

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
 Data File : VN065591.D
 Acq On : 25 Jan 2021 21:01
 Operator : JC/MD
 Sample : VSTDCCC050
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 27 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: VN065591.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.836	21	30	44	rBV	120104	154561	7.09%	0.261%
2	2.036	81	92	103	rBV	156403	218299	10.01%	0.369%
3	2.168	122	133	144	rBV	147608	216584	9.93%	0.366%
4	2.531	235	246	258	rVB	106469	193026	8.85%	0.326%
5	2.676	279	291	305	rVB	80336	153029	7.02%	0.259%
6	2.991	375	389	406	rBV	141256	307451	14.09%	0.520%
7	3.380	496	510	529	rBV	129386	279567	12.82%	0.473%
8	3.570	556	569	590	rVB	74937	177234	8.13%	0.300%
9	3.701	593	610	626	rVV3	249440	785541	36.01%	1.328%
10	3.782	627	635	655	rVB	122706	297066	13.62%	0.502%
11	3.907	660	674	689	rVV	80501	220576	10.11%	0.373%
12	4.004	690	704	728	rVB	141116	370947	17.01%	0.627%
13	4.277	756	789	816	rBV2	210434	637968	29.25%	1.079%
14	4.502	838	859	886	rBV2	144338	436377	20.01%	0.738%
15	4.766	915	941	971	rBV2	44538	166104	7.61%	0.281%
16	4.991	974	1011	1048	rBV4	331648	1757065	80.55%	2.971%
17	5.846	1239	1277	1290	rBV2	590454	2181307	100.00%	3.688%
18	6.785	1540	1569	1588	rBV3	454682	1461077	66.98%	2.470%
