

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN100618\
 Data File : VN051697.D
 Acq On : 5 Oct 2018 19:57
 Operator : MD\SY
 Sample : J5084-06
 Misc : 5.91µ/5.00mL/100µL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 27 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 B-10(7-7.5)

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.622	1496	1508	1521	rVB5	12978	34346	1.07%	0.131%
2	7.590	1790	1809	1820	rBV	457295	1142221	35.64%	4.354%
3	7.664	1821	1832	1848	rVV	696445	1666096	51.99%	6.352%
4	7.734	1850	1854	1871	rVB3	32364	74567	2.33%	0.284%
5	7.876	1883	1898	1907	rBV5	18078	41163	1.28%	0.157%
6	8.027	1925	1945	1968	rBV2	454096	1084100	33.83%	4.133%
7	8.207	1988	2001	2020	rBV2	58509	157466	4.91%	0.600%
8	8.587	2101	2119	2151	rBV	941277	2005209	62.57%	7.644%
9	9.082	2251	2273	2284	rBV9	28711	80421	2.51%	0.307%
10	9.519	2397	2409	2428	rVB3	46735	102729	3.21%	0.392%
11	9.654	2441	2451	2467	rVB3	55918	122968	3.84%	0.469%
12	9.869	2500	2518	2525	rBV4	17660	41846	1.31%	0.160%
