

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
 Data File : VN065619.D
 Acq On : 27 Jan 2021 10:30
 Operator : JC/MD
 Sample : VSTDCCC050
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 2 Sample Multiplier: 1

Instrument :
 MSVOA_N
 LabSampleId :
 VSTDCCC050

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\82N012521W.M
 Title : SW846 8260

Signal : TIC: VN065619.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.837	21	30	42	rBV	129687	166087	7.23%	0.264%
2	2.036	82	92	107	rBV	159434	221679	9.65%	0.353%
3	2.168	122	133	145	rBV	149481	219885	9.57%	0.350%
4	2.296	164	173	187	rVB	15140	24564	1.07%	0.039%
5	2.541	237	249	271	rVB	118605	226972	9.88%	0.361%
6	2.679	281	292	309	rVB	85597	159321	6.93%	0.253%
7	2.994	375	390	409	rBV	149192	323542	14.08%	0.515%
8	3.377	495	509	531	rVB	136856	297904	12.97%	0.474%
9	3.570	555	569	587	rVB	72365	172086	7.49%	0.274%
10	3.705	591	611	625	rBV3	268146	852964	37.13%	1.357%
11	3.779	627	634	652	rVB	149238	344819	15.01%	0.548%
12	3.907	660	674	689	rBV	79711	204245	8.89%	0.325%
13	4.004	690	704	731	rVB	147073	382937	16.67%	0.609%
14	4.274	755	788	823	rBV3	223594	671301	29.22%	1.068%
15	4.499	836	858	891	rVB	154503	460661	20.05%	0.733%
16	4.753	917	937	966	rVB2	45110	160766	7.00%	0.256%
17	4.988	971	1010	1043	rBV5	349748	1843700	80.25%	2.933%
18	5.843	1236	1276	1289	rBV2	614837	2297454	100.00%	3.654%
19	6.779	1541	1567	1586	rBV3	499655	1587799	69.11%	2.526%
20	6.885	1587	1600	1652	rVV3	227554	888684	38.68%	1.414%
21	7.161	1652	1686	1719	rVV5	320570	1319615	57.44%	2.099%
22	7.325	1719	1737	1760	rVB	176089	464542	20.22%	0.739%
23	7.531	1779	1801	1813	rBV2	230584	716421	31.18%	1.140%
24	7.615	1814	1827	1843	rVV2	461933	1260448	54.86%	2.005%
25	7.737	1843	1865	1891	rVB4	352453	1485654	64.67%	2.363%
26	7.997	1924	1946	1961	rBV3	515069	1304181	56.77%	2.074%
27	8.084	1961	1973	1978	rVV	156038	333827	14.53%	0.531%
28	8.126	1980	1986	2006	rVB	215857	432073	18.81%	0.687%
29	8.547	2101	2117	2143	rBV	317228	665450	28.96%	1.058%
30	8.798	2179	2195	2214	rBV	301343	621030	27.03%	0.988%
31	9.042	2254	2271	2278	rBV	397993	879164	38.27%	1.398%
32	9.168	2297	2310	2322	rBV2	424278	860695	37.46%	1.369%
33	9.232	2322	2330	2347	rVB	203282	370468	16.13%	0.589%
34	9.367	2359	2372	2388	rVB	213889	421168	18.33%	0.670%
35	9.589	2428	2441	2450	rBV	52389	100956	4.39%	0.161%
36	9.659	2450	2463	2494	rVV	853553	1527448	66.48%	2.430%

