

Data Path : W:\HPCHEM1\MSVOA N\DATA\VN092115\
 Data File : VN027360.D
 Acq On : 22 Sep 2015 5:43
 Operator : MD\FY
 Sample : G3754-05
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-7BS

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 : W:\HPCHEM1\MSVOA_N\METHODS\82N092115W.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	1.941	98	109	127	rBV	213443	425501	7.86%	1.094%
2	7.677	1870	1893	1905	rBV	658359	1639549	30.29%	4.216%
3	7.751	1905	1916	1943	rVB	1056872	2510758	46.38%	6.456%
4	8.133	2013	2035	2062	rBV3	1534667	4584532	84.69%	11.787%
5	8.680	2187	2205	2232	rBV	1662670	3503293	64.72%	9.007%
6	10.191	2658	2675	2689	rBV	2986194	5413180	100.00%	13.918%
7	10.255	2689	2695	2709	rVB	84787	158290	2.92%	0.407%
8	10.898	2886	2895	2908	rBV4	70335	149542	2.76%	0.384%
9	11.516	3072	3087	3107	rBV	2314550	4033080	74.50%	10.370%
10	11.619	3107	3119	3133	rVB	617646	1020593	18.85%	2.624%
11	11.734	3138	3155	3169	rBV	206142	390960	7.22%	1.005%
