

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012621\
 Data File : VN065617.D
 Acq On : 26 Jan 2021 20:31
 Operator : JC/MD
 Sample : VSTDCCC050
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_N
 LabSampleId :
 VSTDCCC050

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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: VN065617.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	20	30	45	rVB	111925	144540	6.53%	0.236%
2	2.036	81	92	105	rBV	144281	200455	9.06%	0.328%
3	2.168	122	133	144	rBV	137248	203018	9.17%	0.332%
4	2.534	236	247	271	rVB	108874	209326	9.46%	0.342%
5	2.676	280	291	310	rVB	78611	149149	6.74%	0.244%
6	2.991	374	389	404	rBV	143701	312049	14.10%	0.510%
7	3.380	495	510	527	rBV2	130316	285226	12.89%	0.466%
8	3.570	555	569	590	rVB	70804	167606	7.57%	0.274%
9	3.701	591	610	626	rBV3	257271	809583	36.58%	1.323%
10	3.782	627	635	655	rVB	123452	294041	13.29%	0.480%
11	3.907	660	674	688	rVV2	83441	222603	10.06%	0.364%
12	4.004	689	704	725	rVB	140681	365518	16.52%	0.597%
13	4.277	758	789	817	rBV4	212283	643999	29.10%	1.052%
14	4.502	837	859	885	rBV	148693	441267	19.94%	0.721%
15	4.766	915	941	968	rBV3	44228	159653	7.21%	0.261%
16	4.991	975	1011	1043	rBV4	335347	1784926	80.66%	2.917%
17	5.846	1236	1277	1290	rBV2	584142	2187455	98.85%	3.574%
18	6.785	1541	1569	1588	rBV3	466769	1502619	67.90%	2.455%
19	6.891	1589	1602	1650	rVB3	219885	851152	38.46%	1.391%
20	7.168	1657	1688	1719	rBV5	312303	1281987	57.93%	2.095%