19	6.891	1588	1602	1615	rBV2	196155	552784	25.34%	0.935%
20	7.164	1656	1687	1720	rBV4	313497	1278856	58.63%	2.162%
21	7.328	1720	1738	1764	rVB	167572	438893	20.12%	0.742%
22	7.534	1780	1802	1814	rBV2	223144	693883	31.81%	1.173%
23	7.618	1815	1828	1843	rVV2	433495	1182349	54.20%	1.999%
24	7.740	1843	1866	1896	rVB4	335087	1420963	65.14%	2.402%
25	7.997	1928	1946	1962	rBV3	492865	1254178	57.50%	2.120%
26	8.087	1962	1974	1979	rVV	148222	315940	14.48%	0.534%
27	8.129	1981	1987	2007	rVB	208895	410252	18.81%	0.694%
28	8.550	2103	2118	2139	rVB	315770	653466	29.96%	1.105%
29	8.801	2180	2196	2218	rVB	278062	576656	26.44%	0.975%
30	9.045	2254	2272	2279	rBV	377506	837643	38.40%	1.416%
31	9.171	2298	2311	2322	rBV3	408996	827323	37.93%	1.399%
32	9.235	2322	2331	2348	rVB	194413	363374	16.66%	0.614%
33	9.370	2358	2373	2392	rVB	199161	394731	18.10%	0.667%
34	9.592	2427	2442	2451	rBV	51729	99962	4.58%	0.169%
35	9.662	2451	2464	2484	rVB	805631	1450355	66.49%	2.452%
36	9.807	2495	2509	2525	rBV	292636	546407	25.05%	0.924%

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Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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37	9.952	2538	2554	2573	rBV	998581	1792094	82.16%	3.030%