13	10.091	2573	2587	2598	rVV	1751139	3204731	100.00%	12.217%
14	10.156	2598	2607	2633	rVV	843567	1572962	49.08%	5.997%
15	10.287	2634	2648	2659	rVB	16763	44338	1.38%	0.169%
16	10.529	2711	2723	2741	rVB	14489	47315	1.48%	0.180%
17	11.406	2980	2996	3018	rBV	1344870	2375089	74.11%	9.054%
18	11.509	3018	3028	3044	rVV	216551	382724	11.94%	1.459%
19	11.619	3047	3062	3084	rVB	728706	1416551	44.20%	5.400%
20	11.947	3144	3164	3180	rVB	409810	702681	21.93%	2.679%
21	12.249	3248	3258	3267	rBV2	30316	51441	1.61%	0.196%
22	12.400	3289	3305	3329	rVB	1254191	2146595	66.98%	8.183%
23	12.590	3355	3364	3374	rVB	95072	145051	4.53%	0.553%
24	12.654	3374	3384	3391	rBV	389227	662203	20.66%	2.524%
25	12.731	3401	3408	3420	rVB2	205893	334905	10.45%	1.277%
26	12.892	3444	3458	3474	rBV	182738	311754	9.73%	1.188%
27	13.040	3493	3504	3515	rVB	669133	1084914	33.85%	4.136%
28	13.172	3529	3545	3550	rBV3	25302	59080	1.84%	0.225%
29	13.233	3559	3564	3572	rVB2	27392	38176	1.19%	0.146%
30	13.287	3572	3581	3586	rBV3	25552	38473	1.20%	0.147%
