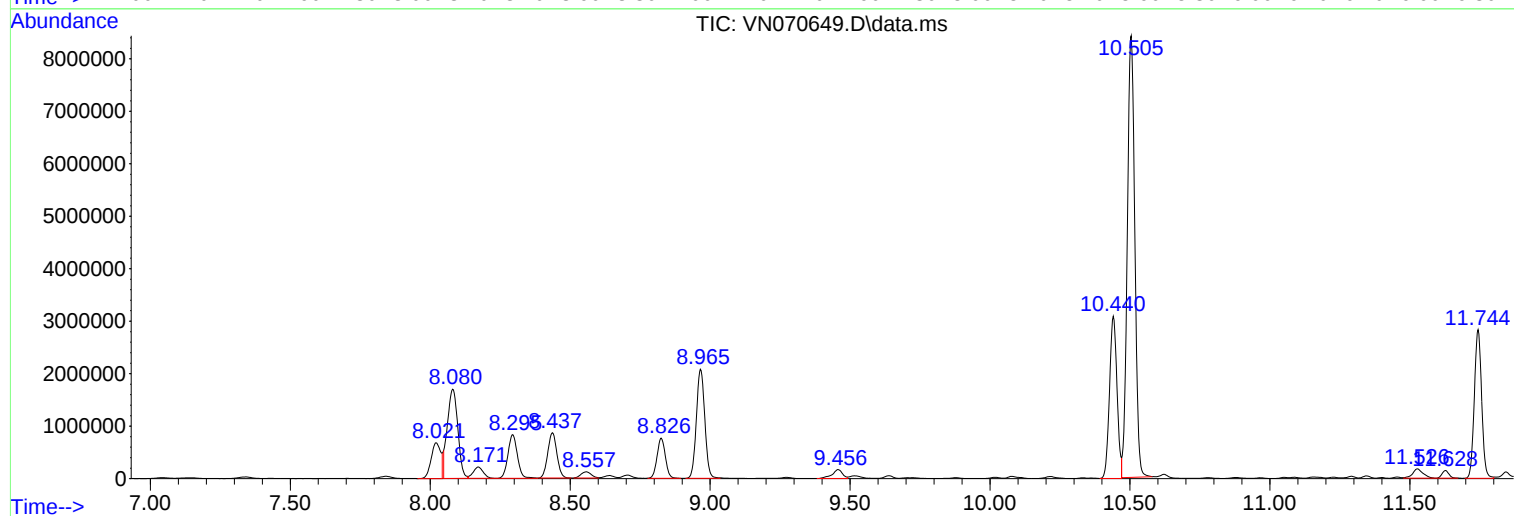
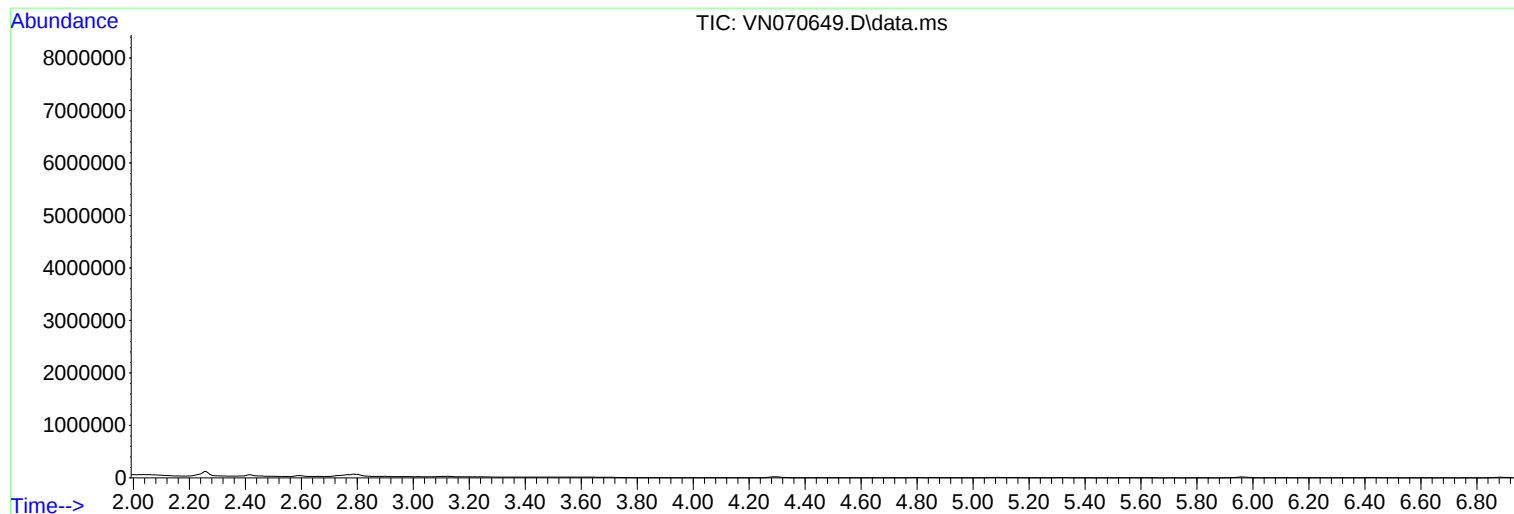
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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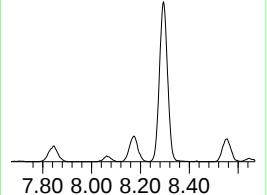
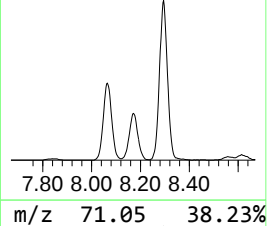
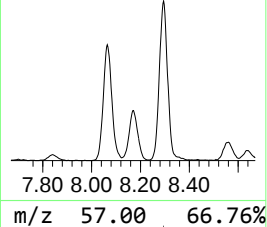
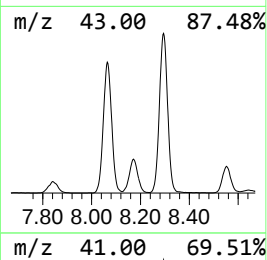
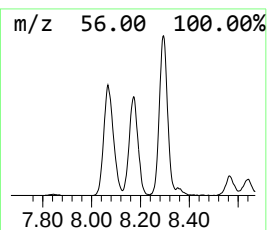
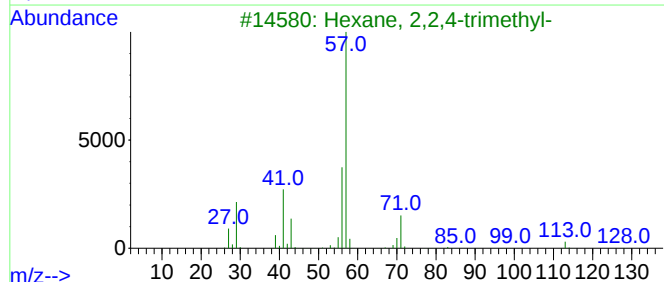
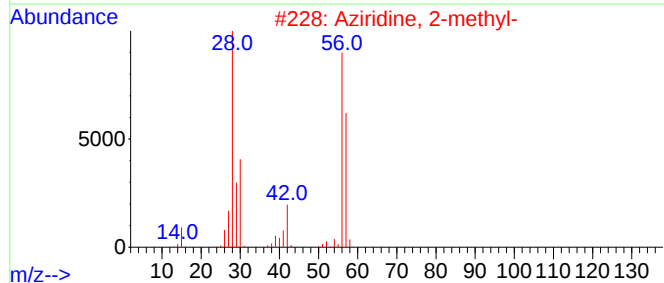
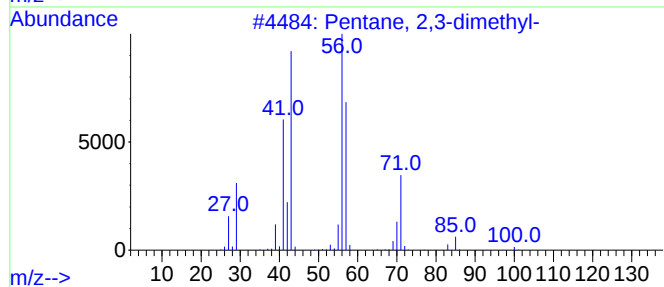
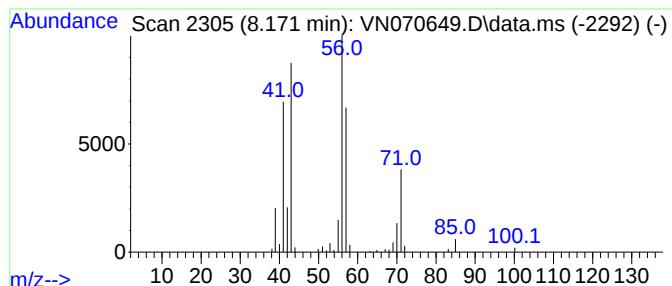
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.171	6.10 ug/l	532032	Pentafluorobenzene	8.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	94