12	12.056	3243	3255	3272	rBV	334113	577763	10.67%	1.486%
13	12.361	3339	3350	3363	rVB	211267	346541	6.40%	0.891%
14	12.516	3382	3398	3413	rBV	2009414	3302294	61.00%	8.491%
15	12.705	3448	3457	3467	rVB2	39086	71112	1.31%	0.183%
16	12.770	3468	3477	3481	rVV3	53310	84853	1.57%	0.218%
17	12.805	3481	3488	3496	rVV	126113	207494	3.83%	0.533%
18	13.008	3540	3551	3563	rBV	118808	199593	3.69%	0.513%
19	13.159	3568	3598	3607	rVV3	152497	388607	7.18%	0.999%
20	13.207	3609	3613	3622	rVV4	36398	54834	1.01%	0.141%
21	13.281	3624	3636	3650	rVV4	29395	88007	1.63%	0.226%
22	13.352	3650	3658	3669	rVB2	79880	123538	2.28%	0.318%
23	13.467	3681	3694	3715	rBV2	1977053	3681413	68.01%	9.465%
24	13.631	3736	3745	3749	rBV2	112516	164725	3.04%	0.424%
25	13.670	3749	3757	3768	rVB	441751	697132	12.88%	1.792%
26	13.850	3801	3813	3827	rVB	422175	722896	13.35%	1.859%
27	14.014	3856	3864	3873	rBV	45493	66097	1.22%	0.170%
28	14.104	3882	3892	3904	rBV2	197549	380352	7.03%	0.978%
