

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN082620\
 Data File : VN063140.D
 Acq On : 26 Aug 2020 18:11
 Operator : JC/MD
 Sample : L3792-08
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP-2

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\82N081820W.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	1.796	3	7	27	rVB	234154	289463	32.57%	2.768%
2	1.992	56	68	76	rBV2	9747	19316	2.17%	0.185%
3	2.163	115	121	129	rVB2	13901	21377	2.41%	0.204%
4	2.294	153	162	177	rBV2	10939	19344	2.18%	0.185%
5	3.777	605	623	659	rBV	201101	542360	61.03%	5.186%
6	4.024	682	700	726	rBV2	45880	141329	15.90%	1.351%
7	4.732	896	920	955	rBV2	45096	171431	19.29%	1.639%
8	6.780	1536	1557	1582	rBV3	20247	68760	7.74%	0.657%
9	7.330	1707	1728	1754	rBV	223602	593152	66.75%	5.671%
10	7.551	1779	1797	1808	rBV	111425	276822	31.15%	2.647%
11	7.629	1808	1821	1845	rVB	187697	447779	50.39%	4.281%
12	7.998	1916	1936	1955	rBV3	254408	671255	75.54%	6.418%
13	8.095	1958	1966	1983	rVB4	8111	19912	2.24%	0.190%
14	8.410	2056	2064	2074	rVB2	4611	9016	1.01%	0.086%
15	8.551	2092	2108	2131	rBV	298222	615531	69.27%	5.885%
16	9.005	2235	2249	2264	rBV4	8265	18641	2.10%	0.178%
17	9.165	2289	2299	2315	rVB3	6322	14391	1.62%	0.138%
18	9.680	2446	2459	2474	rVB2	9979	18974	2.14%	0.181%
19	9.953	2534	2544	2563	rVB	33401	63561	7.15%	0.608%
20	10.059	2563	2577	2588	rBV	480561	886006	99.71%	8.471%
21	10.124	2588	2597	2624	rVB	187286	352163	39.63%	3.367%
22	10.326	2651	2660	2672	rVB3	17329	29230	3.29%	0.279%
23	10.780	2790	2801	2808	rBV	11075	19845	2.23%	0.190%
24	10.844	2808	2821	2839	rVB8	11345	32306	3.64%	0.309%
25	11.381	2963	2988	3010	rBV	465909	810199	91.17%	7.747%
26	11.493	3010	3023	3024	rBV	15213	23014	2.59%	0.220%
27	11.558	3035	3043	3046	rBV2	24679	35699	4.02%	0.341%
28	11.593	3046	3054	3067	rVB	81960	153172	17.24%	1.465%
29	11.693	3075	3085	3095	rBV3	14875	28789	3.24%	0.275%
30	11.924	3146	3157	3172	rBV4	55691	114990	12.94%	1.099%
31	12.175	3224	3235	3242	rBV3	9729	19048	2.14%	0.182%
32	12.220	3243	3249	3262	rVB9	10742	22046	2.48%	0.211%
33	12.378	3285	3298	3309	rBV	384276	647818	72.90%	6.194%
34	12.435	3309	3316	3331	rVB	27122	49451	5.56%	0.473%

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Integration Parameters: RTEINT.P

Integrator: RTE
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Sampling : 1
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Max Peaks: 100
Peak Location: TOP

