

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011422\
 Data File : VN070624.D
 Acq On : 14 Jan 2022 15:38
 Operator : JC/MD
 Sample : N1141-04 10X
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 12 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: VN070624.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	2225	2249	2257	rBV2	596554	1427918	11.62%	3.075%
2	8.080	2260	2271	2291	rVV2	1203360	3047017	24.80%	6.561%
3	8.171	2291	2305	2330	rVB3	162844	414511	3.37%	0.893%
4	8.292	2330	2350	2384	rBV2	633507	1513149	12.31%	3.258%
5	8.437	2385	2404	2428	rBV2	749547	1714311	13.95%	3.692%
6	8.555	2432	2448	2464	rBV5	89194	230485	1.88%	0.496%
7	8.826	2531	2549	2578	rBV2	590532	1246096	10.14%	2.683%
8	8.965	2582	2601	2632	rBV	1469846	3101706	25.24%	6.679%
9	9.459	2756	2785	2797	rBV3	140512	361033	2.94%	0.777%
10	10.440	3133	3151	3162	rBV	2618233	4811740	39.16%	10.361%
11	10.505	3162	3175	3206	rVB	6651969	12287837	100.00%	26.460%
12	11.527	3545	3556	3581	rVB5	149620	359841	2.93%	0.775%
13	11.629	3584	3594	3617	rVB	126590	219167	1.78%	0.472%
14	11.744	3621	3637	3658	rBV	2081556	3756704	30.57%	8.089%
15	11.843	3665	3674	3695	rVB	111476	197279	1.61%	0.425%
16	11.956	3699	3716	3738	rBV5	1084442	2197043	17.88%	4.731%
17	12.280	3815	3837	3853	rBV3	236143	717132	5.84%	1.544%
18	12.731	3993	4005	4031	rVB	2034436	3778773	30.75%	8.137%
19	12.983	4089	4099	4107	rBV	174704	306468	2.49%	0.660%
20	13.050	4113	4124	4138	rVB4	736100	1275746	10.38%	2.747%
21	13.369	4233	4243	4255	rBV	281876	447058	3.64%	0.963%
22	13.675	4344	4357	4377	rVB	1626099	2875148	23.40%	6.191%
23	13.994	4470	4476	4489	rVB4	106631	153179	1.25%	0.330%

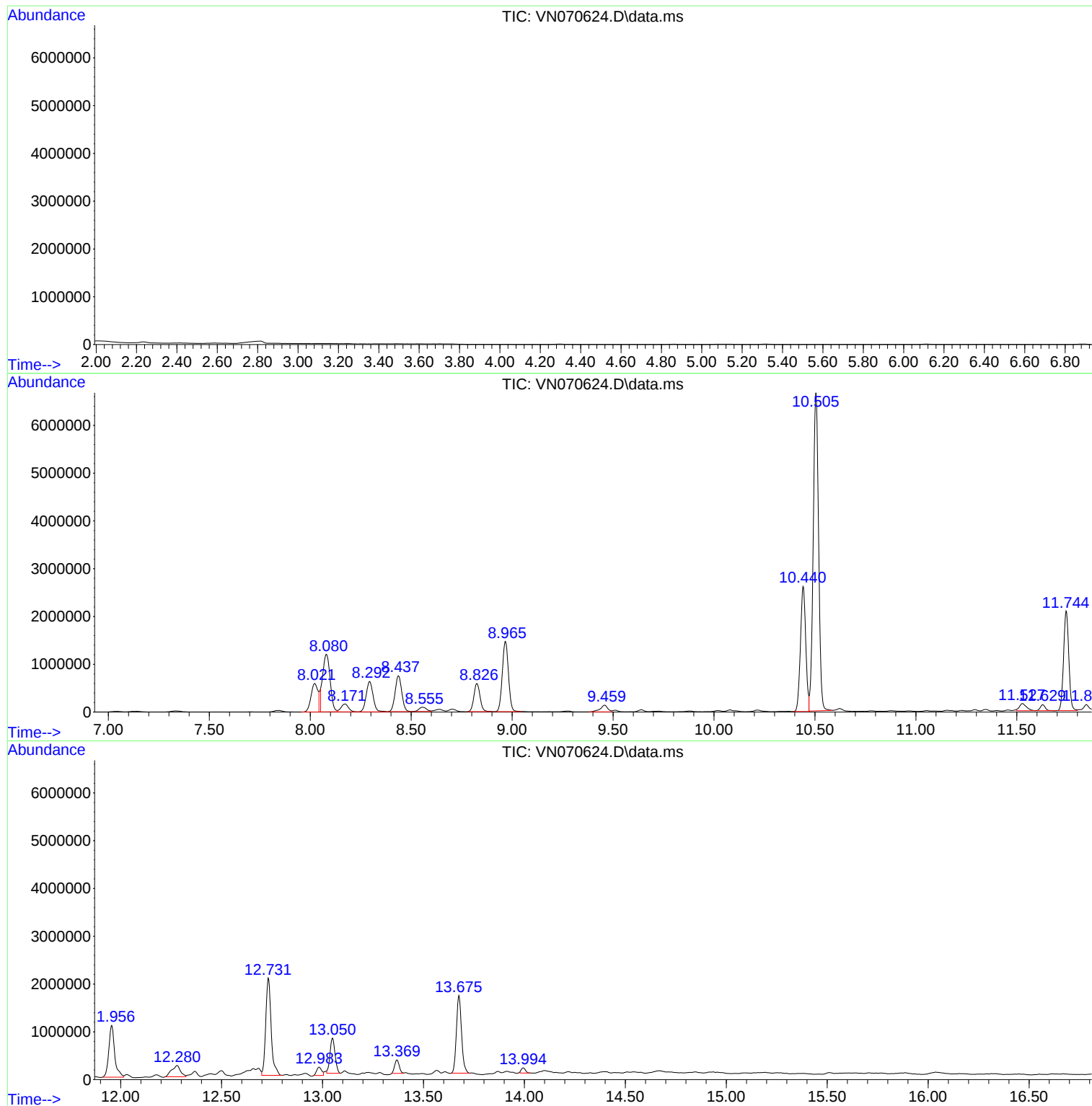
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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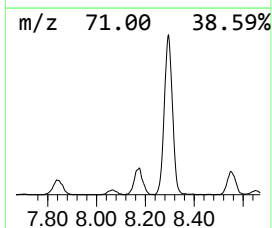
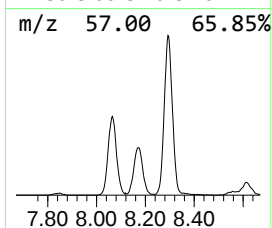
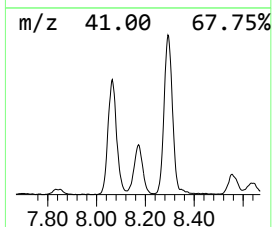
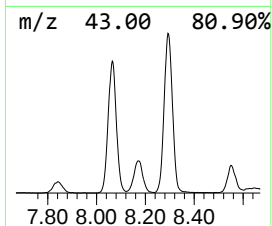
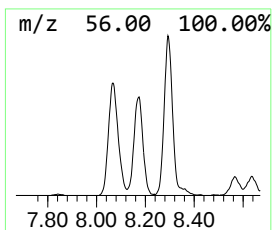
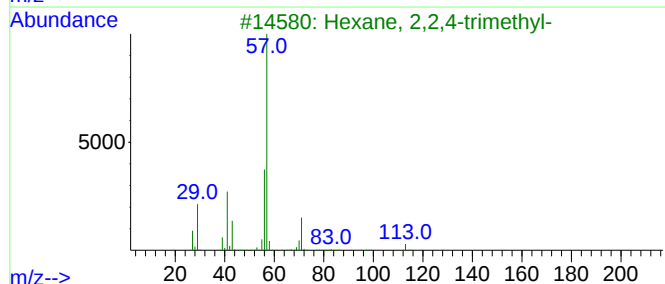