29	14.252	3928	3938	3948	rVB3	35845	79691	1.47%	0.205%
30	14.381	3969	3978	3982	rBV2	89404	146460	2.71%	0.377%
31	14.490	4006	4012	4018	rBV3	36872	57502	1.06%	0.148%
32	14.528	4018	4024	4033	rVB	71460	103893	1.92%	0.267%
33	14.612	4039	4050	4060	rBV2	87770	147024	2.72%	0.378%
34	14.728	4072	4086	4096	rVB4	77929	167780	3.10%	0.431%

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Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

35	14.795	4096	4107	4115	rBV	207508	348597	6.44%	0.896%
36	14.876	4116	4132	4155	rVB3	480350	1243021	22.96%	3.196%
37	14.988	4155	4167	4177	rBV7	56810	115663	2.14%	0.297%
38	15.287	4248	4260	4274	rVB	281950	505205	9.33%	1.299%
39	15.406	4288	4297	4320	rVB	34684	110147	2.03%	0.283%
40	16.165	4521	4533	4549	rBV5	40170	100893	1.86%	0.259%
41	16.364	4585	4595	4608	rVB4	41210	84782	1.57%	0.218%
42	16.561	4638	4656	4675	rBV	307794	696067	12.86%	1.790%

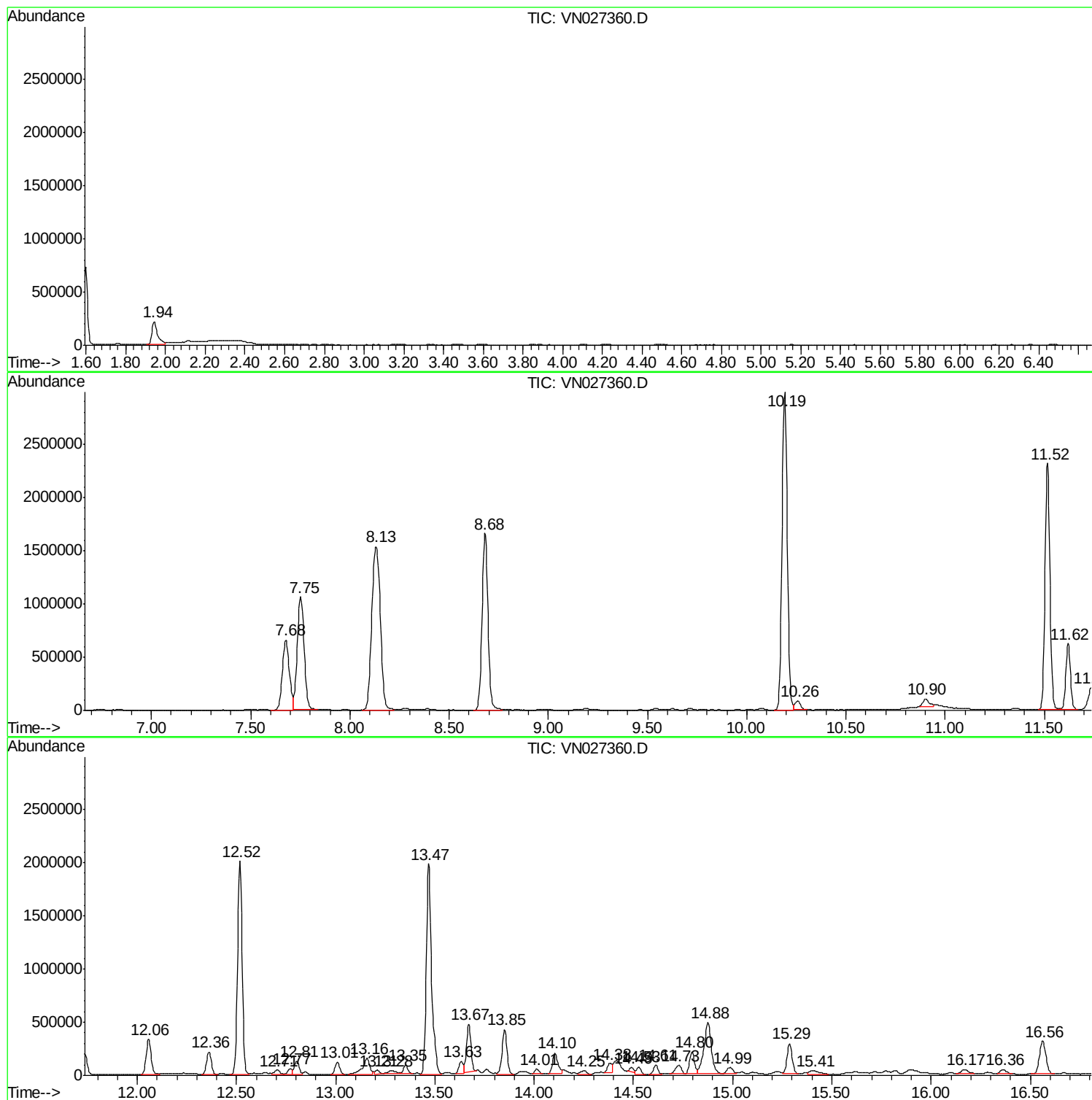
