

Data Path : W:\HPCHEM1\MSVOA N\DATA\VN091715\
 Data File : VN027277.D
 Acq On : 18 Sep 2015 2:15
 Operator : MD\FY
 Sample : G3683-04
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-2R-11

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\82N091515W.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	1.995	103	126	132	rBV3	106425	342520	6.13%	0.597%
2	2.799	358	376	398	rBV	420821	901726	16.14%	1.571%
3	3.149	468	485	506	rBV3	123602	294780	5.28%	0.514%
4	3.590	601	622	640	rBV3	161609	410258	7.34%	0.715%
5	3.841	677	700	716	rBV4	41968	140336	2.51%	0.245%
6	3.928	717	727	746	rVB4	20390	56378	1.01%	0.098%
7	4.487	880	901	915	rBV2	29134	97268	1.74%	0.169%
8	4.612	915	940	941	rBV2	142104	383388	6.86%	0.668%
9	5.136	1076	1103	1130	rBV3	306384	1186333	21.24%	2.067%
10	6.024	1355	1379	1403	rBV3	118454	387824	6.94%	0.676%
11	6.165	1403	1423	1441	rBV6	71211	230556	4.13%	0.402%
12	6.474	1502	1519	1536	rBV3	88979	279672	5.01%	0.487%
13	6.622	1552	1565	1581	rBV4	24523	70221	1.26%	0.122%
14	6.741	1581	1602	1619	rBV	536840	1710958	30.63%	2.981%
15	7.429	1801	1816	1822	rBV3	26166	66587	1.19%	0.116%
16	7.497	1824	1837	1856	rVB	127508	335270	6.00%	0.584%
17	7.677	1875	1893	1904	rBV	664237	1660739	29.73%	2.894%
18	7.754	1904	1917	1936	rVV2	1312539	3391794	60.72%	5.910%
19	7.850	1938	1947	1966	rVB5	116334	306018	5.48%	0.533%
20	7.976	1968	1986	1998	rBV2	97063	238706	4.27%	0.416%
21	8.123	2016	2032	2048	rBV2	1024199	2848139	50.99%	4.963%
22	8.278	2067	2080	2092	rBV6	142714	411820	7.37%	0.718%
23	8.406	2111	2120	2137	rVB6	98708	240826	4.31%	0.420%
24	8.506	2140	2151	2170	rVB8	21241	60948	1.09%	0.106%
25	8.680	2187	2205	2229	rBV	1770696	3908567	69.97%	6.810%
26	8.918	2267	2279	2288	rVV2	69928	149483	2.68%	0.260%
27	8.966	2288	2294	2312	rVB4	41900	94903	1.70%	0.165%
28	9.191	2336	2364	2379	rBV3	278978	810325	14.51%	1.412%
29	9.374	2411	2421	2433	rVB3	57890	107943	1.93%	0.188%
30	9.541	2463	2473	2476	rBV4	37039	59762	1.07%	0.104%
31	9.619	2491	2497	2513	rVB4	57240	109565	1.96%	0.191%
32	9.715	2515	2527	2535	rBV2	207367	396287	7.09%	0.690%
33	9.966	2584	2605	2627	rBV6	82342	281005	5.03%	0.490%
34	10.075	2628	2639	2648	rBV2	109977	203783	3.65%	0.355%

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35	10.191	2661	2675	2689	rBV	3050308	5586010	100.00%	9.733%
36	10.294	2703	2707	2720	rVB2	60447	92844	1.66%	0.162%
37	10.390	2721	2737	2750	rVB6	50100	145743	2.61%	0.254%
38	10.541	2776	2784	2796	rBV5	31459	56172	1.01%	0.098%
39	10.622	2797	2809	2825	rVB5	99505	231225	4.14%	0.403%
40	10.840	2853	2877	2881	rBV6	21752	64964	1.16%	0.113%
41	10.885	2882	2891	2903	rVB	110041	192880	3.45%	0.336%
42	10.975	2904	2919	2928	rBV9	32099	82879	1.48%	0.144%
43	11.516	3072	3087	3105	rBV	2356634	4104989	73.49%	7.153%
44	11.619	3111	3119	3139	rVB4	104910	202644	3.63%	0.353%
45	11.728	3139	3153	3163	rBV3	36093	89524	1.60%	0.156%
46	12.056	3236	3255	3264	rBV4	37842	93746	1.68%	0.163%
47	12.239	3297	3312	3319	rBV10	29199	59626	1.07%	0.104%
48	12.361	3339	3350	3364	rVB	845560	1355563	24.27%	2.362%
49	12.519	3385	3399	3416	rBV	1972842	3295002	58.99%	5.741%
50	12.705	3444	3457	3471	rVB	791894	1288974	23.08%	2.246%
51	13.008	3538	3551	3567	rBV	150427	264096	4.73%	0.460%
52	13.107	3567	3582	3593	rBV10	26998	79642	1.43%	0.139%
53	13.290	3626	3639	3649	rBV4	110160	222682	3.99%	0.388%
54	13.467	3682	3694	3712	rBV	1971942	3231487	57.85%	5.631%
55	13.564	3715	3724	3733	rVV	60882	102788	1.84%	0.179%
56	13.635	3734	3746	3749	rVV	252091	371999	6.66%	0.648%
57	13.670	3750	3757	3766	rVV	1044522	1679884	30.07%	2.927%
58	13.715	3766	3771	3788	rVV4	173079	431754	7.73%	0.752%
59	13.799	3788	3797	3808	rVB	194429	319989	5.73%	0.558%
60	14.014	3853	3864	3875	rBV	671125	1037550	18.57%	1.808%
61	14.078	3875	3884	3889	rVV	204795	317130	5.68%	0.553%
62	14.126	3890	3899	3910	rVB2	639857	1103824	19.76%	1.923%
63	14.194	3911	3920	3929	rVB7	44218	73170	1.31%	0.127%
64	14.262	3929	3941	3948	rBV	88862	158374	2.84%	0.276%
65	14.339	3949	3965	3983	rVB	679962	1162034	20.80%	2.025%
66	14.422	3983	3991	3997	rBV2	60257	89323	1.60%	0.156%
67	14.561	4019	4034	4041	rBV4	72471	177210	3.17%	0.309%
68	14.612	4041	4050	4060	rBV3	306656	520809	9.32%	0.907%
69	14.728	4072	4086	4097	rBV3	848285	1971239	35.29%	3.435%
70	14.789	4097	4105	4115	rVB5	68308	128757	2.30%	0.224%
71	14.882	4126	4134	4144	rBV3	114648	175916	3.15%	0.307%