21	7.328	1721	1738	1761	rVB	171335	451136	20.39%	0.737%
22	7.534	1780	1802	1814	rBV2	230683	718628	32.47%	1.174%
23	7.618	1815	1828	1843	rVV4	439502	1207969	54.59%	1.974%
24	7.740	1843	1866	1889	rVB4	347396	1448642	65.46%	2.367%
25	7.997	1925	1946	1962	rBV3	510924	1288839	58.24%	2.106%
26	8.087	1962	1974	1979	rVV	151992	325896	14.73%	0.533%
27	8.129	1980	1987	2005	rVB	206750	441514	19.95%	0.721%
28	8.547	2102	2117	2134	rBV	333999	695416	31.43%	1.136%
29	8.798	2179	2195	2216	rBV	291853	613814	27.74%	1.003%
30	9.045	2253	2272	2278	rBV	368971	793345	35.85%	1.296%
31	9.167	2298	2310	2322	rBV2	416181	839361	37.93%	1.371%
32	9.235	2322	2331	2346	rVB	198297	365664	16.52%	0.597%
33	9.367	2360	2372	2388	rVB	204192	407546	18.42%	0.666%
34	9.592	2427	2442	2451	rBV	51989	101446	4.58%	0.166%
35	9.663	2451	2464	2488	rVB	805104	1444568	65.28%	2.360%
36	9.807	2495	2509	2529	rBV	301817	561408	25.37%	0.917%

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Integrator: RTE

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37	9.952	2540	2554	2573	rBV	1002370	1812410	81.90%	2.961%
38	10.058	2574	2587	2597	rVV	462654	848120	38.33%	1.386%
39	10.122	2597	2607	2624	rVB	611135	1106302	49.99%	1.808%
40	10.351	2665	2678	2685	rBV	294080	515448	23.29%	0.842%
41	10.399	2685	2693	2709	rVB	318289	535259	24.19%	0.875%
42	10.531	2721	2734	2744	rBV	311257	560357	25.32%	0.916%
43	10.598	2744	2755	2767	rVV	432985	776864	35.11%	1.269%