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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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37	9.804	2494	2508	2528	rVV	316417	585762	25.50%	0.932%
38	9.949	2538	2553	2572	rBV	1039930	1868063	81.31%	2.971%
39	10.055	2573	2586	2596	rVV	461644	838330	36.49%	1.333%
40	10.119	2596	2606	2630	rVB	620705	1137258	49.50%	1.809%
41	10.348	2663	2677	2685	rBV	305581	543404	23.65%	0.864%
42	10.396	2685	2692	2717	rVV	329399	552326	24.04%	0.879%
43	10.528	2717	2733	2744	rVV	316596	581888	25.33%	0.926%
44	10.598	2744	2755	2767	rVV	457845	826178	35.96%	1.314%
45	10.672	2767	2778	2785	rVV	305060	548872	23.89%	0.873%
46	10.721	2785	2793	2813	rVV	771227	1310049	57.02%	2.084%
47	10.823	2813	2825	2832	rVV	305221	511569	22.27%	0.814%
48	10.868	2832	2839	2854	rVV	201357	362470	15.78%	0.577%
49	10.975	2858	2872	2895	rVB	144668	264362	11.51%	0.420%
50	11.380	2983	2998	3000	rBV	502524	755554	32.89%	1.202%
51	11.479	3017	3029	3046	rVB2	1051027	1791245	77.97%	2.849%
52	11.589	3046	3063	3089	rBV	1163897	2253776	98.10%	3.585%
53	11.923	3148	3167	3191	rBV3	950033	2127748	92.61%	3.384%
54	12.039	3191	3203	3213	rVV	399501	625932	27.24%	0.996%
55	12.097	3213	3221	3238	rVB	145011	257036	11.19%	0.409%
56	12.219	3244	3259	3268	rBV	725466	1181208	51.41%	1.879%
57	12.270	3268	3275	3295	rVV	209387	354964	15.45%	0.565%
58	12.370	3295	3306	3326	rVB	310608	523251	22.78%	0.832%
59	12.495	3326	3345	3358	rBV4	598386	1848860	80.47%	2.941%
60	12.560	3358	3365	3378	rVV	722465	1180397	51.38%	1.878%
61	12.643	3378	3391	3400	rVV	570950	946132	41.18%	1.505%
62	12.701	3400	3409	3416	rVV	727701	1196927	52.10%	1.904%
63	12.743	3416	3422	3449	rVB	563159	896489	39.02%	1.426%
64	12.962	3477	3490	3497	rBV	665842	1102116	47.97%	1.753%
65	13.007	3497	3504	3528	rVV	885066	1495827	65.11%	2.379%
66	13.142	3532	3546	3560	rBV	640665	1010916	44.00%	1.608%
67	13.257	3567	3582	3591	rBV2	1106839	1853450	80.67%	2.948%
68	13.325	3591	3603	3624	rVB2	588477	1455872	63.37%	2.316%
69	13.582	3670	3683	3690	rBV	633181	1022869	44.52%	1.627%
70	13.621	3690	3695	3714	rVB	455904	734638	31.98%	1.169%
71	13.843	3752	3764	3780	rVB	306553	522398	22.74%	0.831%
72	14.238	3874	3887	3904	rVB2	101203	192332	8.37%	0.306%
73	14.550	3970	3984	3998	rBV	687206	1091250	47.50%	1.736%
74	14.875	4074	4085	4105	rBV	342110	575717	25.06%	0.916%
75	14.978	4105	4117	4131	rVB2	236815	386348	16.82%	0.615%
76	15.097	4141	4154	4175	rBV	410471	712307	31.00%	1.133%

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ALS Vial : 2 Sample Multiplier: 1

Instrument :
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LabSampleId :
VSTDCCC050