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72	14.988	4151	4167	4175	rBV3	217901	430050	7.70%	0.749%
73	15.027	4175	4179	4188	rVV2	103641	167932	3.01%	0.293%
74	15.101	4192	4202	4213	rVB4	205967	458830	8.21%	0.799%
75	15.194	4223	4231	4238	rBV2	34315	60766	1.09%	0.106%
76	15.287	4250	4260	4271	rVB	495395	867927	15.54%	1.512%
77	15.397	4287	4294	4299	rBV4	43562	75004	1.34%	0.131%
78	15.580	4340	4351	4365	rBV5	52174	106772	1.91%	0.186%
79	15.872	4434	4442	4452	rVB3	54264	85026	1.52%	0.148%
80	16.097	4499	4512	4524	rBV5	91572	219006	3.92%	0.382%
81	16.297	4557	4574	4581	rBV9	43588	118667	2.12%	0.207%
82	16.358	4581	4593	4621	rVB	410625	925169	16.56%	1.612%
83	16.564	4641	4657	4673	rBV	491338	1139747	20.40%	1.986%

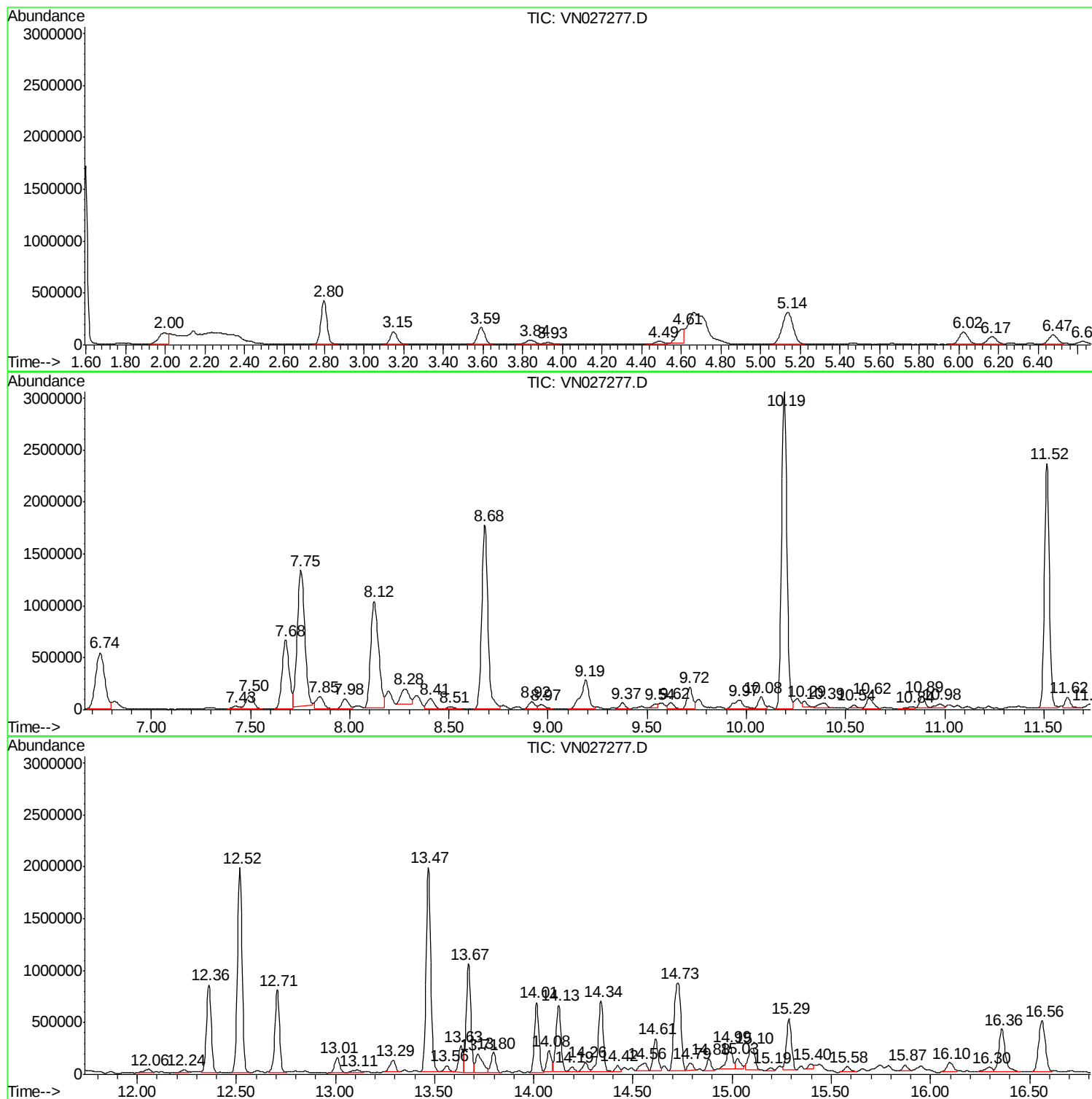
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Quant Method : W:\HPCHEM1\MSVOA_N\METHODS\82N091515W.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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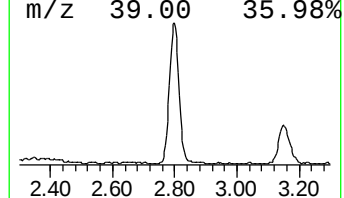
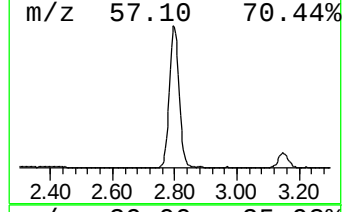
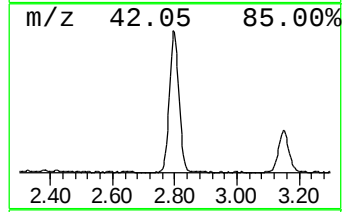
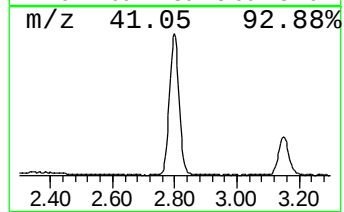
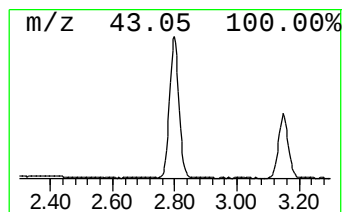
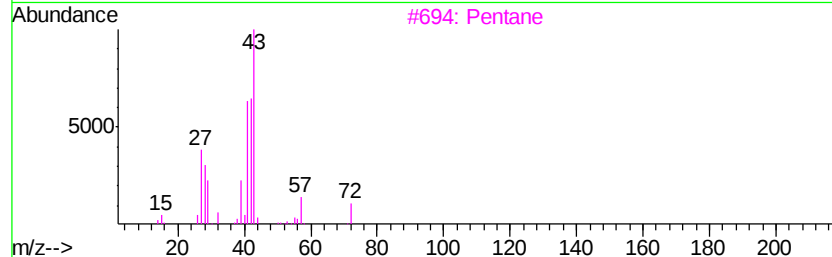
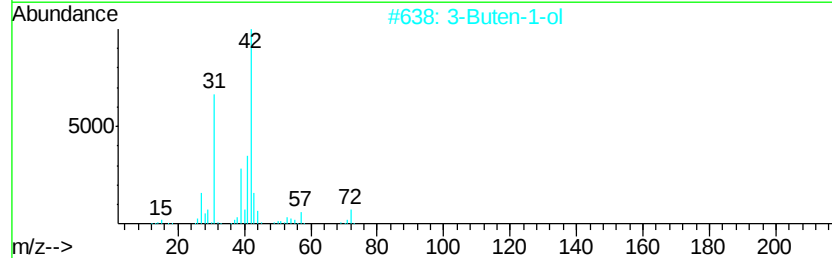
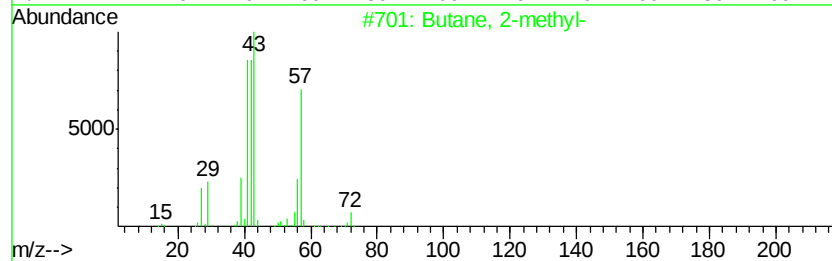
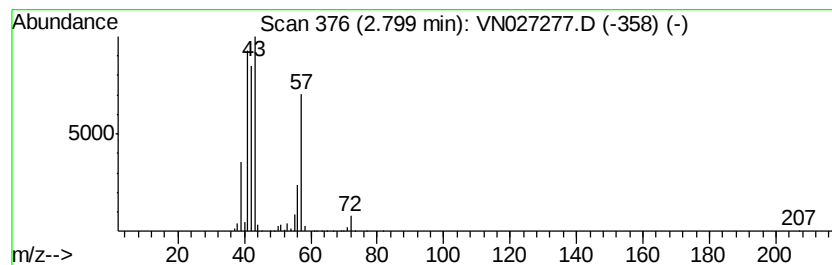
Quant Method : W:\HPCHEM1\MSVOA_N\METHODS\82N091515W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.80	13.29 ug/l	901726	Pentafluorobenzene	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		Pentane	72	C5H12	000109-66-0	42
4		1-Butene	56	C4H8	000106-98-9	14
5		Pyruvic acid, butyl ester	144	C7H12O3	020279-44-1	10