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35	12.570	3347	3358	3366	rBV2	8893	14713	1.66%	0.141%
36	12.632	3370	3377	3381	rVV2	7076	9449	1.06%	0.090%
37	12.677	3382	3391	3392	rVV6	10179	15456	1.74%	0.148%
38	12.702	3393	3399	3408	rVV4	15159	29080	3.27%	0.278%
39	12.763	3410	3418	3419	rVV6	9515	12850	1.45%	0.123%
40	12.805	3422	3431	3442	rVV	137531	217926	24.52%	2.084%
41	12.886	3442	3456	3470	rVB7	14903	37088	4.17%	0.355%
42	12.969	3470	3482	3486	rBV8	5981	10869	1.22%	0.104%
43	13.014	3486	3496	3503	rVV	58189	98459	11.08%	0.941%
44	13.053	3504	3508	3524	rVV6	28017	69388	7.81%	0.663%
45	13.140	3526	3535	3543	rVB6	9542	18388	2.07%	0.176%
46	13.233	3557	3564	3577	rVB8	8506	16466	1.85%	0.157%
47	13.320	3577	3591	3605	rBV	479208	815063	91.72%	7.793%
48	13.394	3607	3614	3617	rBV7	6851	10336	1.16%	0.099%
49	13.525	3645	3655	3668	rBV3	17007	45764	5.15%	0.438%
50	13.699	3691	3709	3721	rBV	238634	395618	44.52%	3.783%
51	13.821	3735	3747	3769	rVB	16932	48253	5.43%	0.461%
52	13.937	3771	3783	3792	rBV9	10320	26890	3.03%	0.257%
53	14.069	3813	3824	3843	rBV2	21104	48095	5.41%	0.460%
54	14.194	3855	3863	3870	rBV4	13960	22262	2.51%	0.213%
55	14.558	3967	3976	3986	rBV9	4191	9183	1.03%	0.088%
56	14.631	3989	3999	4009	rVV3	17187	28926	3.26%	0.277%
57	14.712	4016	4024	4037	rVB4	17646	30259	3.41%	0.289%
58	14.821	4037	4058	4067	rBV6	25782	52533	5.91%	0.502%
59	14.873	4068	4074	4084	rVB9	6503	11266	1.27%	0.108%
60	15.104	4133	4146	4162	rBV	511621	888627	100.00%	8.496%
61	15.194	4163	4174	4189	rVB2	26861	58140	6.54%	0.556%
62	16.123	4450	4463	4478	rBV	31446	65614	7.38%	0.627%
63	16.213	4479	4491	4509	rVV4	17733	47094	5.30%	0.450%
64	16.313	4511	4522	4537	rVB	28567	58559	6.59%	0.560%