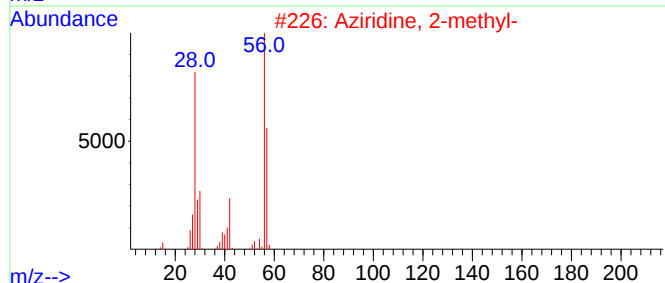
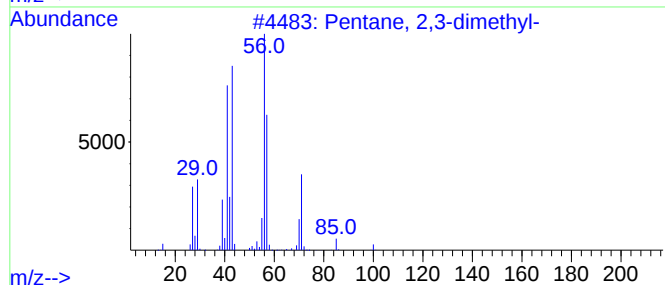
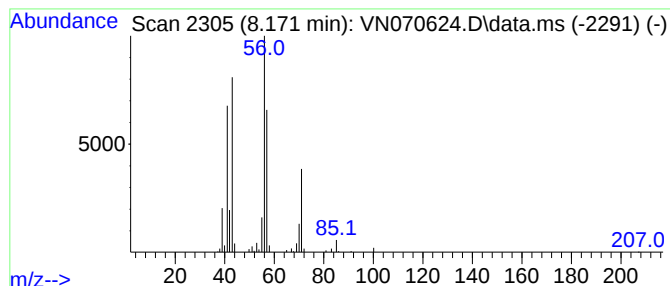
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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	6.80 ug/l	414511	Pentafluorobenzene	8.083

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	46
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45
4			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
5			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38



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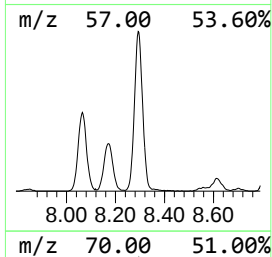
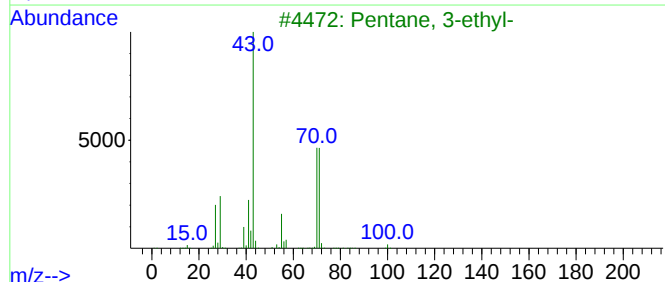
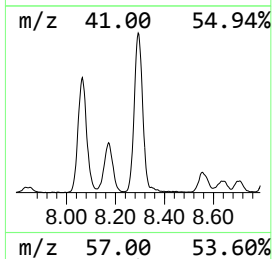
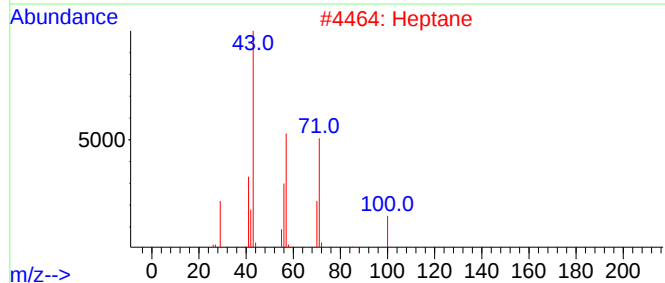
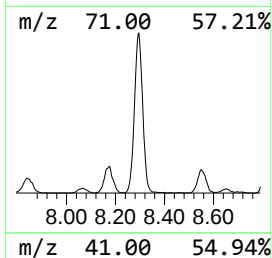
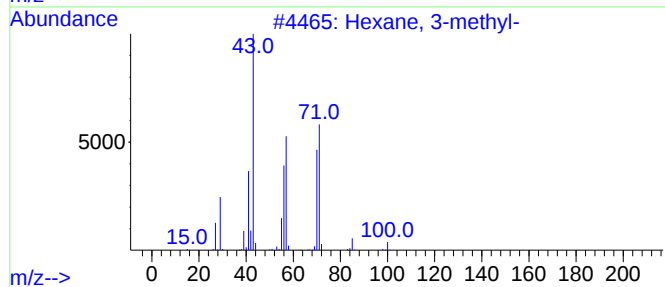
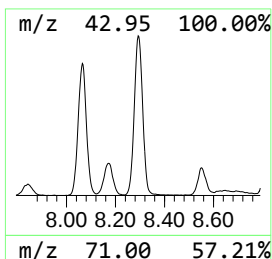
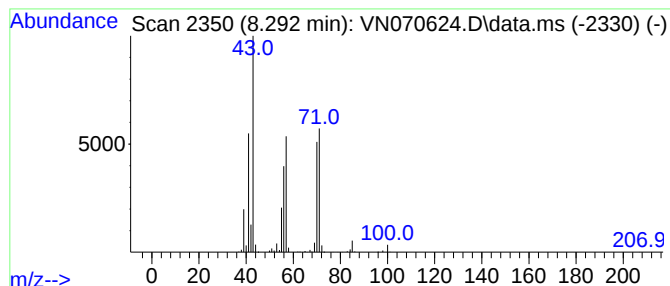
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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.