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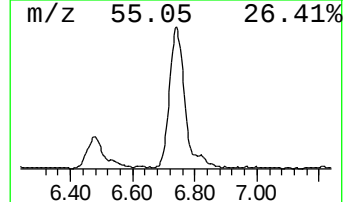
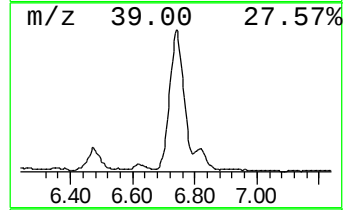
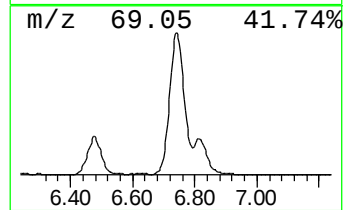
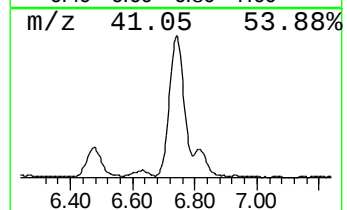
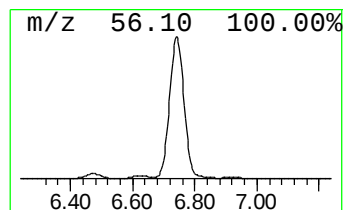
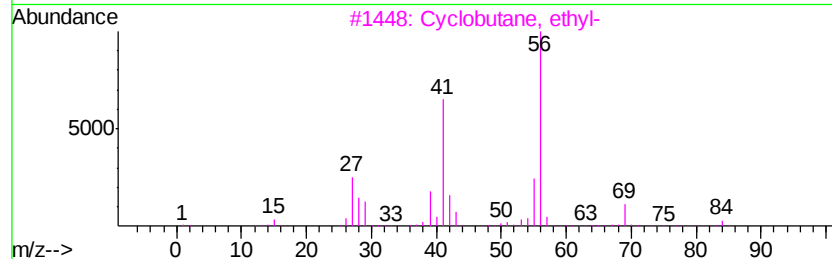
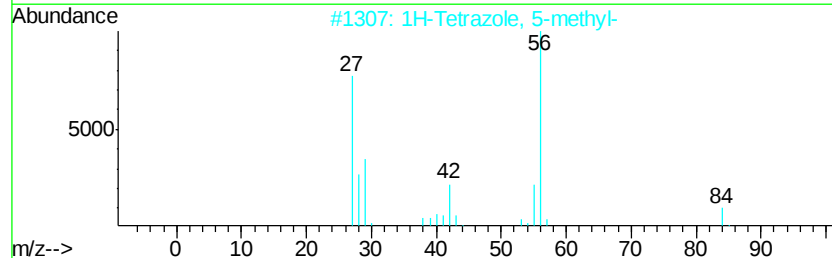
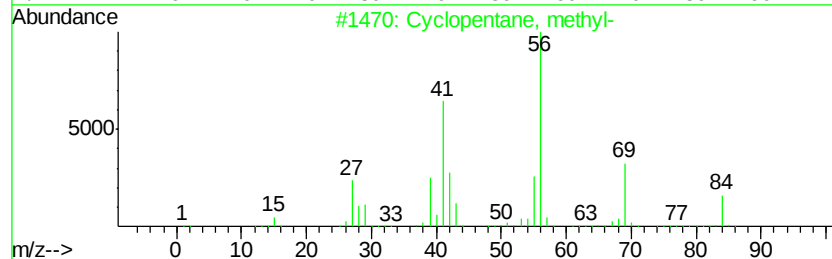
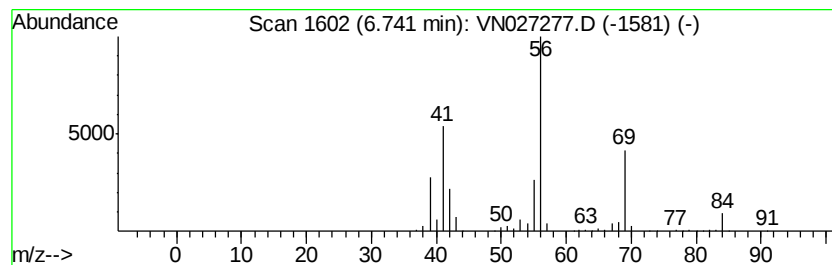
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	25.22 ug/l	1710960	Pentafluorobenzene	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4		Cyclohexane	84	C6H12	000110-82-7	64
5		Cyclobutane	56	C4H8	000287-23-0	53