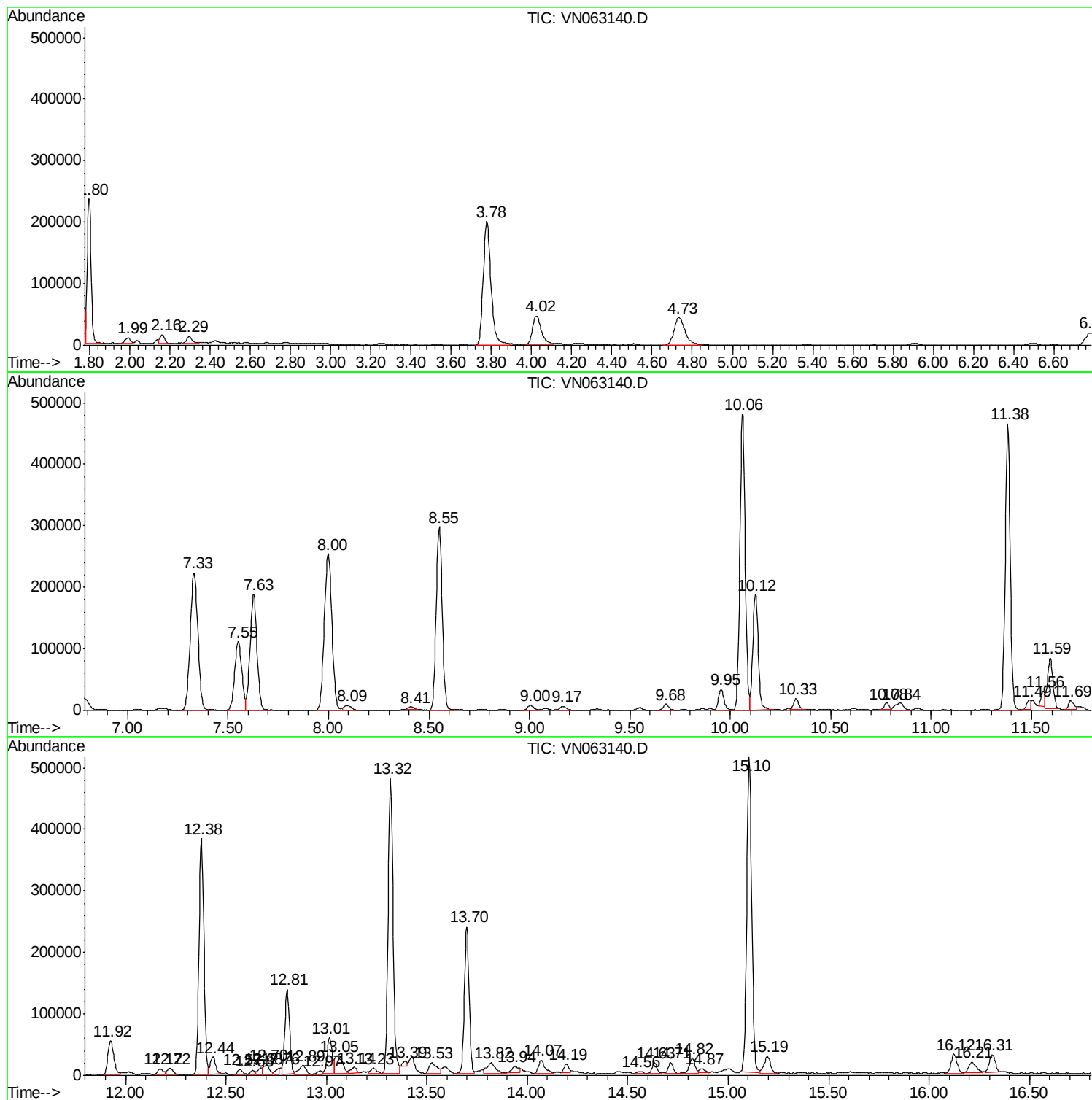
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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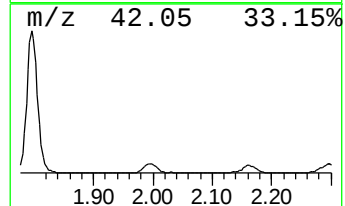
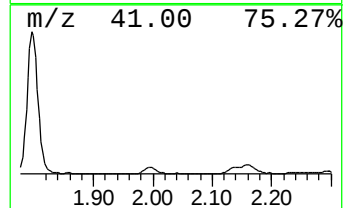
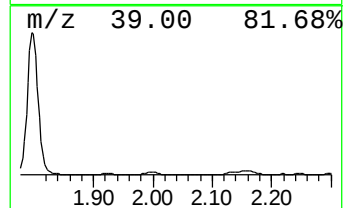
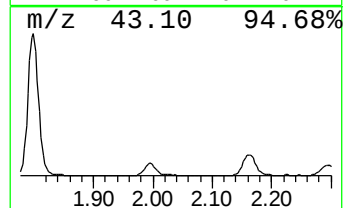