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\82N012521W.M
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77	15.277	4193	4210	4228	rVB	313692	572832	24.93%	0.911%
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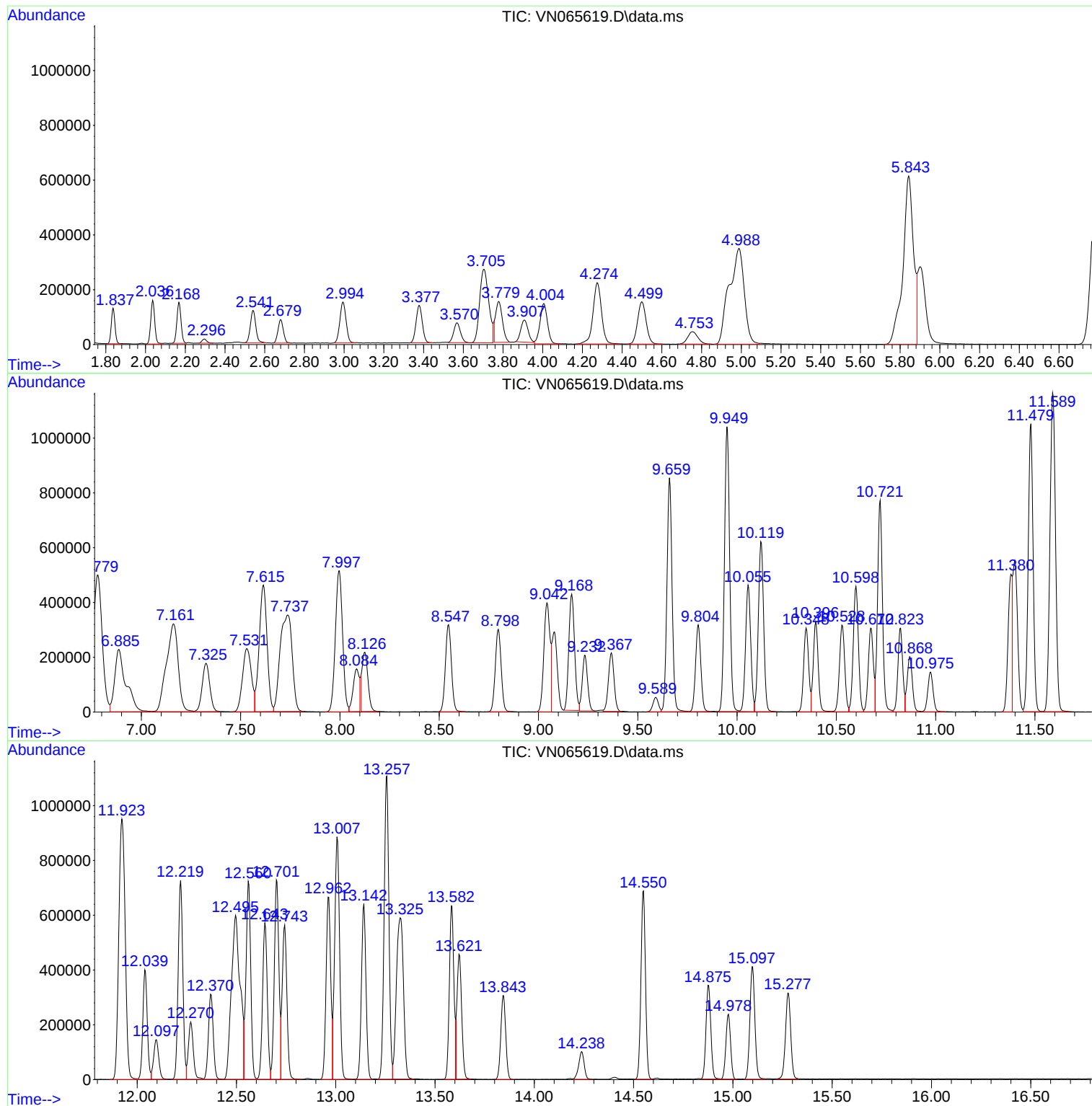
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Instrument :
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LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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Instrument :
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VSTDCCC050