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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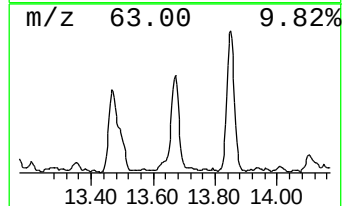
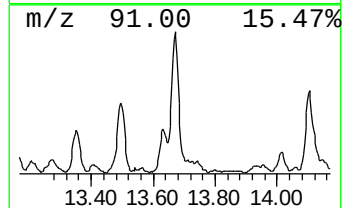
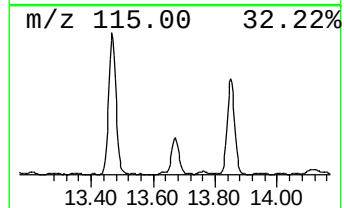
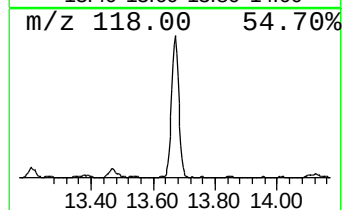
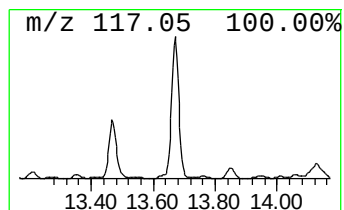
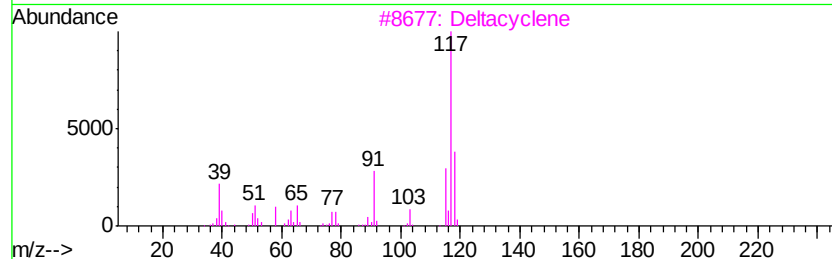
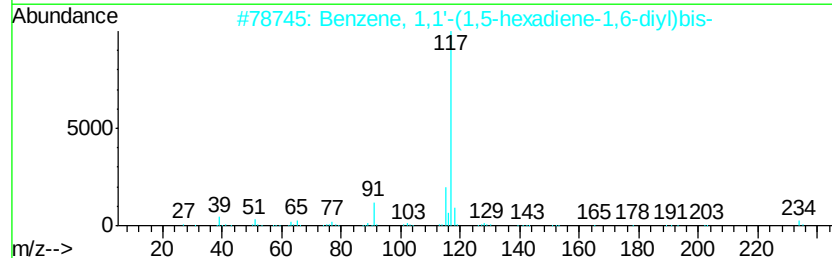
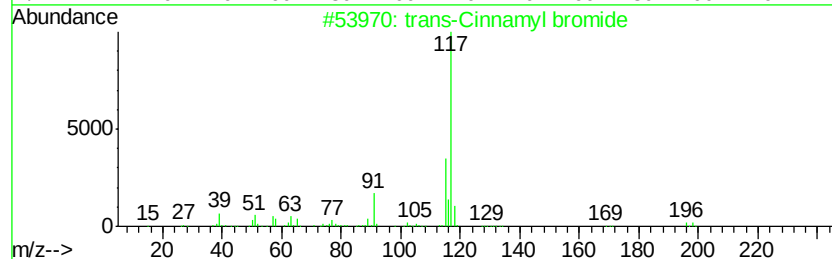
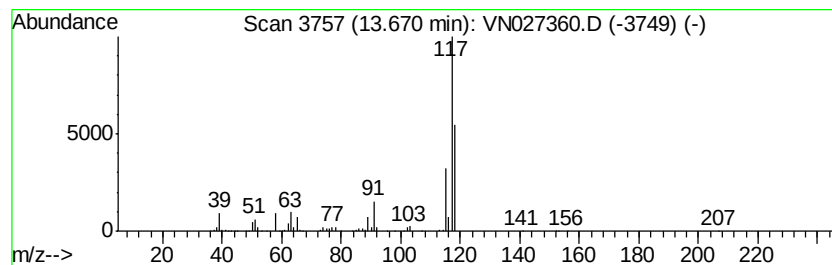
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 trans-Cinnamyl bromide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	9.47 ug/l	697132	1,4-Dichlorobenzene-d4	13.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
2			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	53
3			Deltacyclene	118	C9H10	007785-10-6	45
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	43
5			Indole	117	C8H7N	000120-72-9	38



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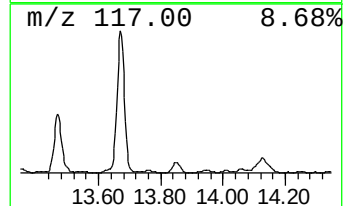