44	10.675	2768	2779	2785	rVV	294864	506577	22.89%	0.828%
45	10.720	2785	2793	2813	rVB	741654	1254223	56.68%	2.049%
46	10.823	2815	2825	2833	rBV	300829	494963	22.37%	0.809%
47	10.872	2833	2840	2852	rVB	188791	332684	15.03%	0.544%
48	10.974	2862	2872	2887	rVB	145138	265519	12.00%	0.434%
49	11.380	2985	2998	3000	rBV	513126	736932	33.30%	1.204%
50	11.479	3017	3029	3043	rBV2	1013784	1706356	77.11%	2.788%
51	11.592	3050	3064	3085	rBV	1120005	2212916	100.00%	3.616%
52	11.923	3154	3167	3183	rBV4	934295	2096233	94.73%	3.425%
53	12.042	3195	3204	3213	rBV	378939	600671	27.14%	0.981%
54	12.097	3214	3221	3237	rVB	160860	291483	13.17%	0.476%
55	12.219	3248	3259	3268	rBV	689465	1122211	50.71%	1.834%
56	12.270	3268	3275	3287	rVB	192711	312707	14.13%	0.511%
57	12.373	3297	3307	3328	rBV	325753	615954	27.83%	1.006%
58	12.495	3330	3345	3358	rVV5	562661	1751429	79.15%	2.862%
59	12.560	3359	3365	3378	rVV	685600	1103788	49.88%	1.804%
60	12.643	3381	3391	3401	rVV	560783	968454	43.76%	1.582%
61	12.701	3401	3409	3416	rVV	711225	1157093	52.29%	1.891%
62	12.743	3416	3422	3441	rVB	523976	835049	37.74%	1.364%
63	12.965	3480	3491	3497	rBV	636073	1053160	47.59%	1.721%
64	13.007	3497	3504	3523	rVB	851354	1461971	66.07%	2.389%
65	13.142	3535	3546	3558	rBV	611817	984631	44.49%	1.609%
66	13.257	3570	3582	3591	rBV2	1059364	1759001	79.49%	2.874%
67	13.325	3591	3603	3619	rVB2	559633	1373071	62.05%	2.244%
68	13.585	3673	3684	3690	rBV	599040	974517	44.04%	1.592%