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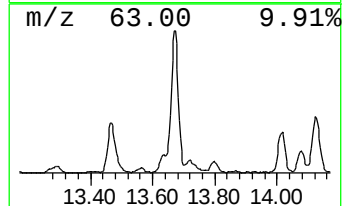
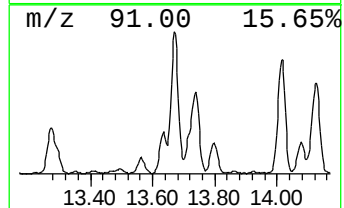
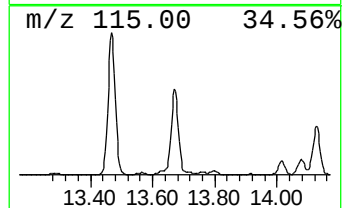
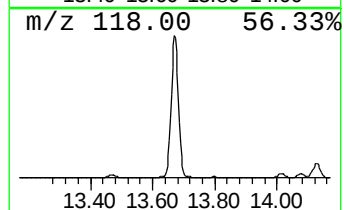
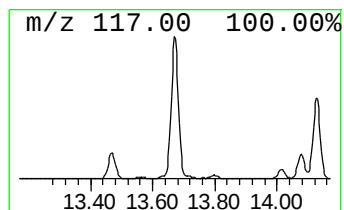
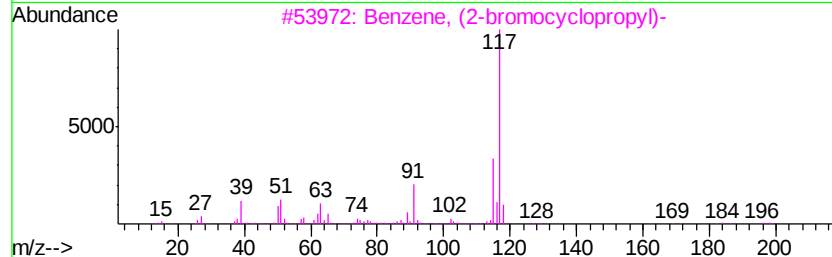
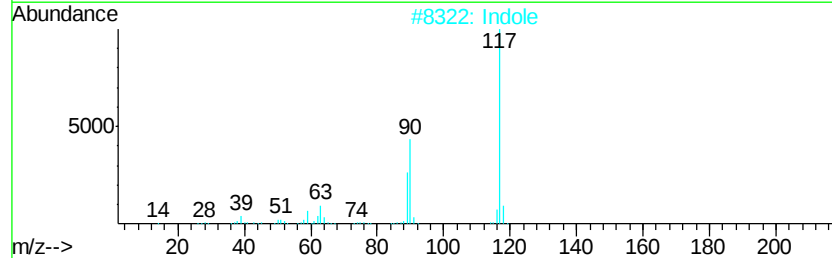
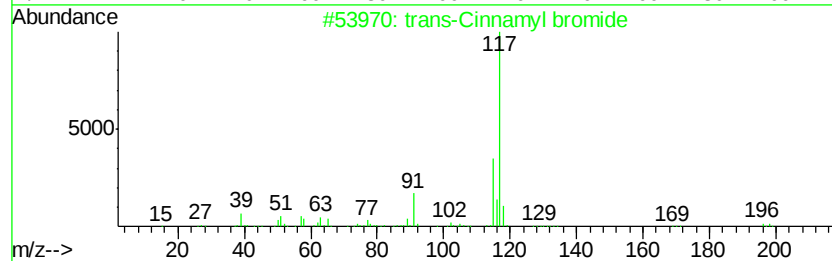
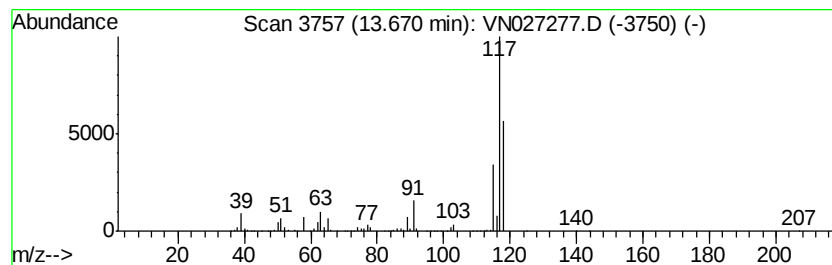
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 trans-Cinnamyl bromide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	25.99 ug/l	1679880	1,4-Dichlorobenzene-d4	13.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
2		Indole	117	C8H7N	000120-72-9	49
3		Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	45
4		Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	40
5		Benzene, (isocyanomethyl)-	117	C8H7N	010340-91-7	40