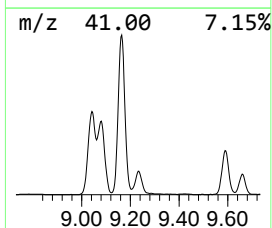
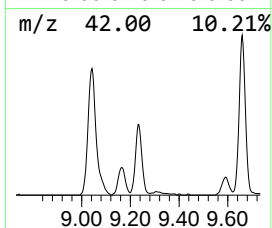
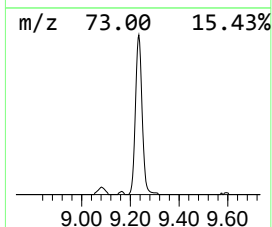
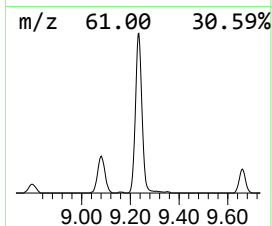
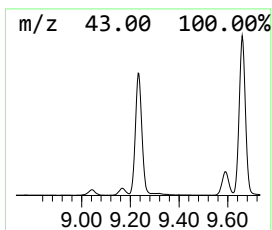
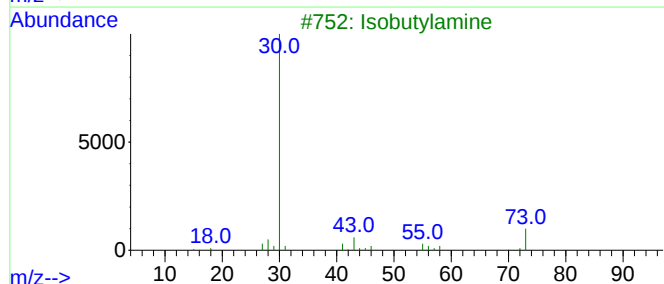
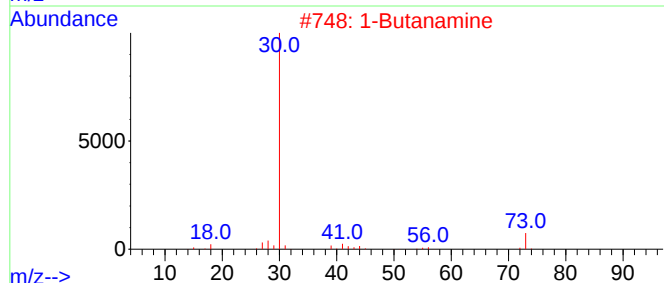
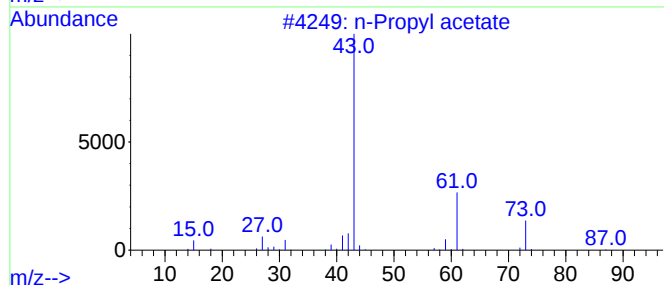
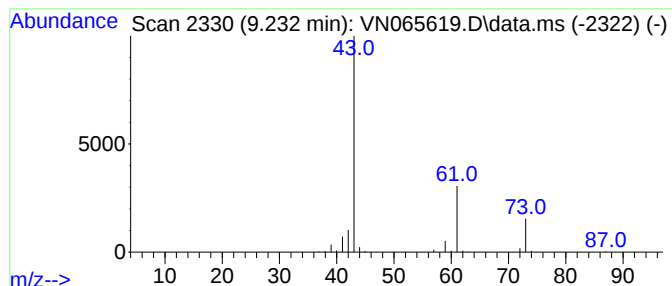
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.232	27.84 ug/l	370468	1,4-Difluorobenzene	8.547

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			1-Butanamine	73	C4H11N	000109-73-9	7
3			Isobutylamine	73	C4H11N	000078-81-9	4
4			5-Methyloxazolidine	87	C4H9NO	058328-22-6	4
5			Hydrogen azide	43	HN3	007782-79-8	4