8.292	24.83 ug/l	1513150	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	59
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	58
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
5			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	50



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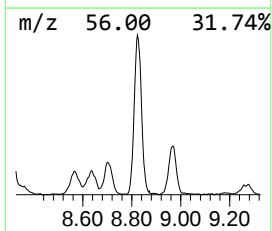
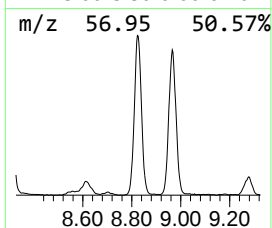
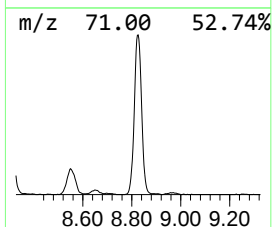
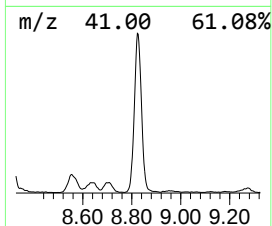
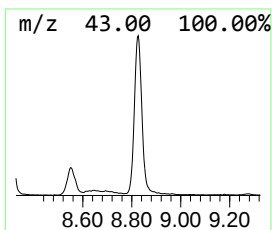
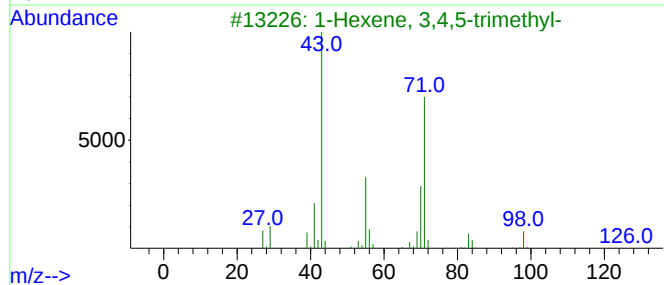
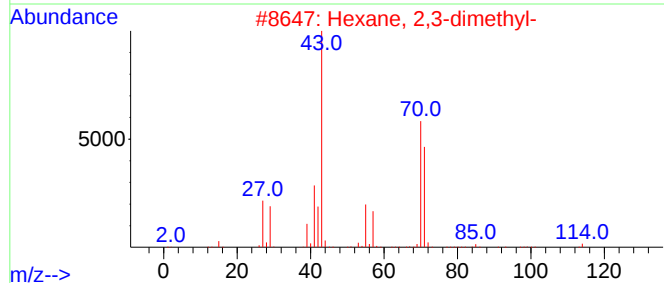
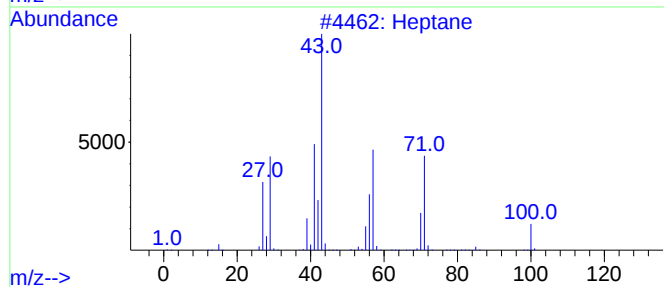
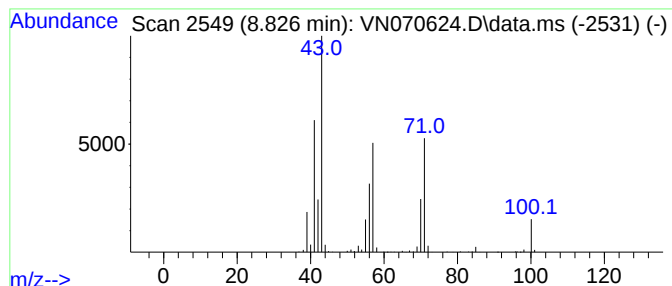
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Peak Number 3 Heptane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.826	20.09 ug/l	1246100	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	94
2			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	40
3			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	38
4			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38