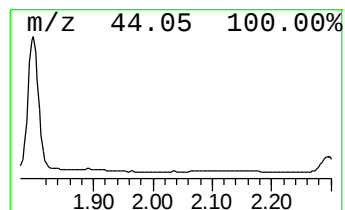
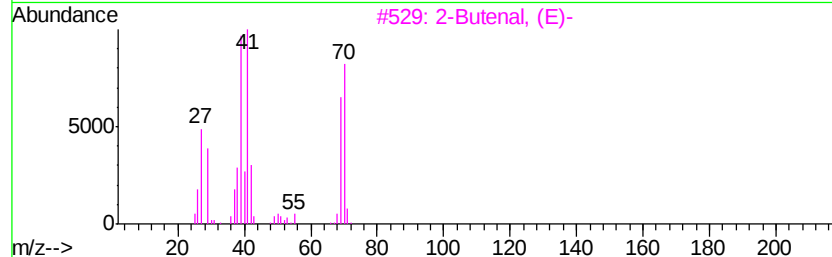
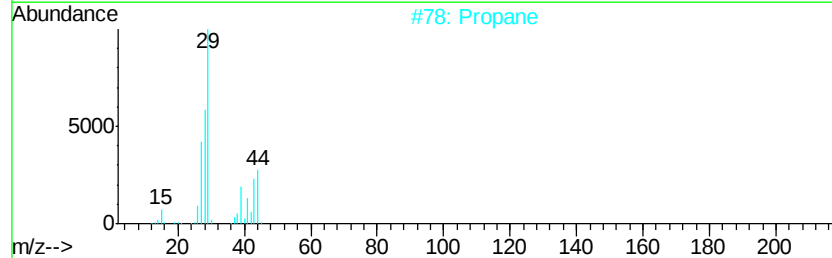
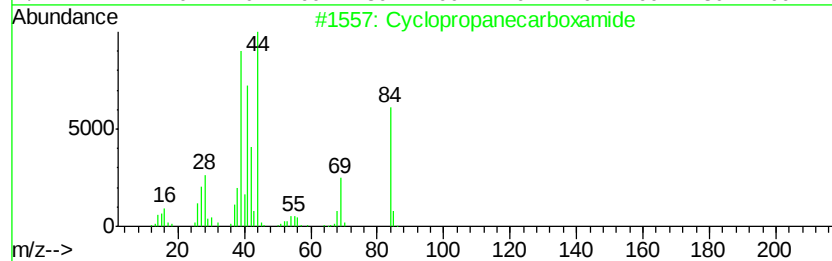
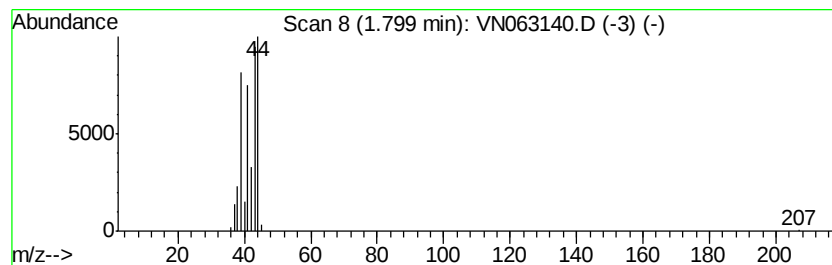
Instrument :
MSVOA_N
ClientSampleId :
COMP-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N081820W.M
Quant Title : SW846 8260