38	10.058	2573	2587	2597	rVV	448028	825869	37.86%	1.396%
39	10.122	2597	2607	2629	rVB	594516	1067065	48.92%	1.804%
40	10.351	2664	2678	2685	rBV	282270	499747	22.91%	0.845%
41	10.399	2685	2693	2716	rVV	310180	523973	24.02%	0.886%
42	10.531	2720	2734	2745	rVV	301287	549221	25.18%	0.929%
43	10.598	2745	2755	2768	rVV	421475	747203	34.25%	1.263%
44	10.675	2768	2779	2785	rVV	290957	504005	23.11%	0.852%
45	10.720	2785	2793	2813	rVV	731573	1268091	58.13%	2.144%
46	10.823	2814	2825	2833	rVV	296973	497777	22.82%	0.842%
47	10.871	2833	2840	2858	rVV	188767	333177	15.27%	0.563%
48	10.974	2858	2872	2887	rVV	137208	244511	11.21%	0.413%
49	11.379	2982	2998	3001	rBV	488903	792615	36.34%	1.340%
50	11.479	3017	3029	3048	rVB2	996239	1675520	76.81%	2.833%
51	11.592	3049	3064	3088	rVV	1074839	2085211	95.59%	3.525%
52	11.926	3151	3168	3191	rBV4	897312	2004316	91.89%	3.389%
53	12.042	3192	3204	3213	rVV	376612	590490	27.07%	0.998%
54	12.097	3213	3221	3238	rVB	138091	246938	11.32%	0.417%
55	12.219	3246	3259	3268	rBV	673317	1097250	50.30%	1.855%
56	12.270	3268	3275	3295	rVV	196839	334430	15.33%	0.565%
57	12.373	3295	3307	3326	rVB	298976	510382	23.40%	0.863%
58	12.495	3326	3345	3359	rBV5	565261	1774571	81.35%	3.000%
59	12.560	3359	3365	3379	rVV	663597	1074684	49.27%	1.817%