2			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
4			Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	38
5			1,4-Dioxaspiro[2.4]heptan-5-one,...	142	C7H10O3	126091-79-0	37



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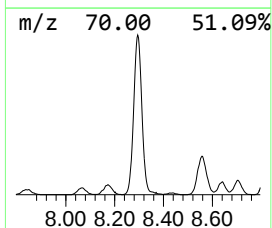
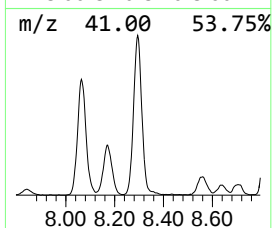
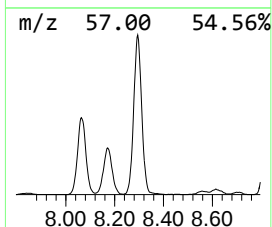
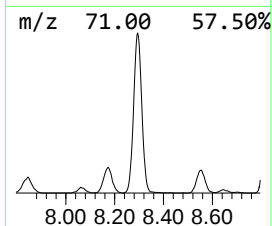
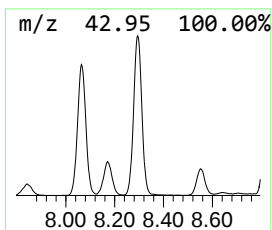
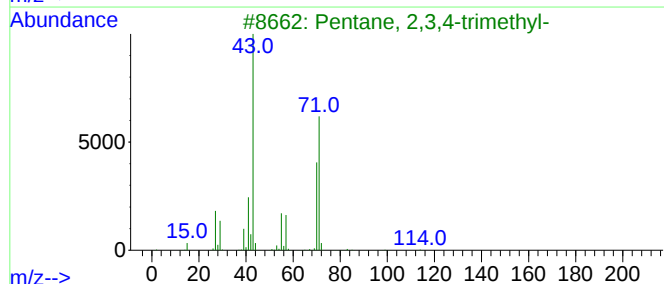
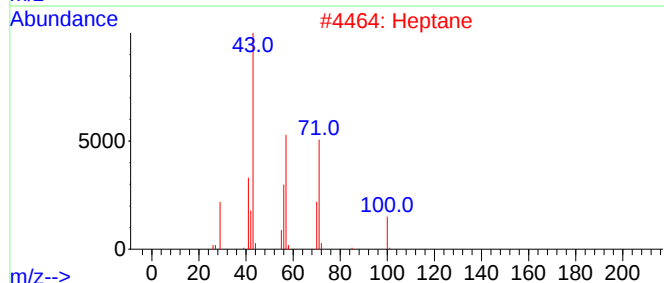
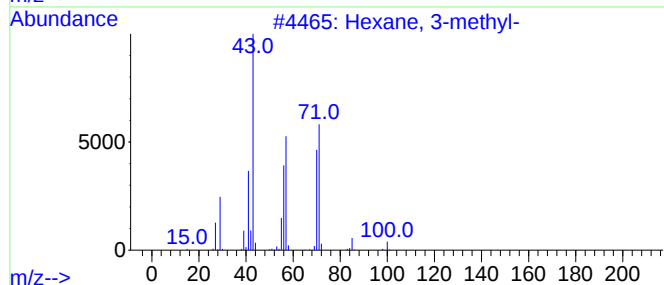
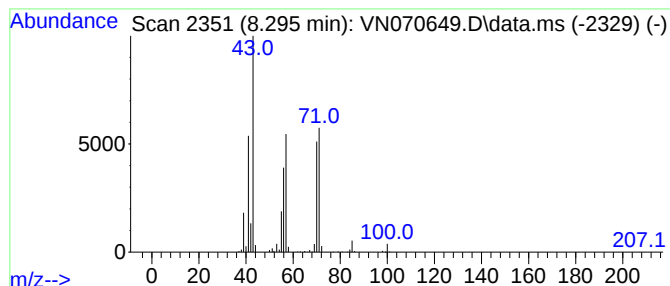