31	13.345	3586	3599	3625	rBV2	1357299	2558083	79.82%	9.752%
32	13.451	3625	3632	3642	rVB2	36141	59401	1.85%	0.226%
33	13.541	3642	3660	3667	rBV2	212719	416308	12.99%	1.587%
34	13.583	3667	3673	3691	rVB4	146758	302696	9.45%	1.154%

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ClientSampleId :
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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

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Title : SW846 8260

35	13.670	3691	3700	3709	rVB8	22129	34106	1.06%	0.130%
36	13.741	3711	3722	3731	rVB2	48108	85108	2.66%	0.324%
37	13.805	3731	3742	3747	rBV2	93041	169172	5.28%	0.645%
38	13.889	3759	3768	3779	rBV2	126004	194029	6.05%	0.740%
39	13.995	3791	3801	3811	rVB3	69686	114797	3.58%	0.438%
40	14.065	3811	3823	3833	rBV3	20132	42775	1.33%	0.163%
41	14.127	3835	3842	3850	rBV2	28229	41198	1.29%	0.157%
42	14.210	3856	3868	3873	rBV	60506	101206	3.16%	0.386%
43	14.249	3873	3880	3887	rVV	85600	133974	4.18%	0.511%
44	14.297	3887	3895	3902	rVV5	57182	94043	2.93%	0.359%