60	12.643	3379	3391	3401	rVV	519212	876159	40.17%	1.481%
61	12.704	3401	3410	3416	rVV	688150	1107195	50.76%	1.872%
62	12.743	3416	3422	3442	rVB	516122	836552	38.35%	1.414%
63	12.965	3476	3491	3497	rBV	641120	1048420	48.06%	1.772%
64	13.010	3497	3505	3519	rVB	831040	1415178	64.88%	2.393%
65	13.141	3533	3546	3560	rBV	597471	958272	43.93%	1.620%
66	13.257	3569	3582	3592	rBV2	1039184	1740712	79.80%	2.943%
67	13.325	3592	3603	3624	rVB2	547484	1369570	62.79%	2.315%
68	13.585	3671	3684	3690	rBV	586447	931713	42.71%	1.575%
69	13.624	3690	3696	3722	rVB	432192	709689	32.54%	1.200%
70	13.846	3752	3765	3778	rVB	301502	508024	23.29%	0.859%
71	14.241	3874	3888	3904	rVB3	100017	186227	8.54%	0.315%
72	14.550	3971	3984	3998	rBV	662366	1039365	47.65%	1.757%
73	14.878	4074	4086	4102	rVB	313794	521068	23.89%	0.881%
74	14.977	4106	4117	4131	rVB2	228601	371573	17.03%	0.628%
75	15.100	4142	4155	4175	rBV	365929	651878	29.88%	1.102%
76	15.280	4191	4211	4229	rBV	293265	527932	24.20%	0.893%

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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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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

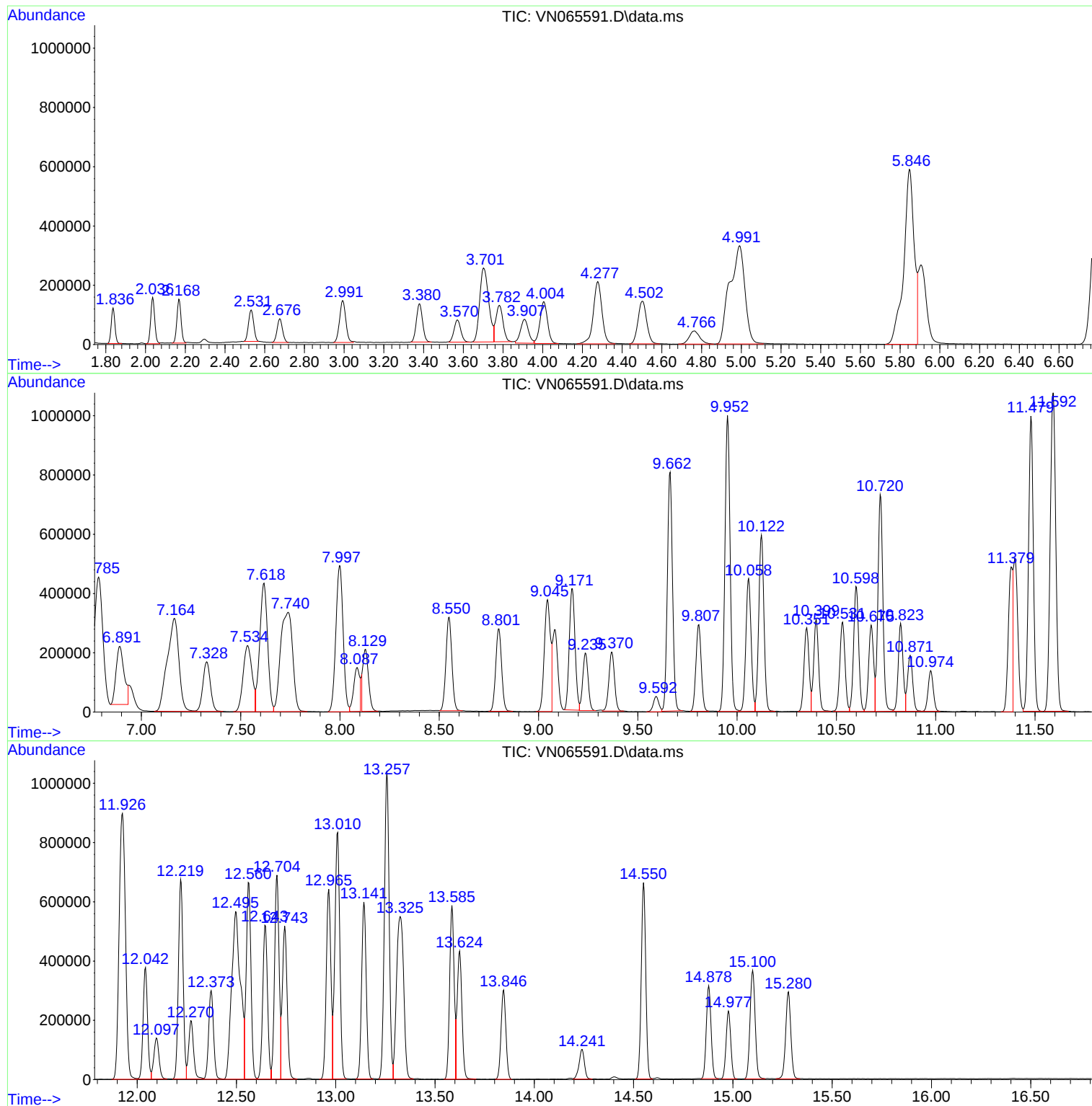