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.295	22.47 ug/l	1959580	Pentafluorobenzene	8.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2			Heptane	100	C7H16	000142-82-5	72
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	53



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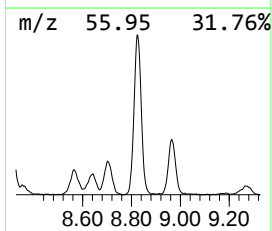
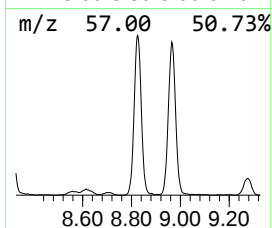
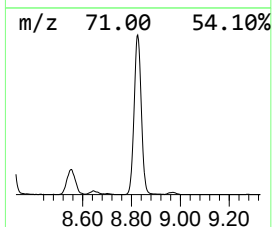
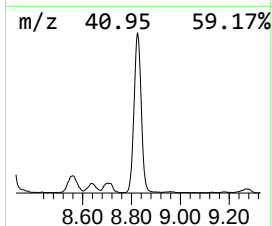
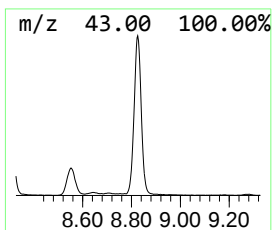
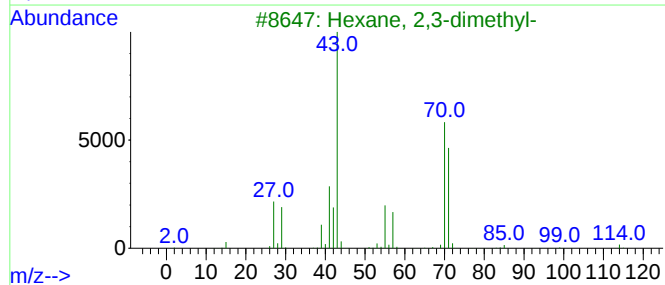
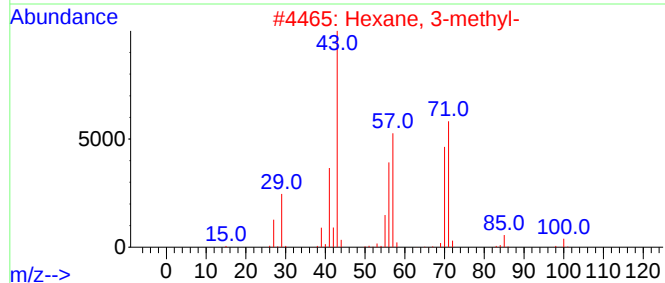
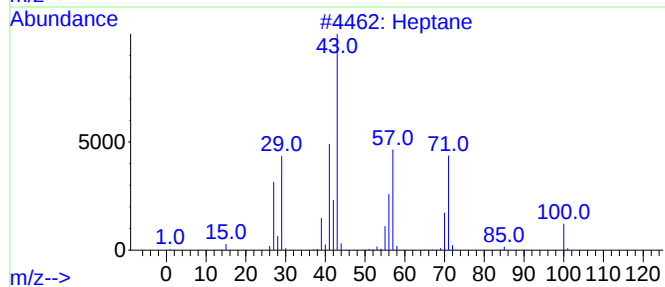