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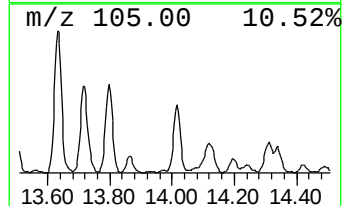
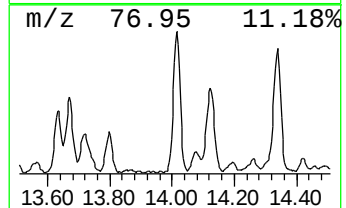
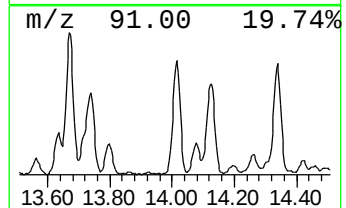
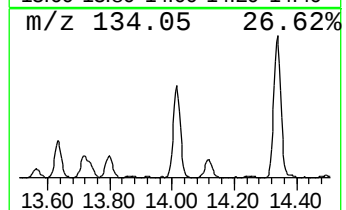
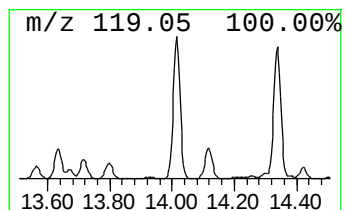
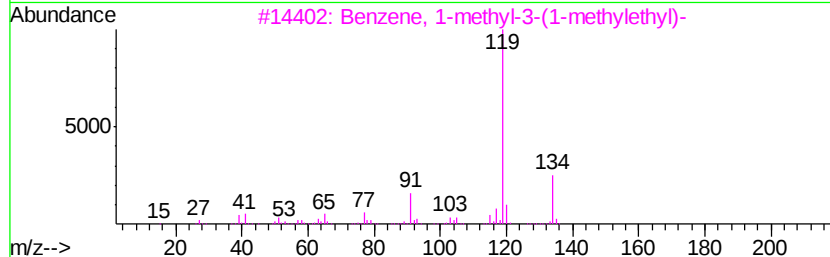
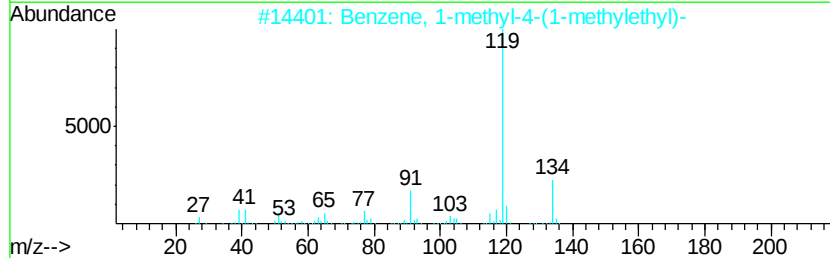
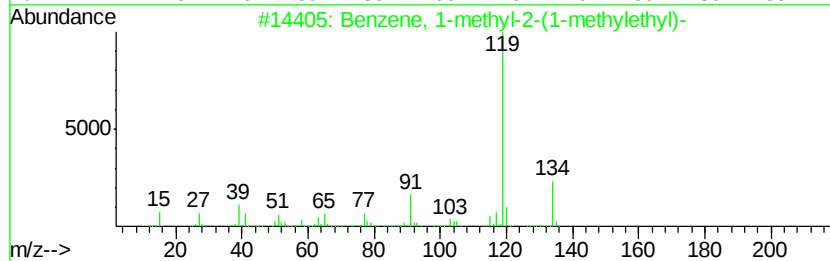
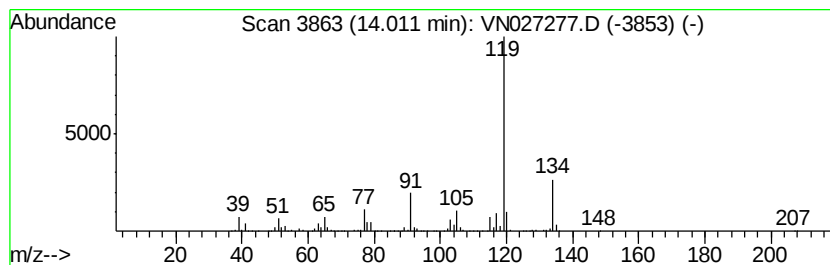
Quant Method : W:\HPCHEM1\MSVOA_N\METHODS\82N091515W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-methyl-2-(1-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	16.05 ug/l	1037550	1,4-Dichlorobenzene-d4	13.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	000527-84-4	95
2		Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	000099-87-6	95
3		Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	94
4		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94
5		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	93



Data Path : W:\HPCHEM1\MSVOA N\DATA\VN091715\
Data File : VN027277.D
Acq On : 18 Sep 2015 2:15
Operator : MD\FY
Sample : G3683-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2R-11