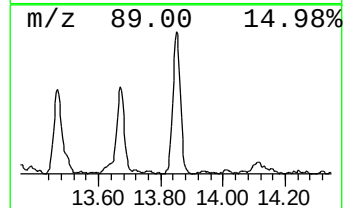
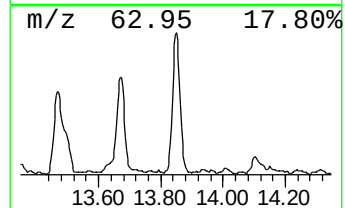
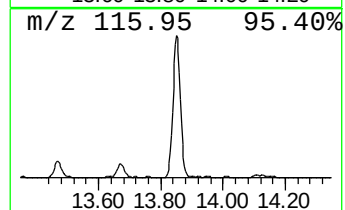
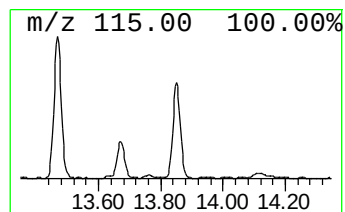
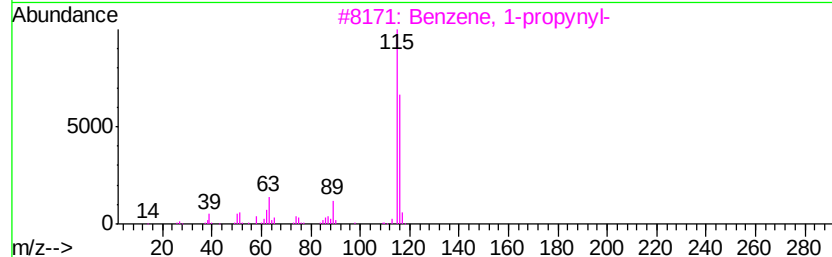
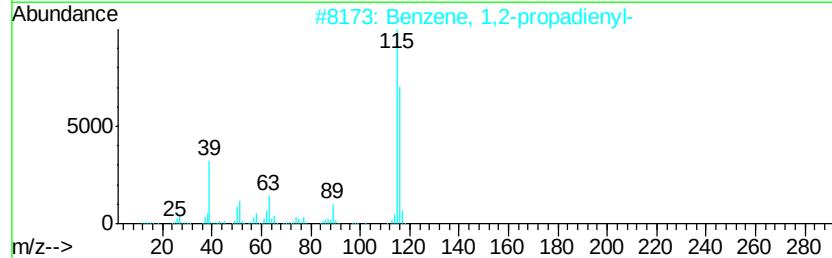
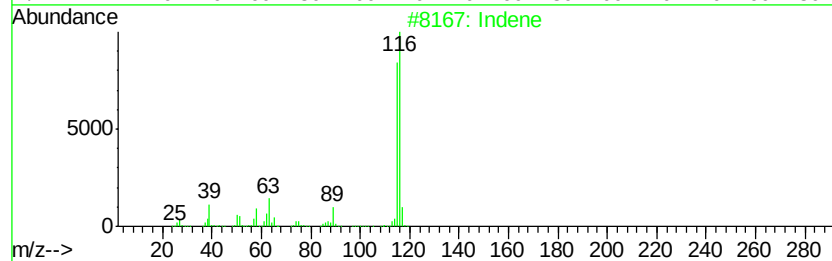
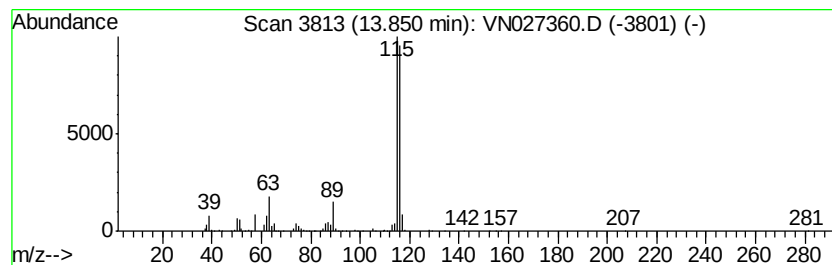
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Peak Number 3 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	9.82 ug/l	722896	1,4-Dichlorobenzene-d4	13.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Indene	116 C9H8	000095-13-6	95
2	Benzene, 1,2-propadienyl-	116 C9H8	002327-99-3	91
3	Benzene, 1-propynyl-	116 C9H8	000673-32-5	91
4	Benzene, 1-ethynyl-2-methyl-	116 C9H8	000766-47-2	91
5	Benzene, 1-ethynyl-4-methyl-	116 C9H8	000766-97-2	80



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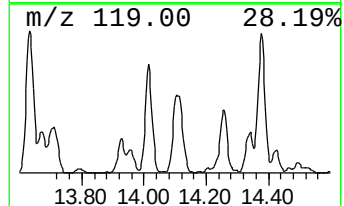
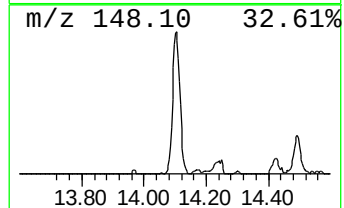