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

Peak Number 1 Cyclopropanecarboxamide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.80	32.32 ug/l	289463	Pentafluorobenzene	7.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cvclopropanecarboxamide	85	C4H7NO	006228-73-5	78
2		Propane	44	C3H8	000074-98-6	74
3		2-Butenal, (E)-	70	C4H6O	000123-73-9	64
4		Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	64
5		Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	50



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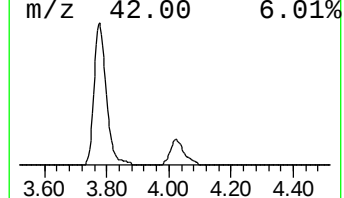
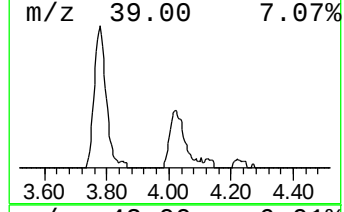
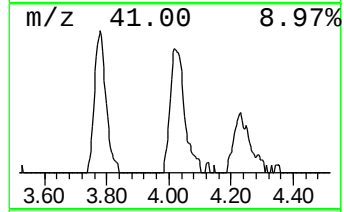
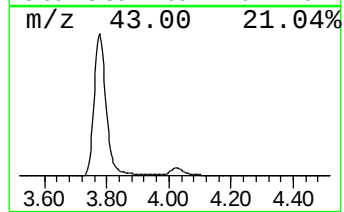
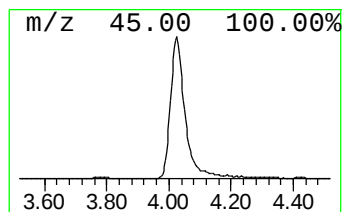
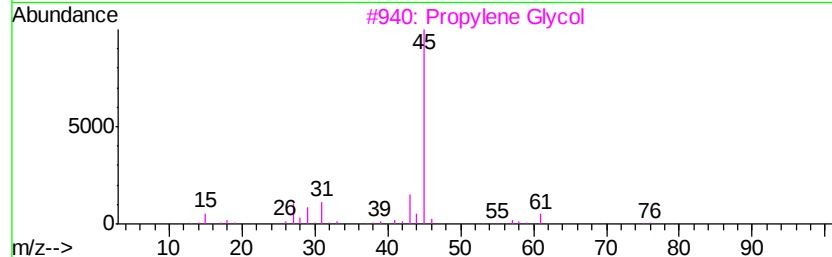
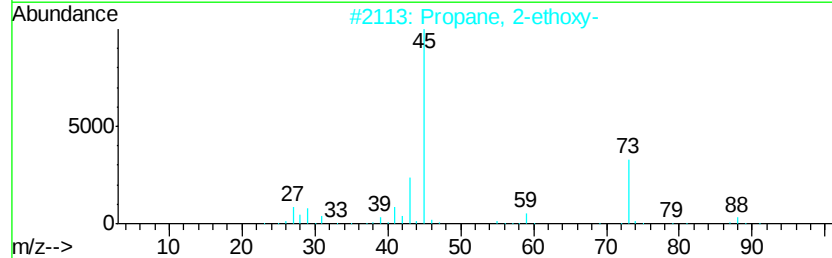
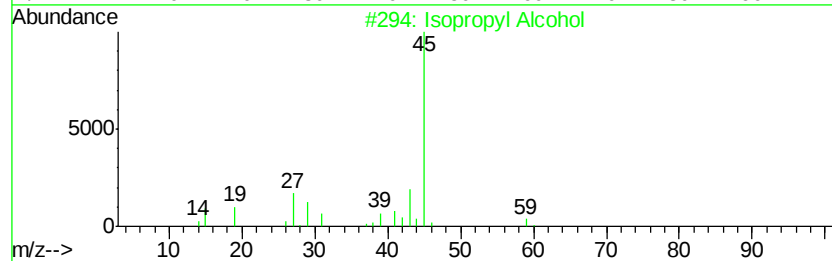
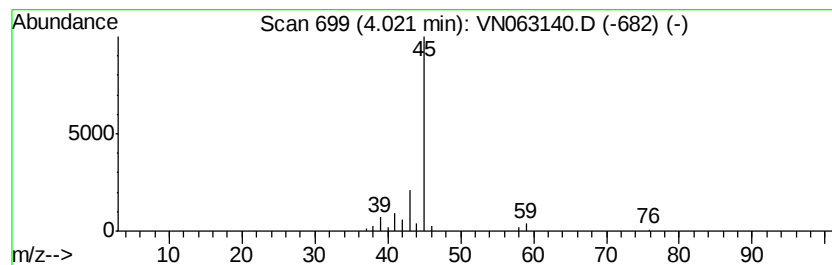
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Quant Title : SW846 8260

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	15.78 ug/l	141329	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5		2-Pentanol	88	C5H12O	006032-29-7	9



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ALS Vial : 15 Sample Multiplier: 1