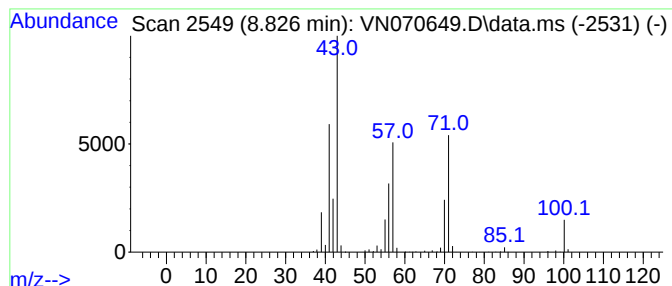
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Quant Title : SW846 8260

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

Peak Number 3 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.826	18.03 ug/l	1562500	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	94
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	47
3			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
5			Pentane, 2-methyl-	86	C6H14	000107-83-5	38



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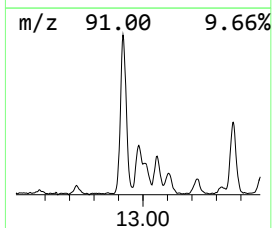
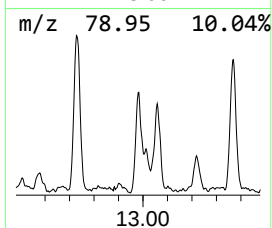
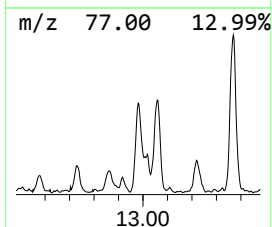