69	13.624	3690	3696	3713	rVB	442830	751769	33.97%	1.228%
70	13.846	3755	3765	3779	rVB2	301914	544491	24.61%	0.890%
71	14.238	3878	3887	3904	rVB3	115004	244994	11.07%	0.400%
72	14.550	3973	3984	3997	rBV	683011	1097656	49.60%	1.794%
73	14.878	4075	4086	4100	rBV	334401	580054	26.21%	0.948%
74	14.977	4108	4117	4138	rVB2	237678	426446	19.27%	0.697%
75	15.100	4142	4155	4169	rBV	429997	791780	35.78%	1.294%
76	15.280	4199	4211	4228	rVB	319228	620455	28.04%	1.014%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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77	16.055	4444	4452	4462	rBV6	15479	28677	1.30%	0.047%
78	16.119	4466	4472	4485	rVV6	13563	33826	1.53%	0.055%
79	16.186	4488	4493	4505	rVB	20245	32360	1.46%	0.053%

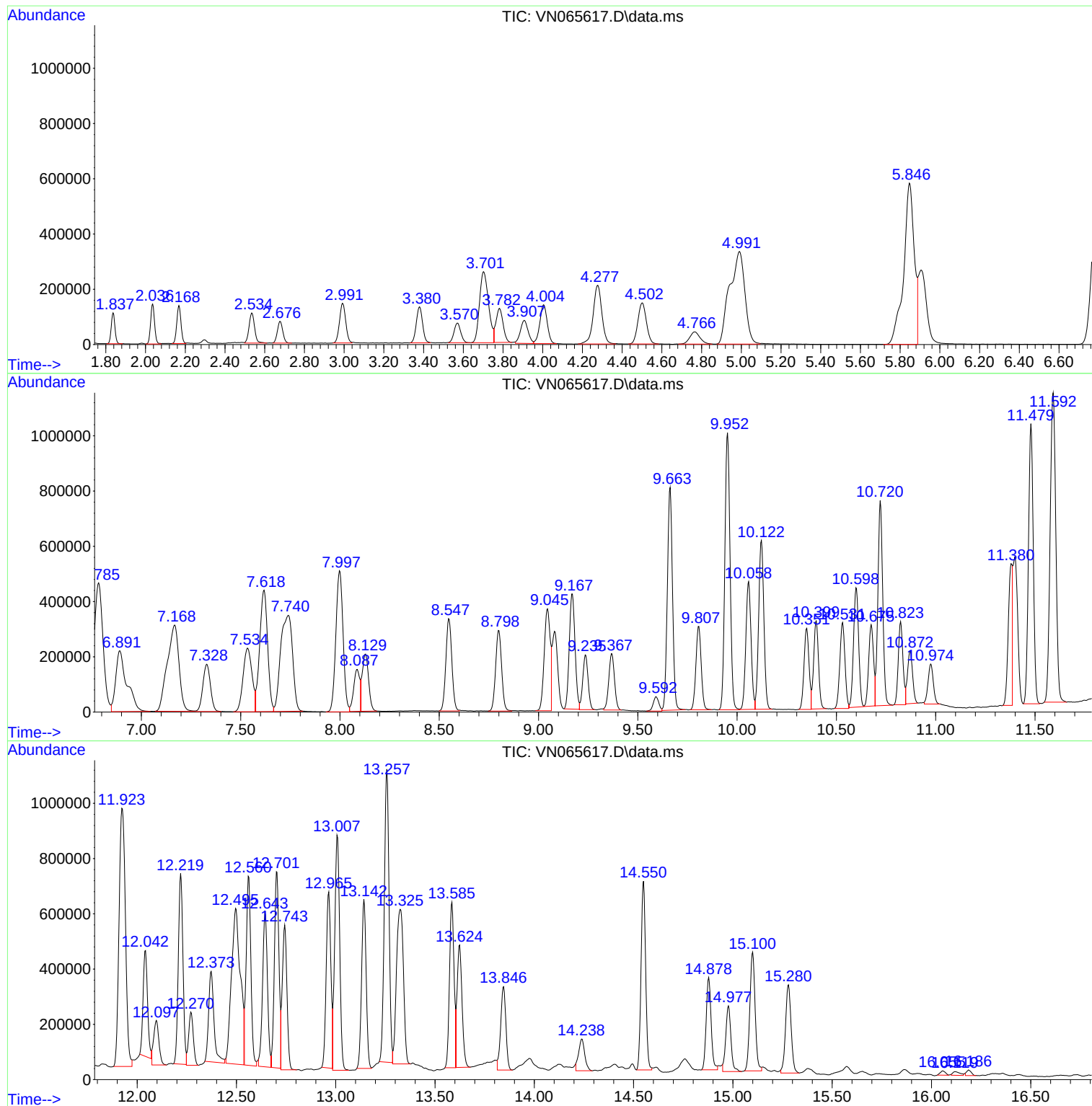
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LabSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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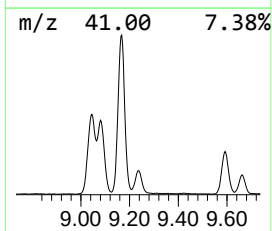
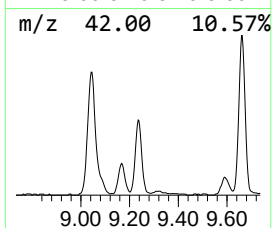
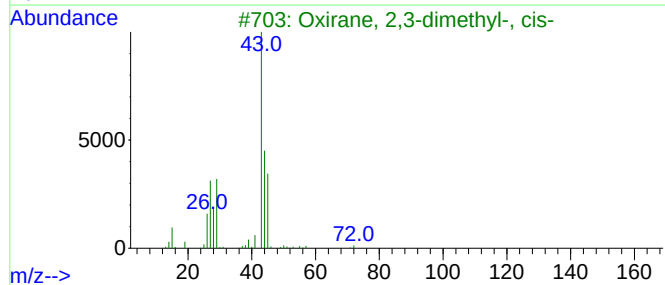
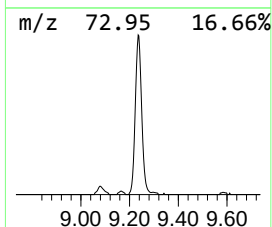
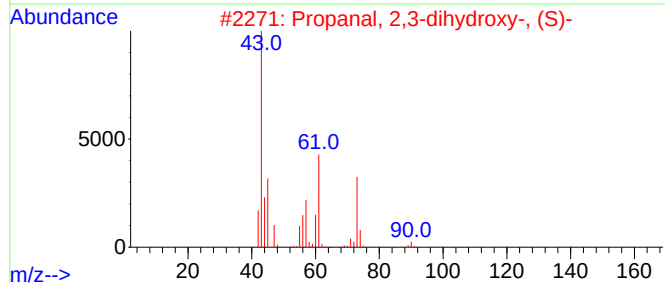
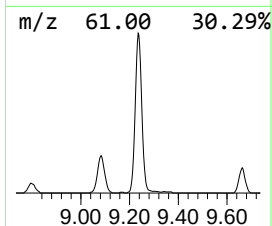
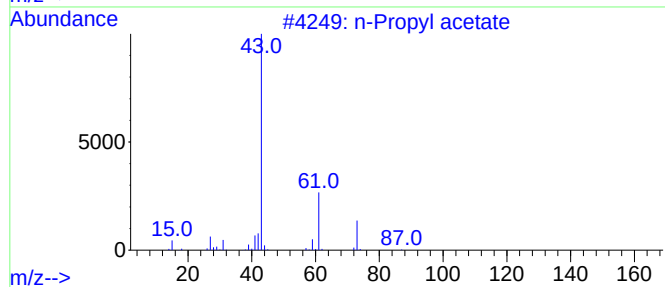
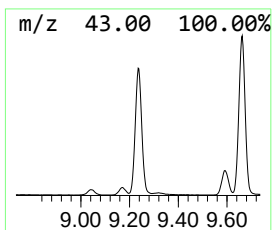
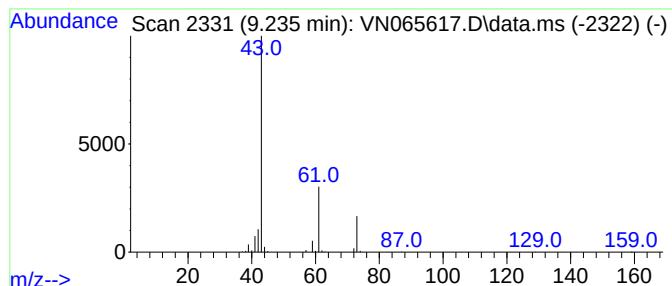
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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.