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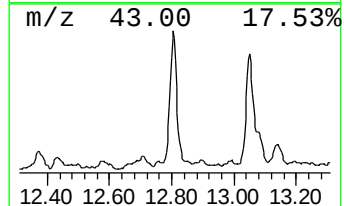
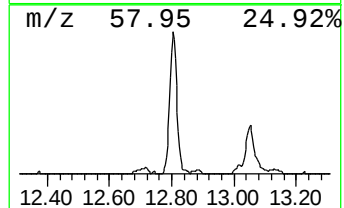
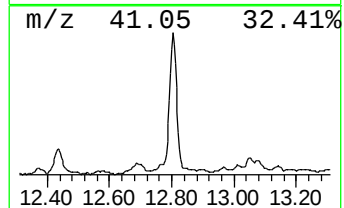
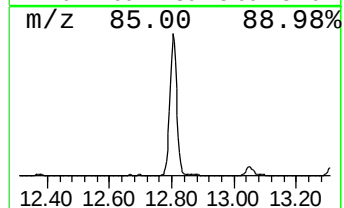
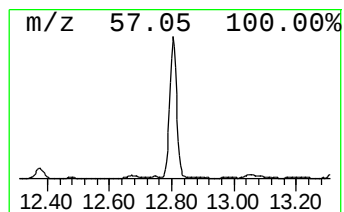
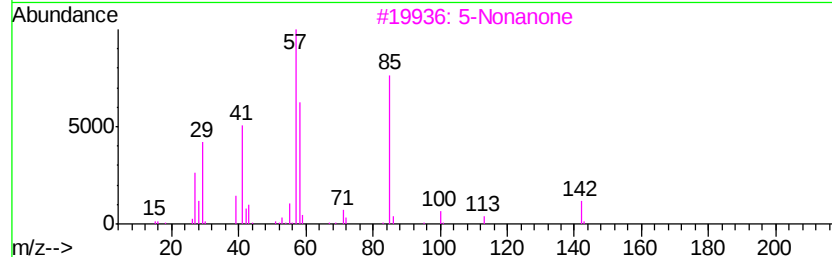
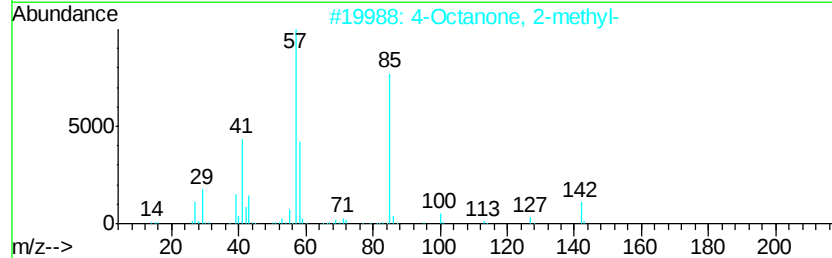
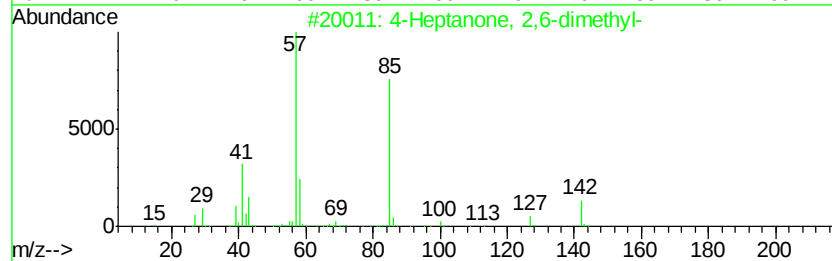
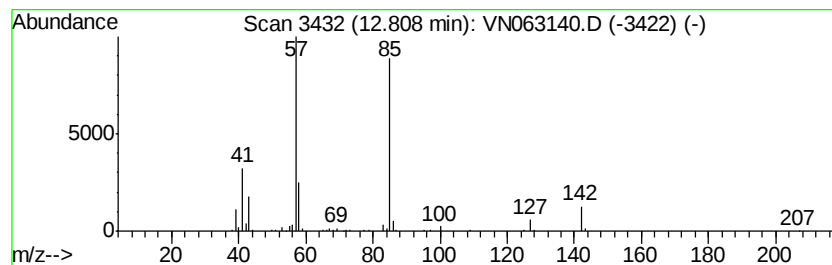
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-Heptanone, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.81	13.37 ug/l	217926	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2		4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
3		5-Nonanone	142	C9H18O	000502-56-7	59
4		2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	47
5		2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	38