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



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Instrument :
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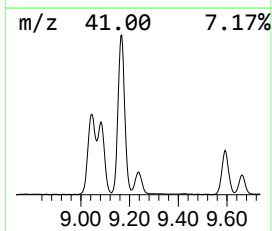
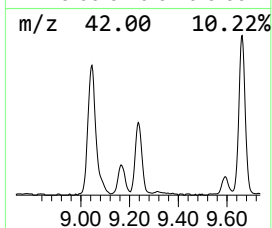
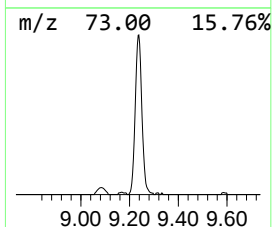
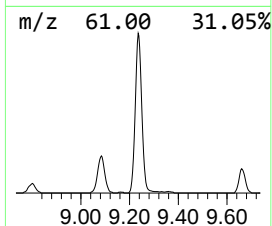
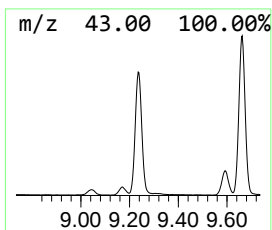
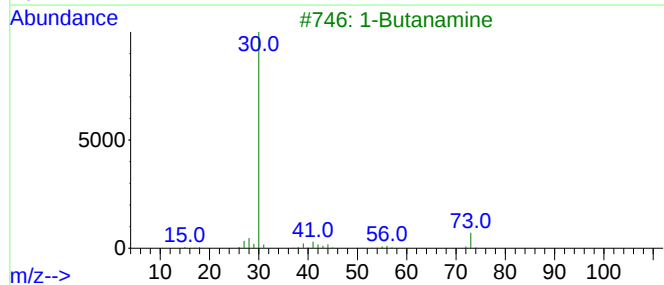
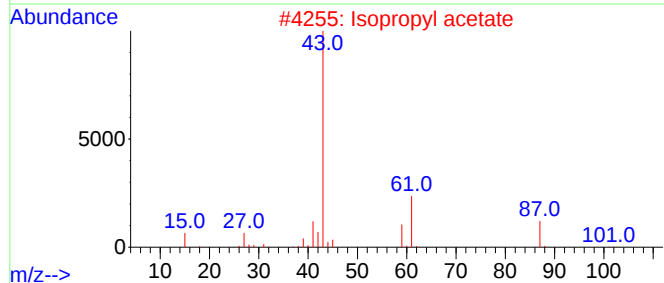
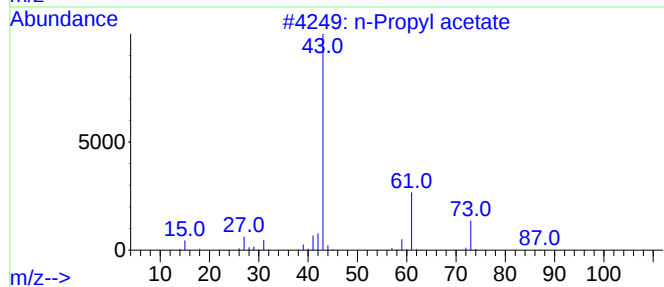
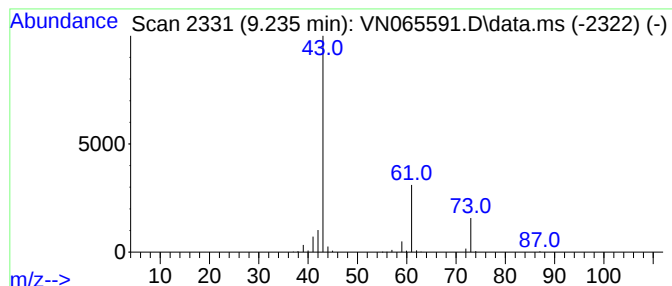
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Quant Title : SW846 8260

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.235	27.80 ug/l	363374	1,4-Difluorobenzene	8.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Propyl acetate	102	C5H10O2	000109-60-4	78
2		Isopropyl acetate	102	C5H10O2	000108-21-4	9
3		1-Butanamine	73	C4H11N	000109-73-9	7
4		Isobutylamine	73	C4H11N	000078-81-9	4
5		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4



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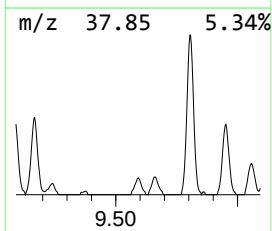
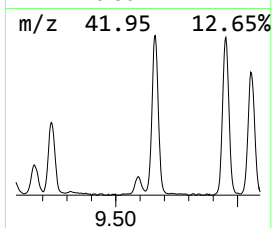
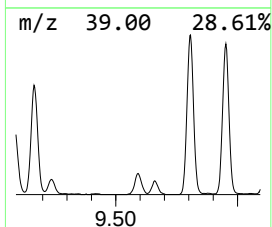
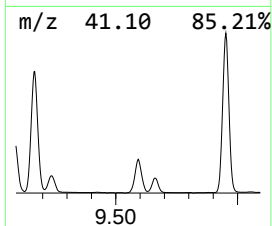