9.235	26.29 ug/l	365664	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			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
3			Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4			1-Butanamine	73	C4H11N	000109-73-9	7
5			Isobutylamine	73	C4H11N	000078-81-9	4



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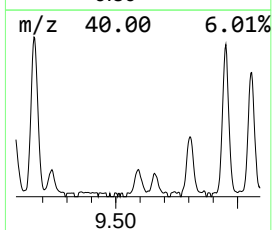
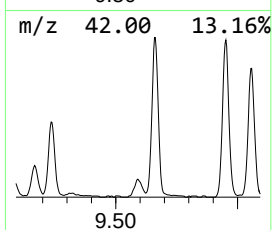
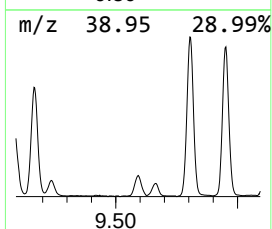
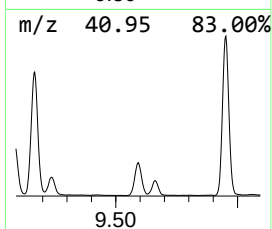
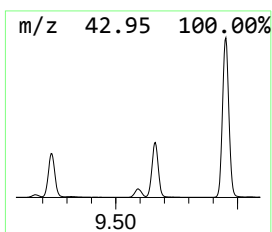
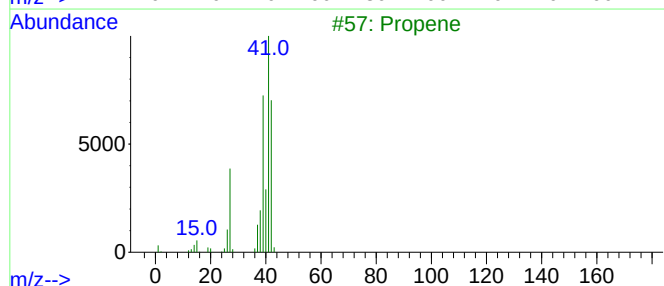
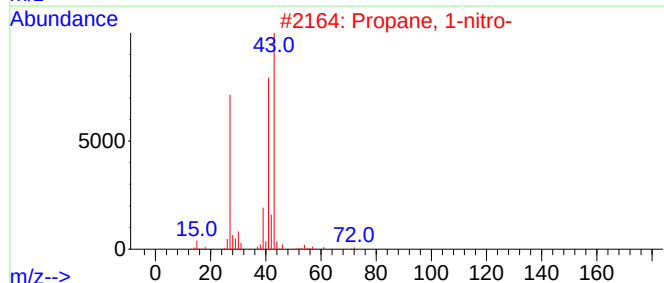
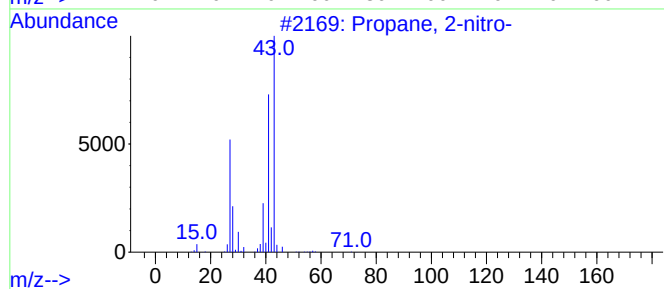
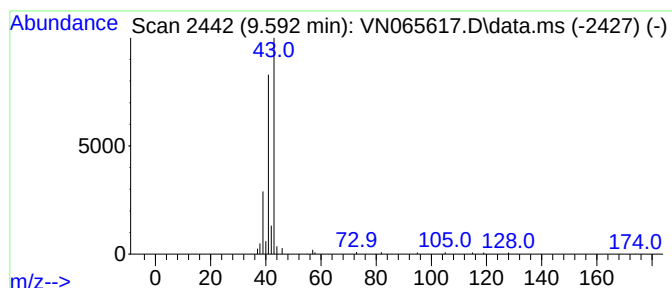
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	7.29 ug/l	101446	1,4-Difluorobenzene	8.547

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 2-nitro-	89	C3H7NO2	000079-46-9	78
2		Propane, 1-nitro-	89	C3H7NO2	000108-03-2	50