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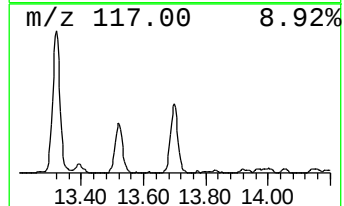
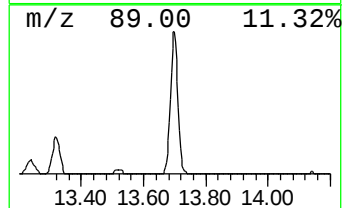
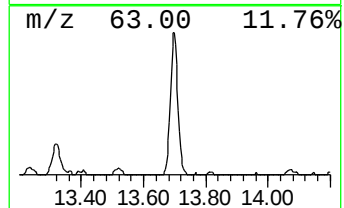
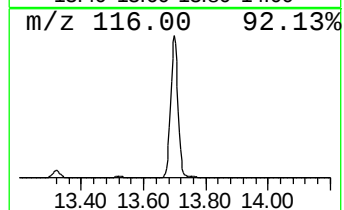
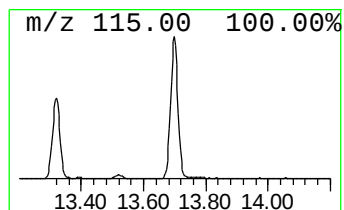
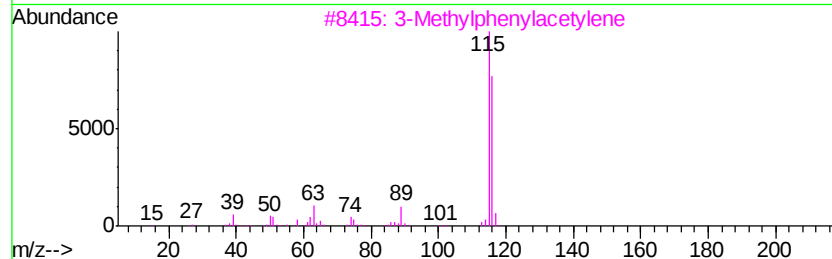
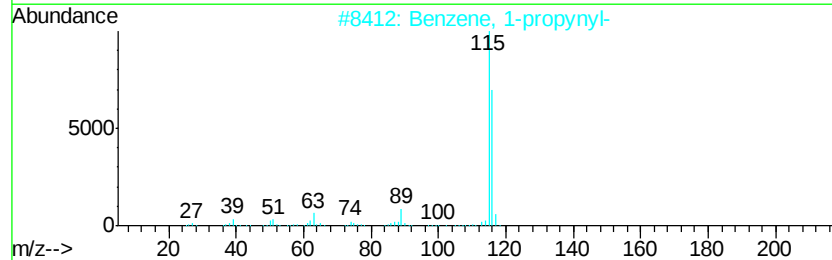
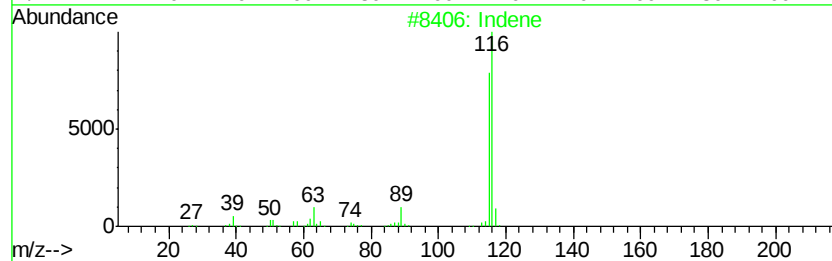
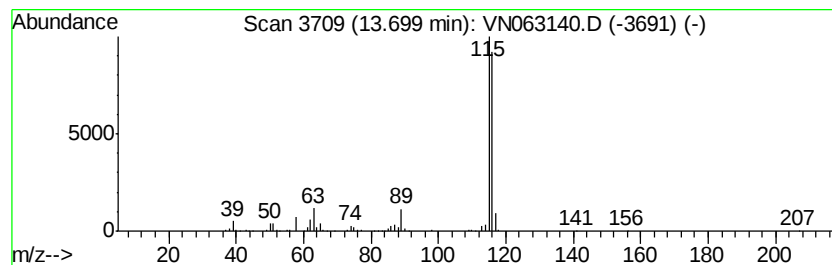
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Peak Number 4 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	24.27 ug/l	395618	1,4-Dichlorobenzene-d4	13.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene		116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-		116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene		116	C9H8	000766-82-5	91
4	2-Methylphenylacetylene		116	C9H8	000766-47-2	91
5	Benzene, 1-ethynyl-4-methyl-		116	C9H8	000766-97-2	90



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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
Cyclopropanecarbo...	1.80	32.3	ug/l	289463	1	7.63	447779	50.0
Isopropyl Alcohol	4.02	15.8	ug/l	141329	1	7.63	447779	50.0
4-Heptanone, 2,6-...	12.81	13.4	ug/l	217926	4	13.32	815063	50.0
Indene	13.70	24.3	ug/l	395618	4	13.32	815063	50.0