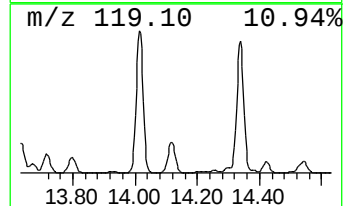
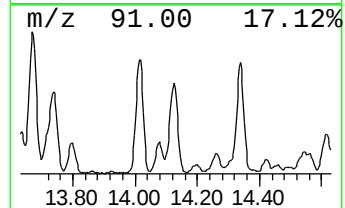
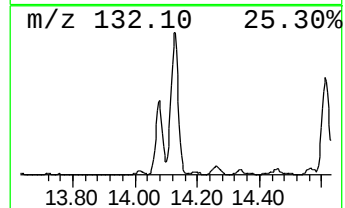
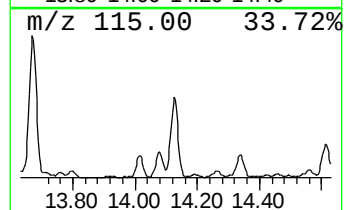
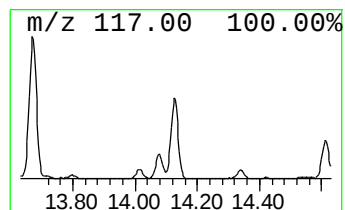
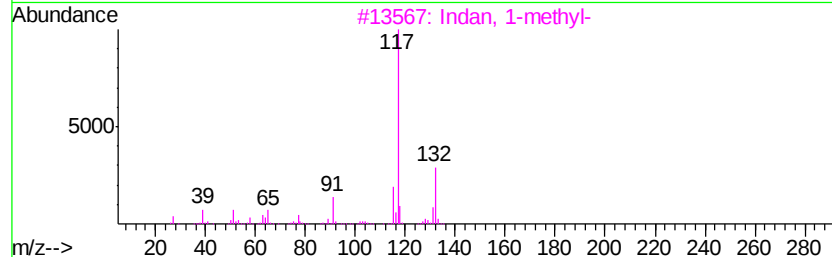
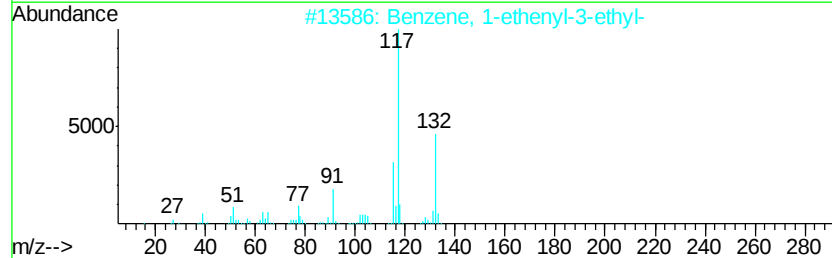
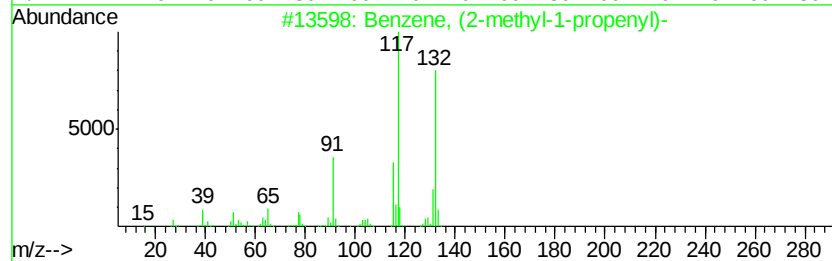
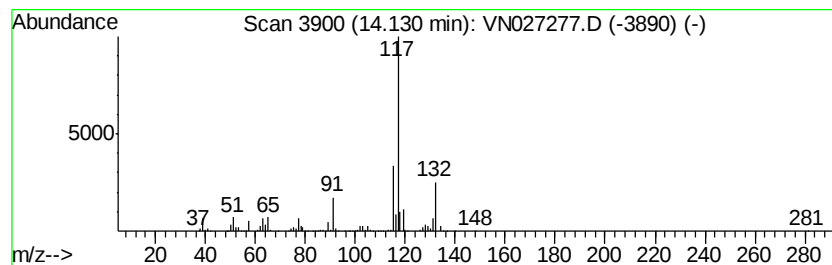
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, (2-methyl-1-propen... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	17.08 ug/l	1103820	1,4-Dichlorobenzene-d4	13.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
2			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83
3			Indan, 1-methyl-	132	C10H12	000767-58-8	81
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	72
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	72



Data Path : W:\HPCHEM1\MSVOA N\DATA\VN091715\
Data File : VN027277.D
Acq On : 18 Sep 2015 2:15
Operator : MD\FY
Sample : G3683-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2R-11

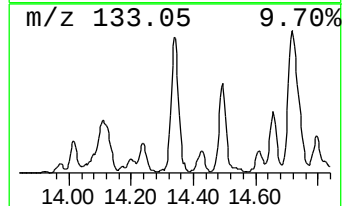
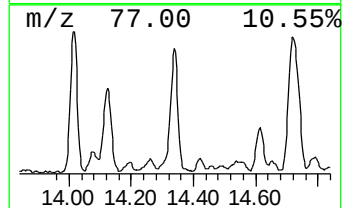
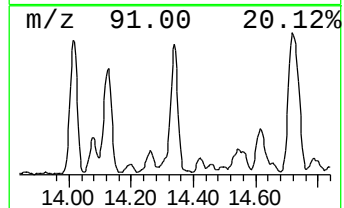
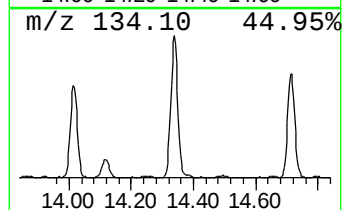
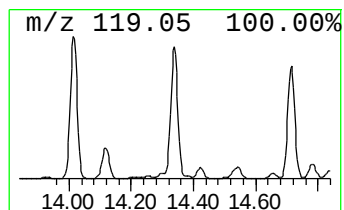
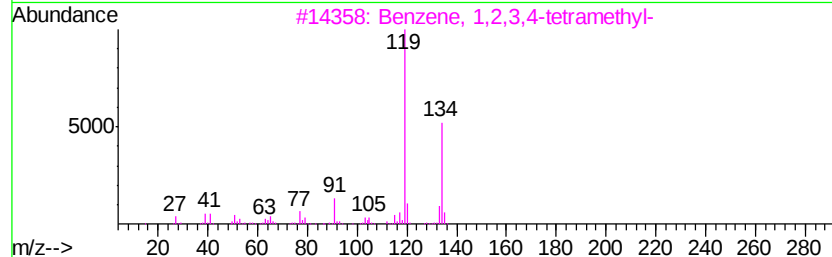
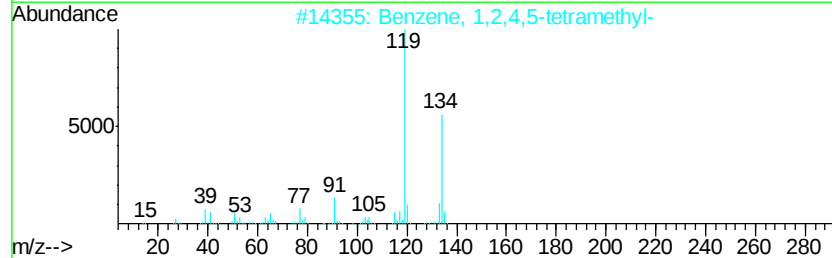
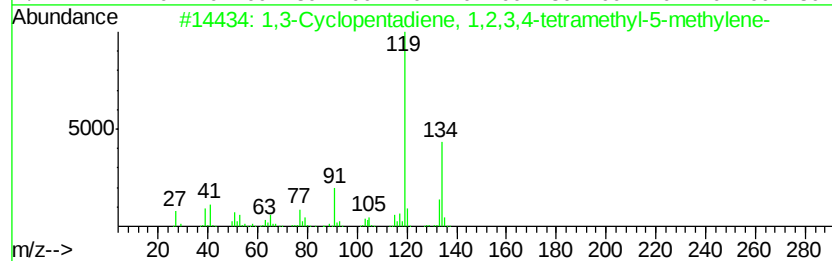
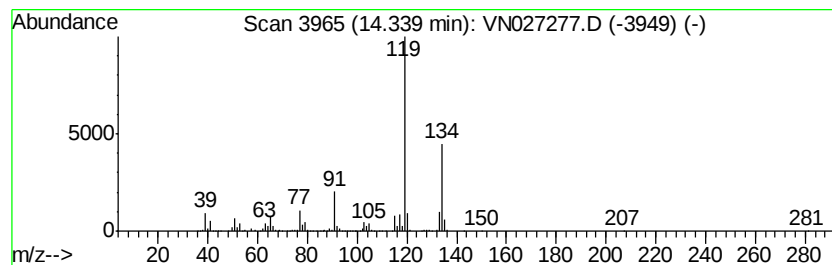
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Quant Title : SW846 8260