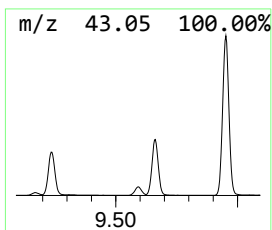
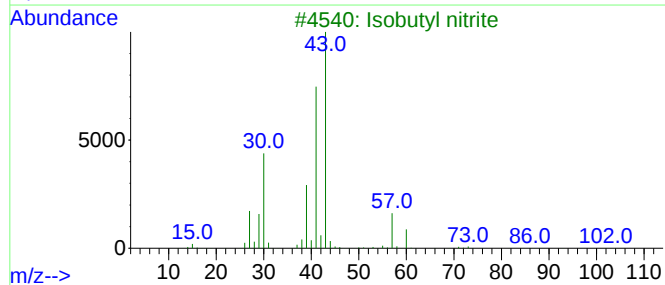
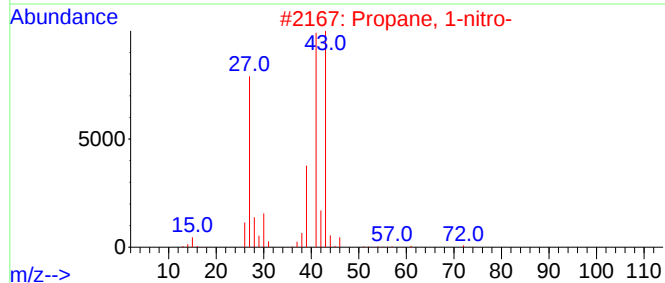
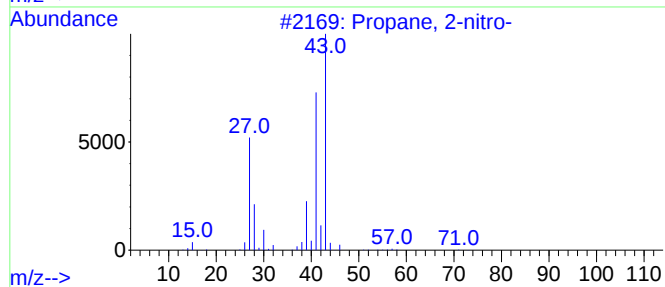
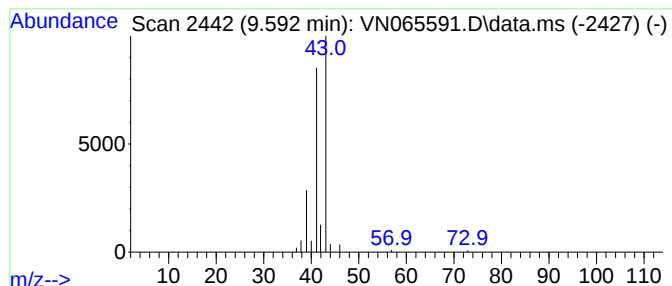
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	7.65 ug/l	99962	1,4-Difluorobenzene	8.550

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	83		
3	Isobutyl nitrite	103	C4H9NO2	000542-56-3	43		
4	Propene	42	C3H6	000115-07-1	9		
5	o-Allylhydroxylamine	73	C3H7NO	006542-54-7	5		



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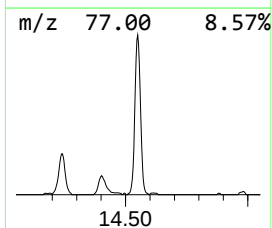
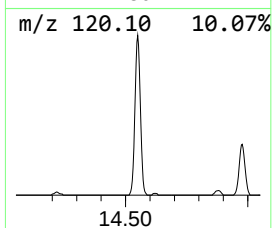
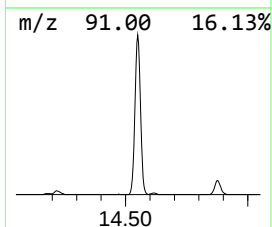
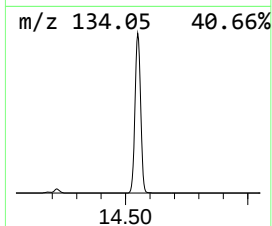
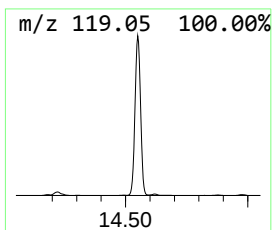
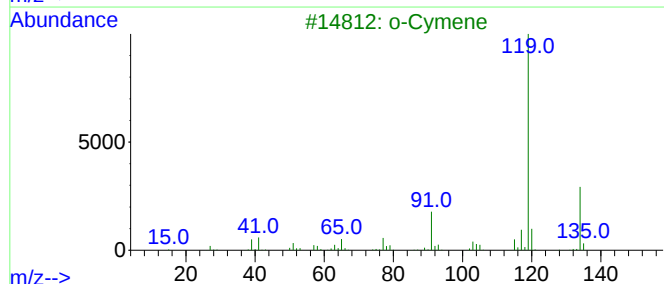
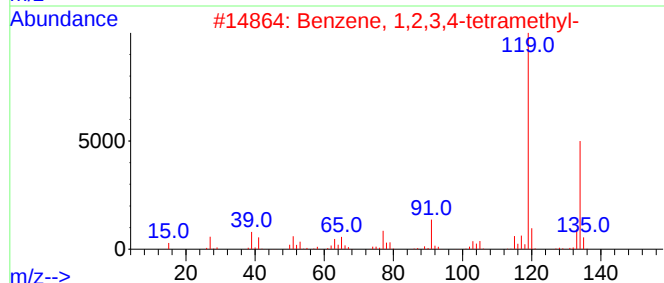
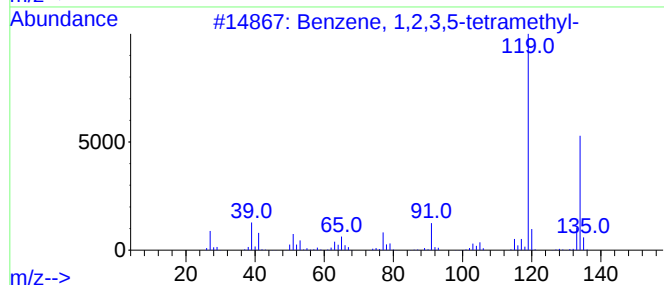
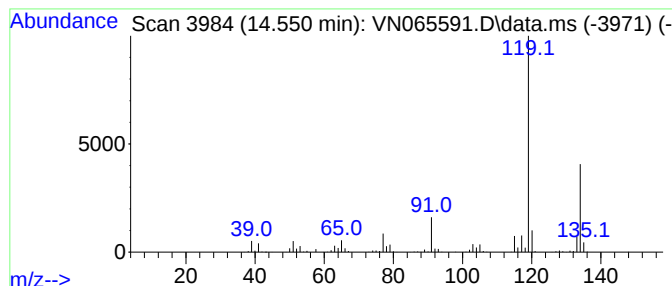
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.550	37.94 ug/l	1039370	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	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	9.235	27.8	ug/l	363374	2	8.550	653466	50.0
Propane, 2-nitro-	9.592	7.6	ug/l	99962	2	8.550	653466	50.0
Benzene, 1,2,3,...	14.550	37.9	ug/l	1039370	4	13.315	1369570	50.0