45	14.332	3902	3906	3914	rVB3	30486	39975	1.25%	0.152%
46	14.477	3943	3951	3958	rVV2	44727	73580	2.30%	0.281%
47	14.522	3960	3965	3974	rVB3	43429	60901	1.90%	0.232%
48	14.586	3974	3985	3997	rBV5	90790	206233	6.44%	0.786%
49	14.647	3998	4004	4014	rVB	30644	49359	1.54%	0.188%
50	14.853	4059	4068	4081	rBV3	38500	87602	2.73%	0.334%
51	14.956	4092	4100	4111	rBV8	29593	49771	1.55%	0.190%
52	15.133	4144	4155	4166	rVB	51223	106632	3.33%	0.407%
53	15.416	4235	4243	4255	rBV3	18389	38221	1.19%	0.146%

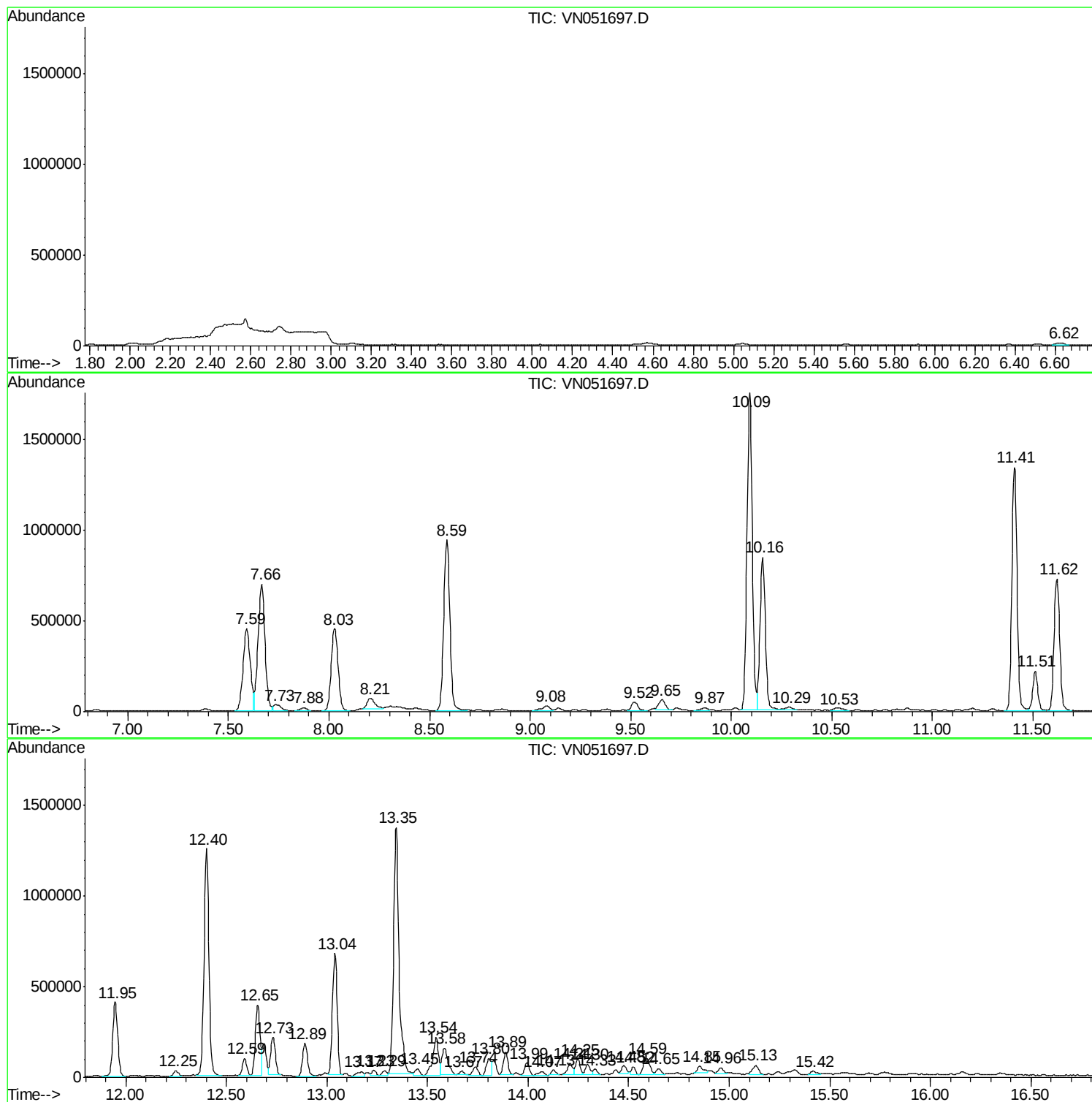
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B-10(7-7.5)

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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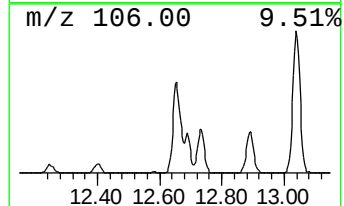
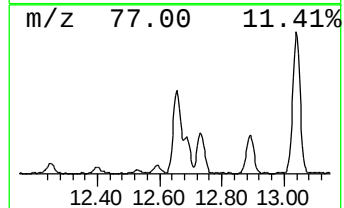
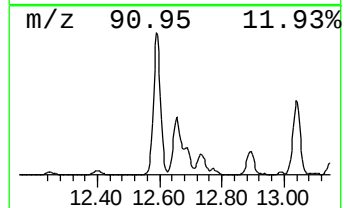
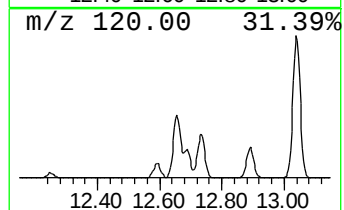
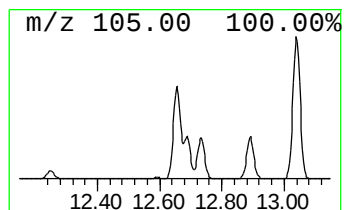
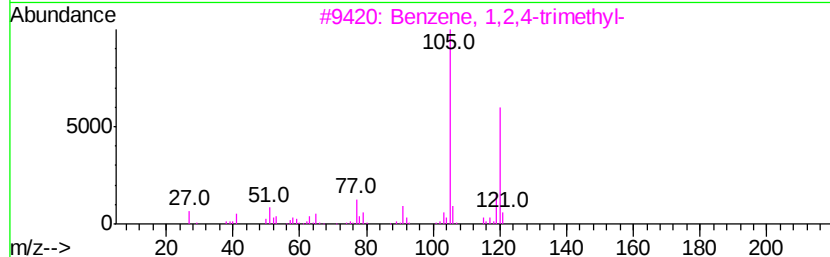
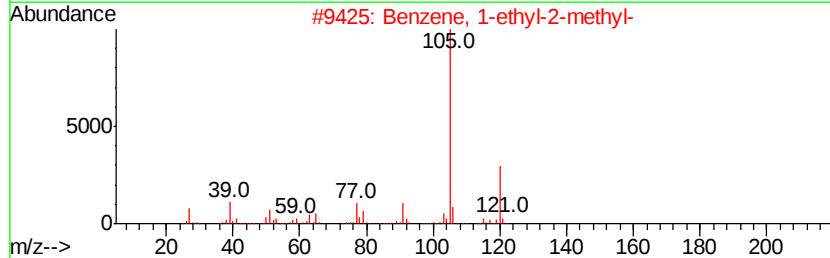