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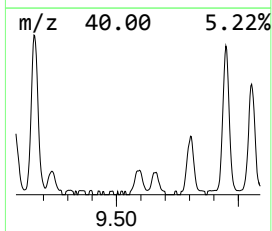
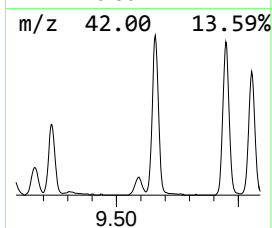
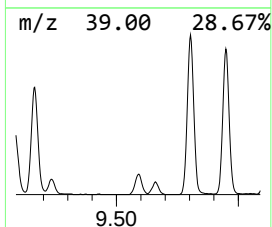
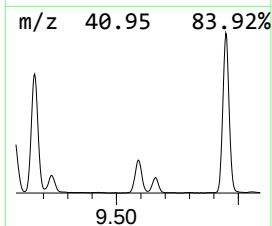
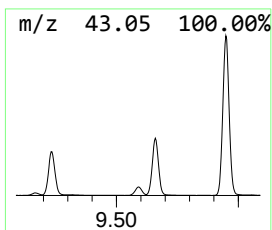
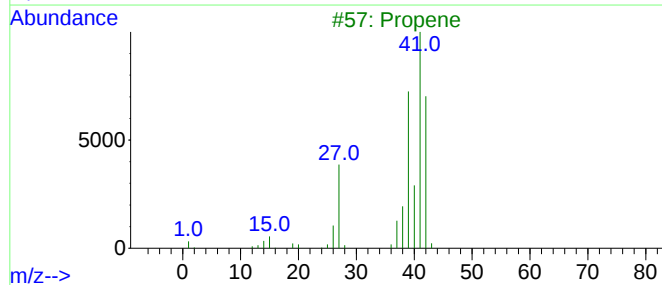
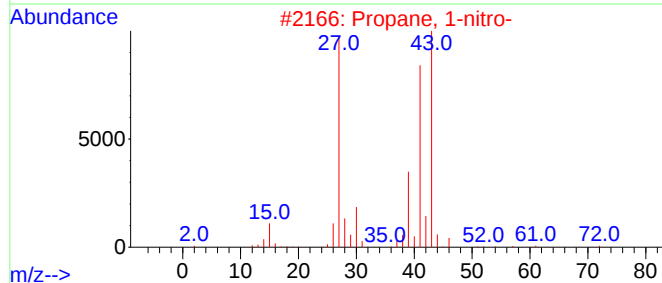
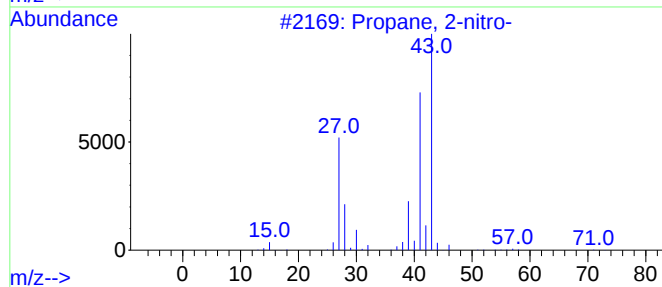
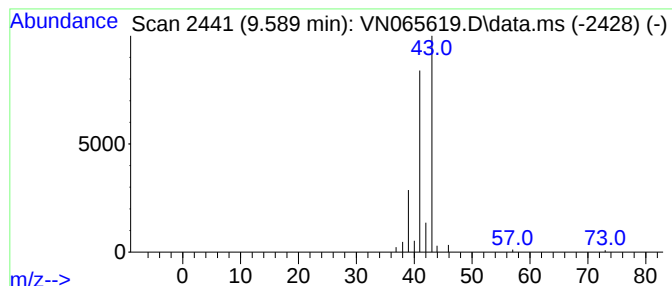
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Quant Title : SW846 8260

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

Peak Number 2 Propane, 2-nitro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.589	7.59 ug/l	100956	1,4-Difluorobenzene	8.547

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	83
2			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	74
3			Propene	42	C3H6	000115-07-1	9
4			Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
5			o-Allylhydroxylamine	73	C3H7NO	006542-54-7	5