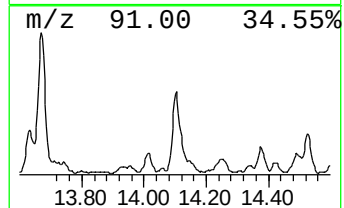
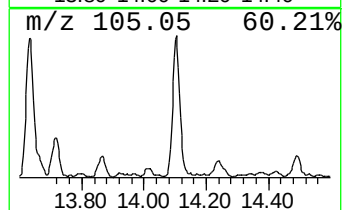
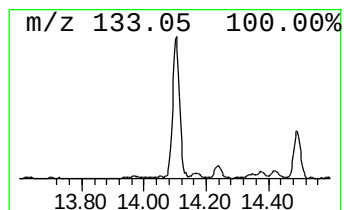
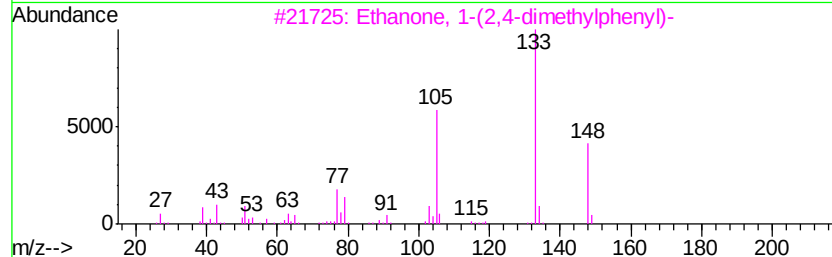
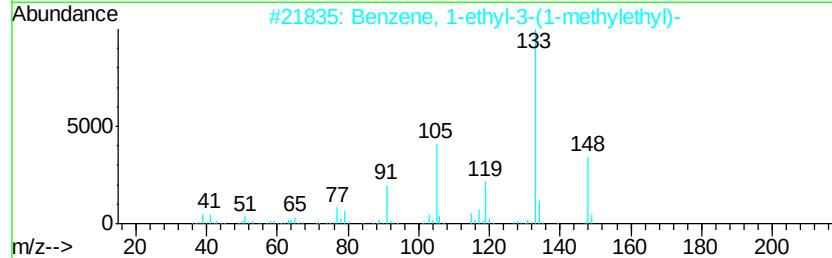
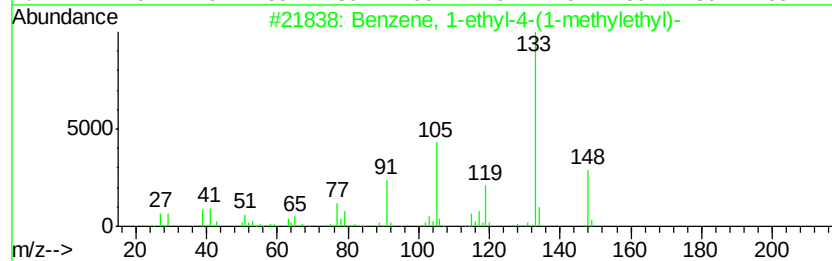
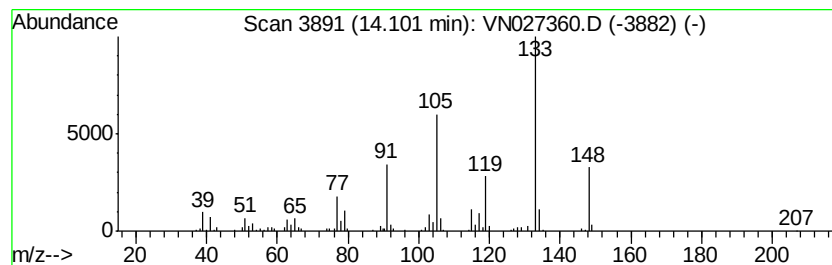
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-4-(1-methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	5.17 ug/l	380352	1,4-Dichlorobenzene-d4	13.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	97
2		Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	96
3		Ethanone, 1-(2,4-dimethylphenyl)-	148	C10H12O	000089-74-7	94
4		Ethanone, 1-(3,4-dimethylphenyl)-	148	C10H12O	003637-01-2	89
5		2-tert-Butyltoluene	148	C11H16	001074-92-6	87



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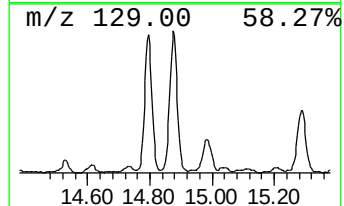
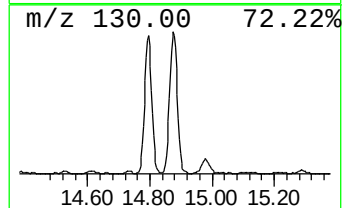
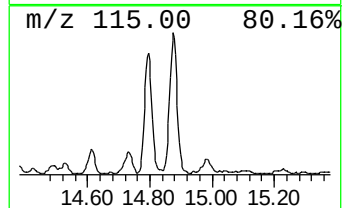