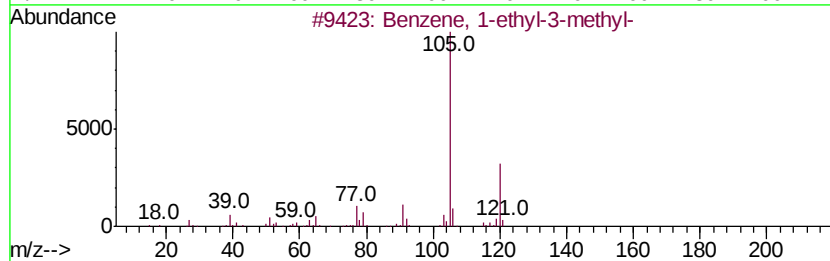
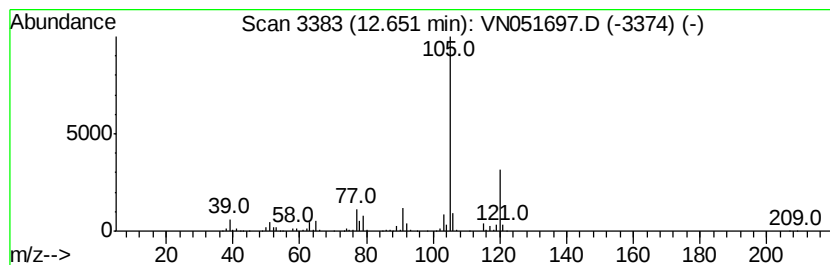
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N100418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	12.94 ug/l	662203	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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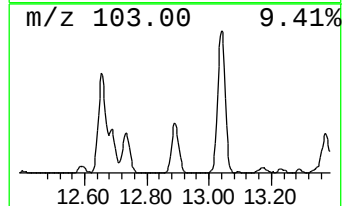
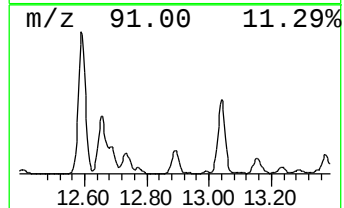
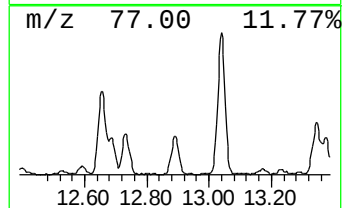
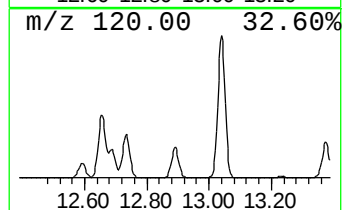
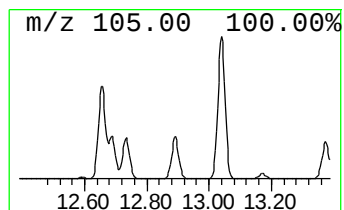
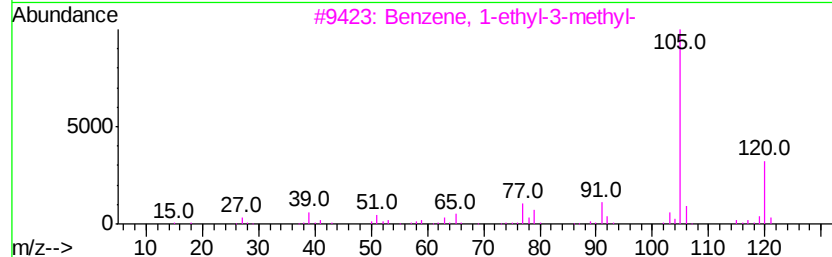
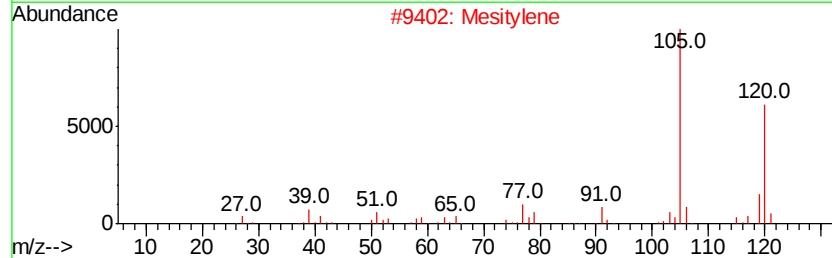
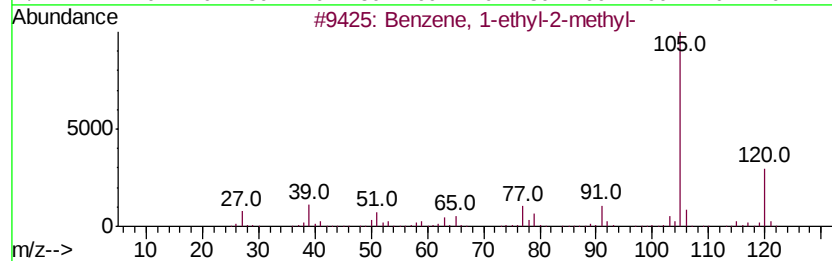
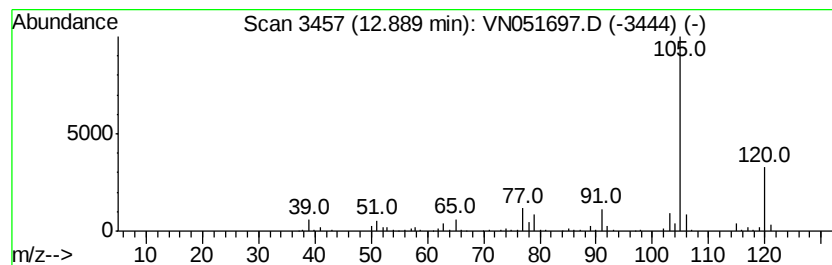
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	6.09 ug/l	311754	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2		Mesitylene	120	C9H12	000108-67-8	91
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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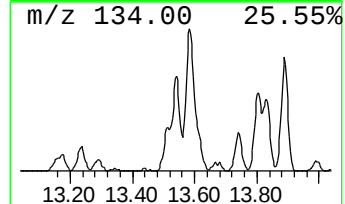