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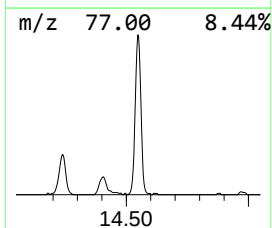
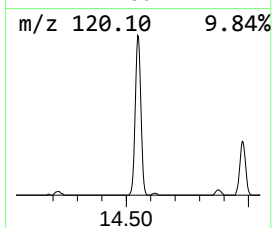
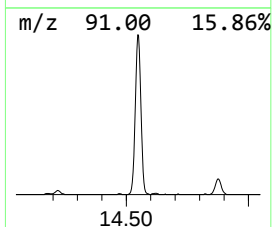
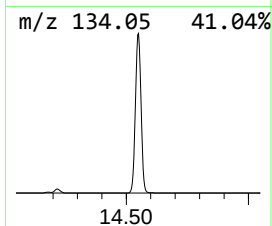
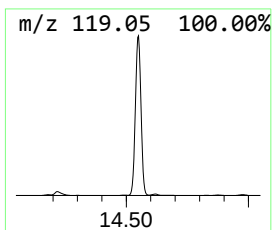
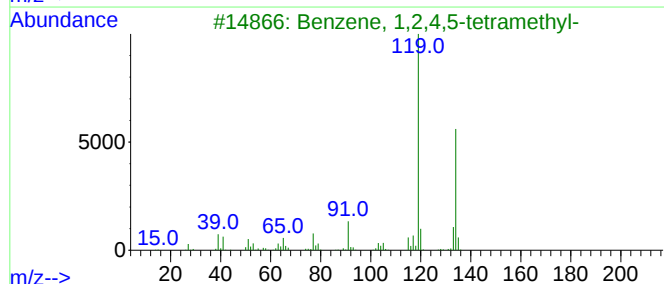
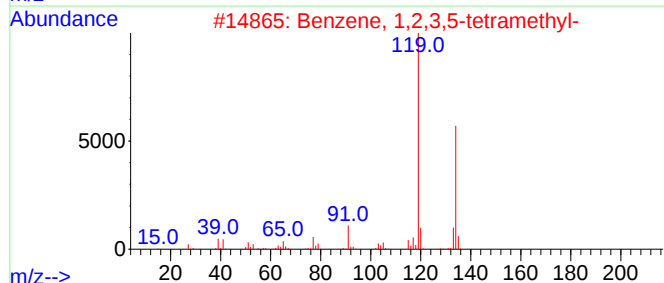
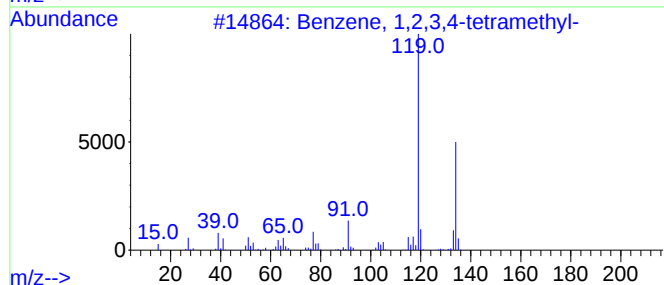
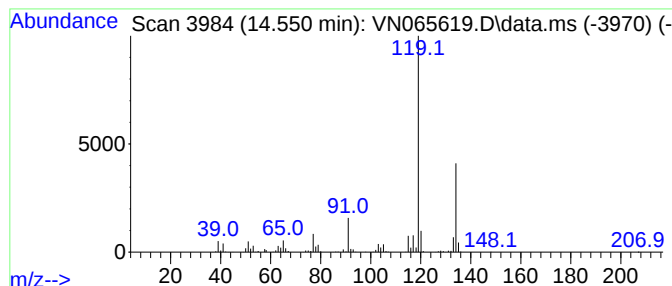
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.550	37.48 ug/l	1091250	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	9.232	27.8	ug/l	370468	2	8.547	665450	50.0
Propane, 2-nitro-	9.589	7.6	ug/l	100956	2	8.547	665450	50.0
Benzene, 1,2,3,...	14.550	37.5	ug/l	1091250	4	13.312	1455870	50.0