3		Propene	42	C3H6	000115-07-1	9
4		Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	9
5		Oxirane, ethyl-	72	C4H8O	000106-88-7	9



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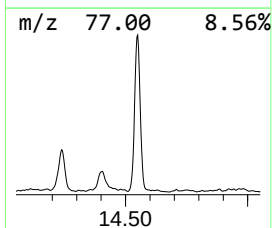
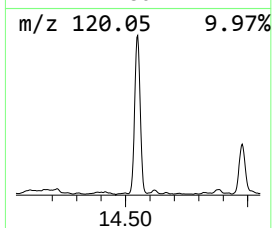
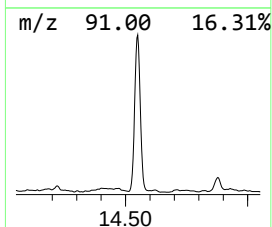
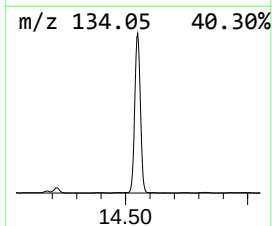
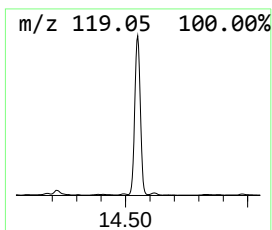
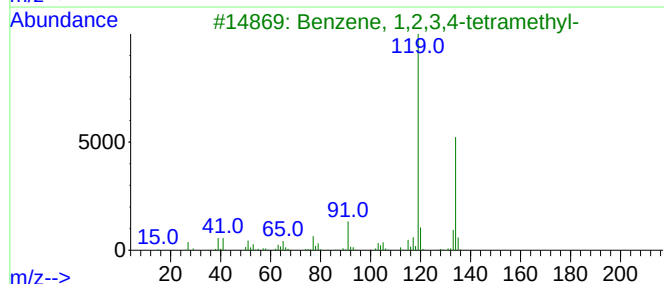
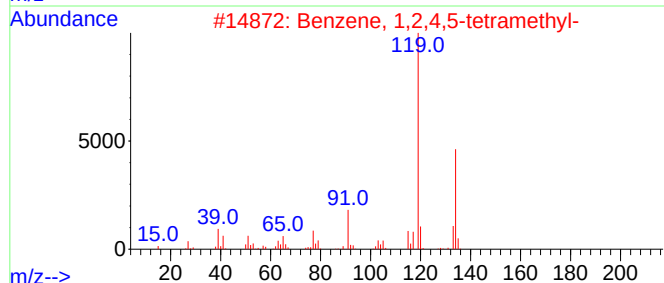
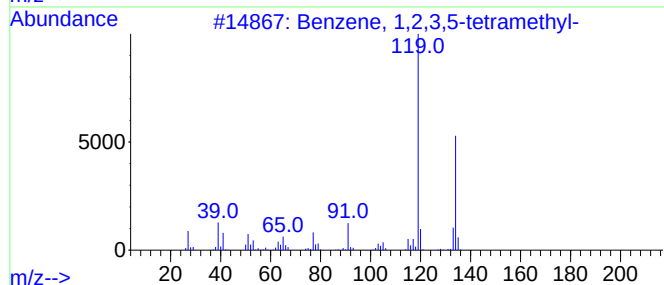
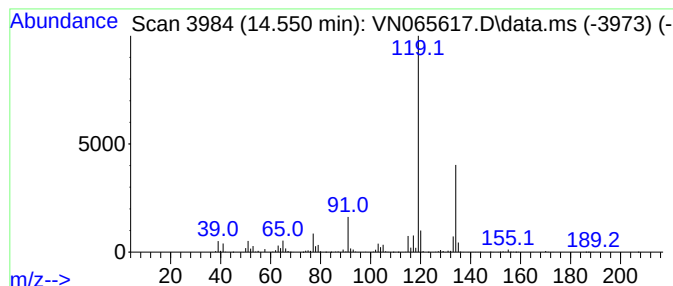
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.550	39.97 ug/l	1097660	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5			o-Cymene	134	C10H14	000527-84-4	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	9.235	26.3	ug/l	365664	2	8.547	695416	50.0
Propane, 2-nitro-	9.592	7.3	ug/l	101446	2	8.547	695416	50.0
Benzene, 1,2,3,...	14.550	40.0	ug/l	1097660	4	13.312	1373070	50.0