5			Pyrrolidine	71	C4H9N	000123-75-1	37



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ALS Vial : 12 Sample Multiplier: 1

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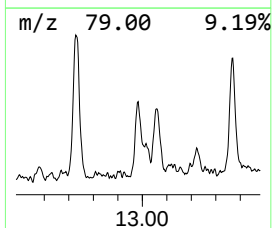
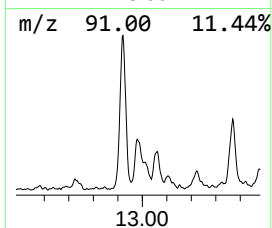
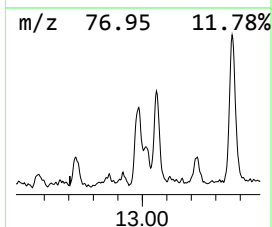
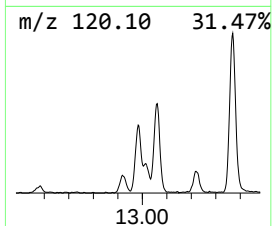
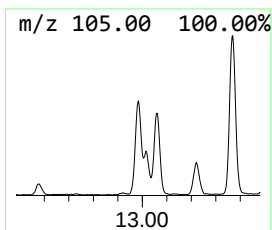
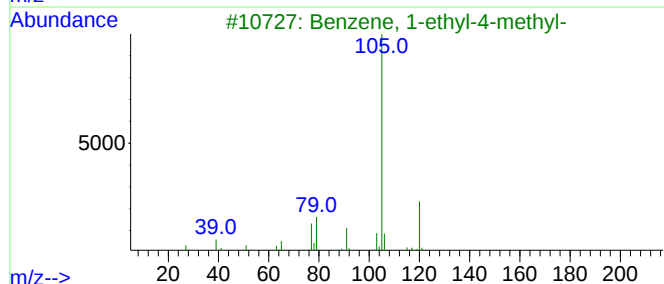
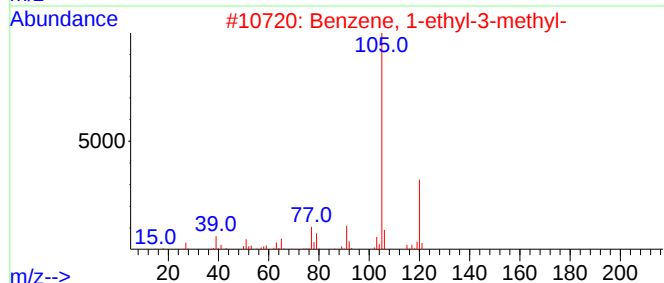
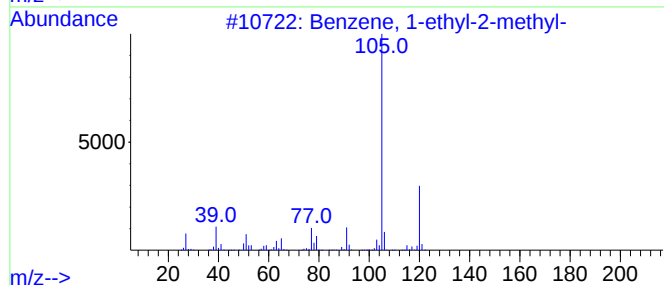
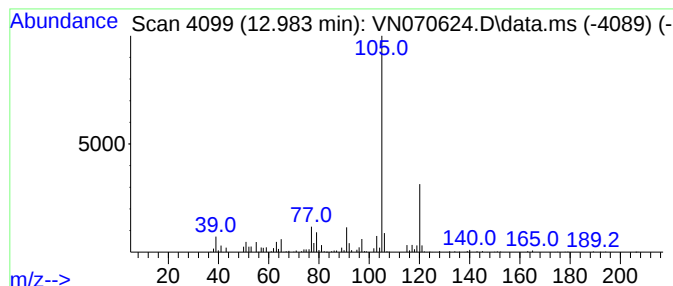
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	5.33 ug/l	306468	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	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5			Mesitylene	120	C9H12	000108-67-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.171	6.8	ug/l	414511	1	8.083	3047020	50.0
Hexane, 3-methyl-	8.292	24.8	ug/l	1513150	1	8.083	3047020	50.0
Heptane	8.826	20.1	ug/l	1246100	2	8.968	3101710	50.0
Benzene, 1-ethy...	12.983	5.3	ug/l	306468	4	13.675	2875150	50.0