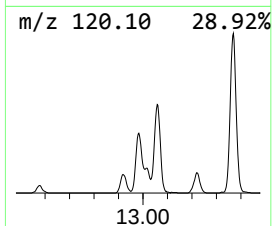
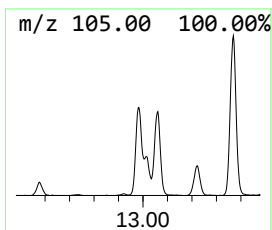
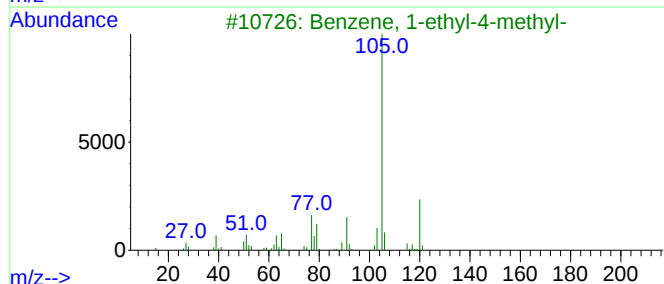
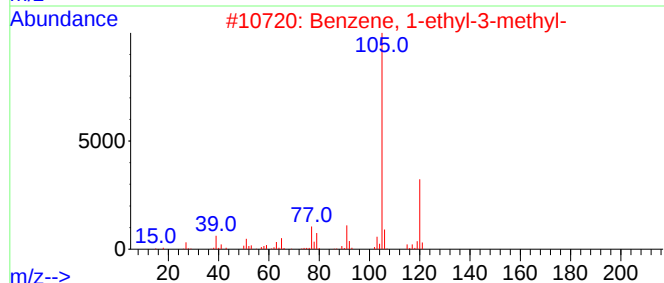
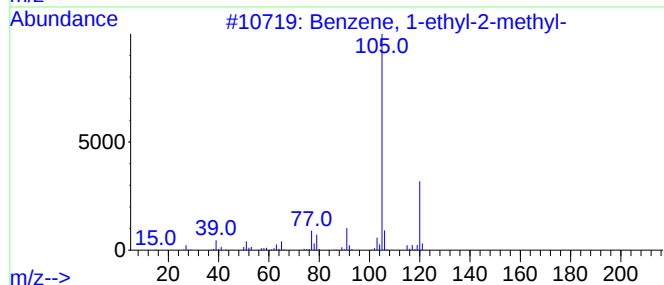
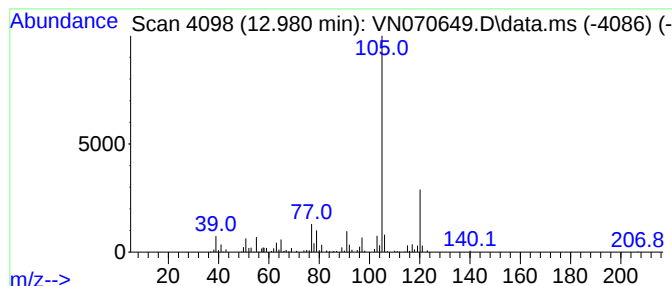
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	5.52 ug/l	409071	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	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.171	6.1	ug/l	532032	1	8.085	4360760	50.0
Hexane, 3-methyl-	8.295	22.5	ug/l	1959580	1	8.085	4360760	50.0
Heptane	8.826	18.0	ug/l	1562500	2	8.965	4333670	50.0
Benzene, 1-ethy...	12.980	5.5	ug/l	409071	4	13.675	3704480	50.0