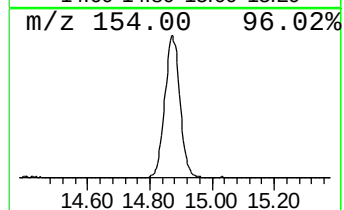
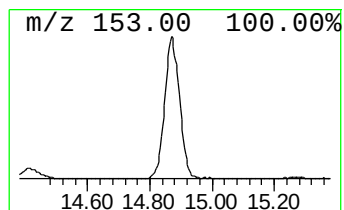
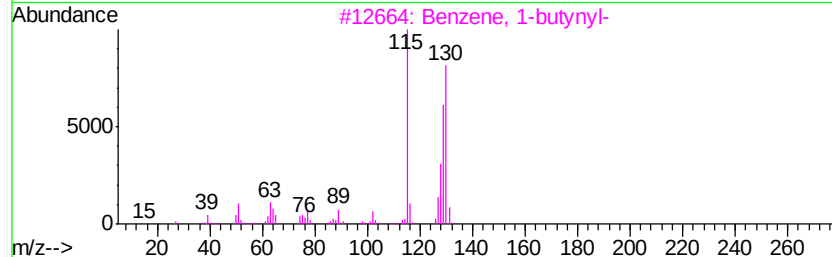
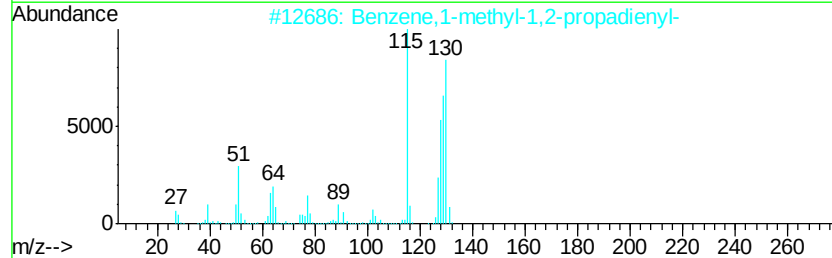
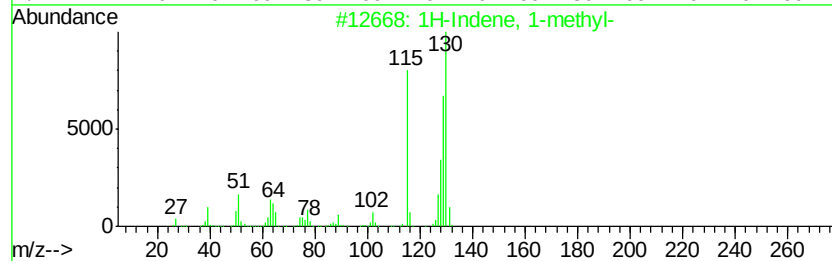
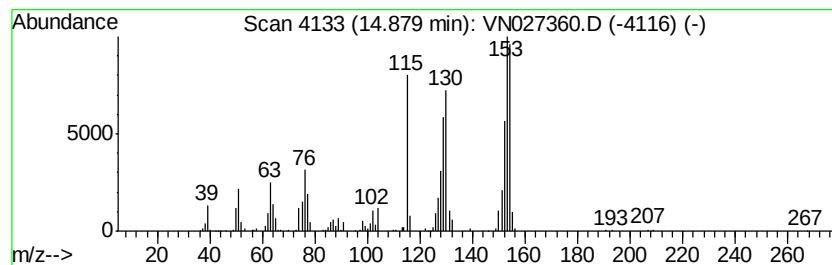
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1H-Indene, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.88	16.88 ug/l	1243020	1,4-Dichlorobenzene-d4	13.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	83
2		Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	74
3		Benzene, 1-butylnyl-	130	C10H10	000622-76-4	49
4		Acenaphthene	154	C12H10	000083-32-9	42
5		1H-Indene, 3-methyl-	130	C10H10	000767-60-2	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
trans-Cinnamyl br...	13.67	9.5	ug/l	697132	4	13.47	3681410	50.0
Indene	13.85	9.8	ug/l	722896	4	13.47	3681410	50.0
Benzene, 1-ethyl-...	14.10	5.2	ug/l	380352	4	13.47	3681410	50.0
1H-Indene, 1-methyl-	14.88	16.9	ug/l	1243020	4	13.47	3681410	50.0