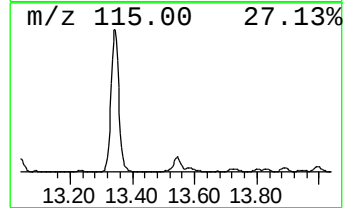
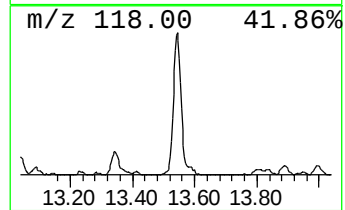
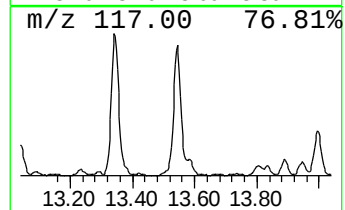
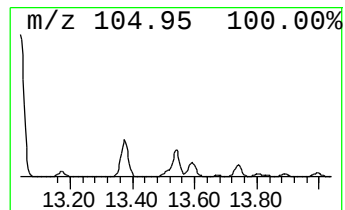
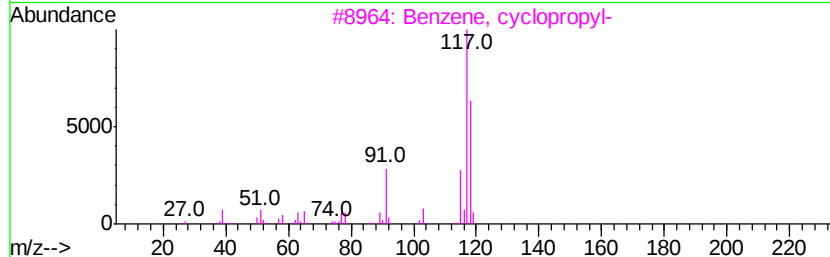
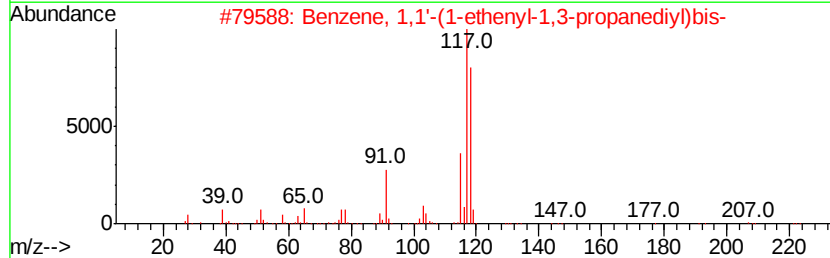
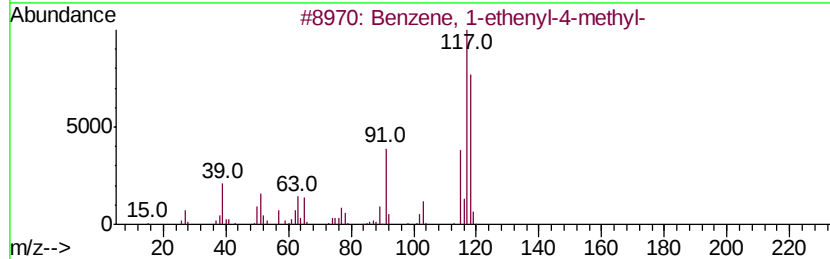
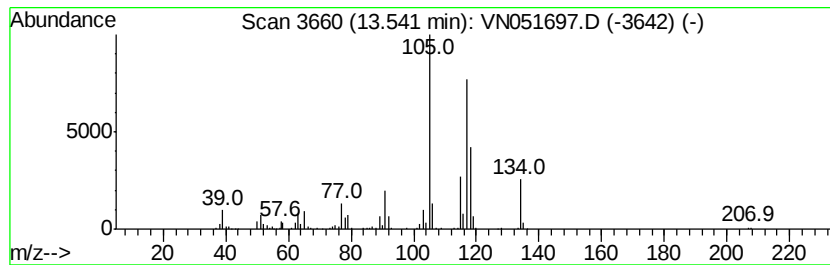
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethenyl-4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	8.14 ug/l	416308	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethenyl-4-methyl-	118 C9H10	000622-97-9 91
2		Benzene, 1,1'-(1-ethenyl-1,3-pro...	222 C17H18	061141-97-7 64
3		Benzene, cyclopropyl-	118 C9H10	000873-49-4 64
4		Benzene, 1-ethenyl-2-methyl-	118 C9H10	000611-15-4 64
5		Benzene, 1-propenyl-	118 C9H10	000637-50-3 64



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-ethyl-...	12.65	12.9	ug/l	662203	4	13.35	2558080	50.0
Benzene, 1-ethyl-...	12.89	6.1	ug/l	311754	4	13.35	2558080	50.0
Benzene, 1-etheny...	13.54	8.1	ug/l	416308	4	13.35	2558080	50.0