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

Peak Number 6 1,3-Cyclopentadiene, 1,2,3,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	17.98 ug/l	1162030	1,4-Dichlorobenzene-d4	13.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	97
2		Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4		Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	95
5		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95



Data Path : W:\HPCHEM1\MSVOA N\DATA\VN091715\
Data File : VN027277.D
Acq On : 18 Sep 2015 2:15
Operator : MD\FY
Sample : G3683-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2R-11

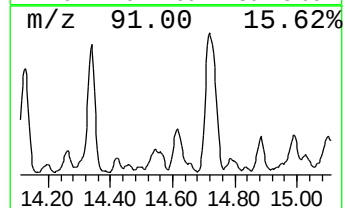
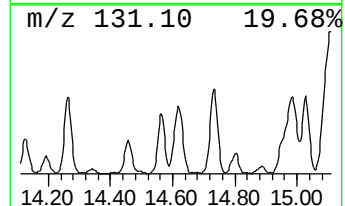
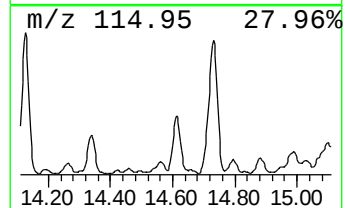
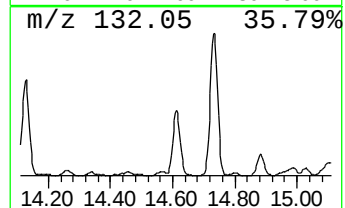
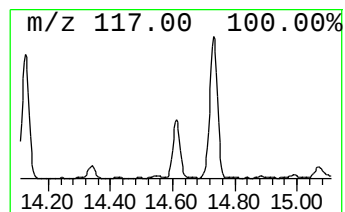
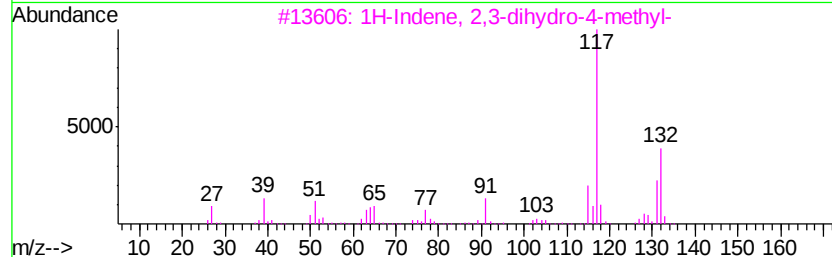
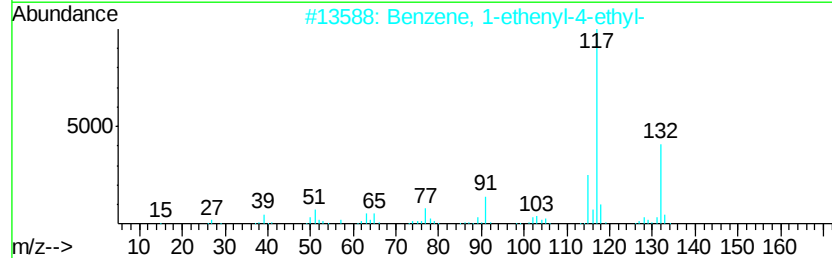
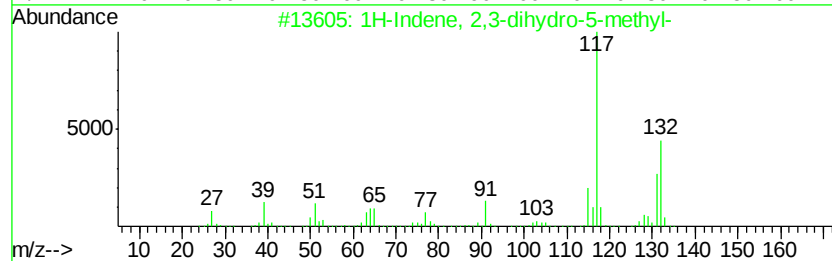
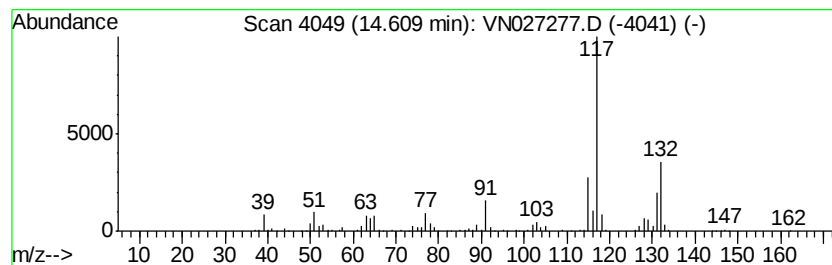
Quant Method : W:\HPCHEM1\MSVOA_N\METHODS\82N091515W.M
Quant Title : SW846 8260

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

Peak Number 7 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	8.06 ug/l	520809	1,4-Dichlorobenzene-d4	13.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
2		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3		1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	91
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87



Data Path : W:\HPCHEM1\MSVOA N\DATA\VN091715\
Data File : VN027277.D
Acq On : 18 Sep 2015 2:15
Operator : MD\FY
Sample : G3683-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2R-11

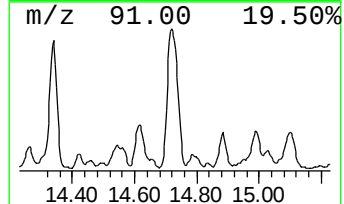
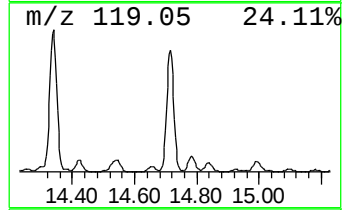
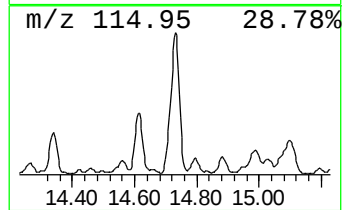
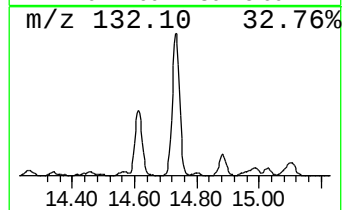
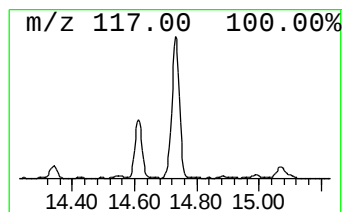
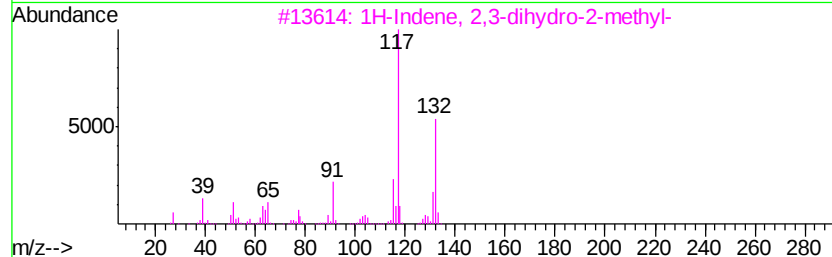
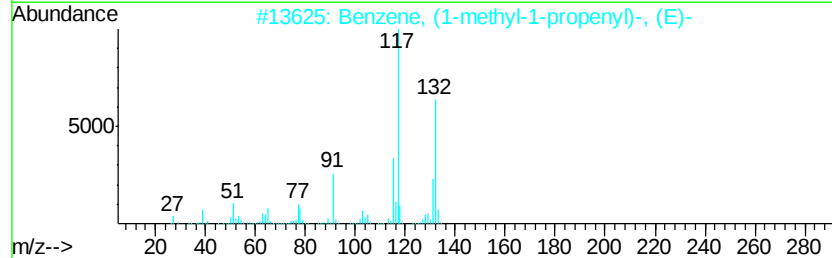
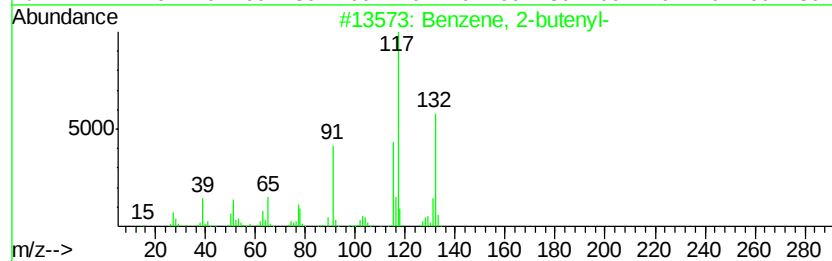
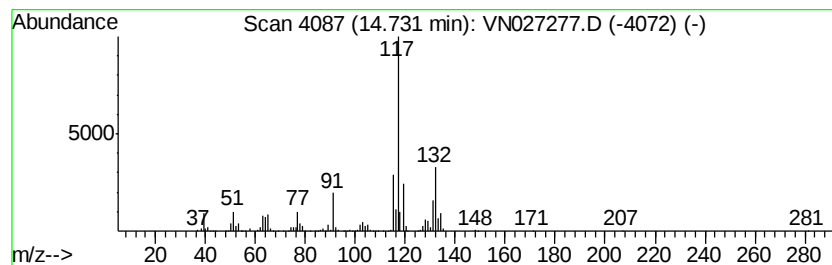
Quant Method : W:\HPCHEM1\MSVOA_N\METHODS\82N091515W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-butenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	30.50 ug/l	1971240	1,4-Dichlorobenzene-d4	13.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
2		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	76
3		1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	76
4		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
5		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70



Data Path : W:\HPCHEM1\MSVOA_N\DATA\VN091715\
Data File : VN027277.D
Acq On : 18 Sep 2015 2:15
Operator : MD\FY
Sample : G3683-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2R-11

Quant Method : W:\HPCHEM1\MSVOA_N\METHODS\82N091515W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	2.80	13.3	ug/l	901726	1	7.75	3391790	50.0
Cyclopentane, met...	6.74	25.2	ug/l	1710960	1	7.75	3391790	50.0
trans-Cinnamyl br...	13.67	26.0	ug/l	1679880	4	13.47	3231490	50.0
Benzene, 1-methyl...	14.01	16.1	ug/l	1037550	4	13.47	3231490	50.0
Benzene, (2-methy...	14.13	17.1	ug/l	1103820	4	13.47	3231490	50.0
1,3-Cyclopentadie...	14.34	18.0	ug/l	1162030	4	13.47	3231490	50.0
1H-Indene, 2,3-di...	14.61	8.1	ug/l	520809	4	13.47	3231490	50.0
Benzene, 2-butenyl-	14.73	30.5	ug/l	1971240	4	13.47	3231490	50.0