

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012721\
 Data File : VN065637.D
 Acq On : 27 Jan 2021 18:14
 Operator : JC/MD
 Sample : VSTDCCC050
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 20 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: VN065637.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	41	rBV	129819	166643	7.31%	0.267%
2	2.036	81	92	106	rBV	161629	230812	10.13%	0.370%
3	2.168	122	133	144	rBV	153367	226759	9.95%	0.363%
4	2.296	163	173	187	rBV	17901	30210	1.33%	0.048%
5	2.541	237	249	271	rVB	123793	231795	10.17%	0.371%
6	2.679	280	292	310	rBV	87478	162742	7.14%	0.261%
7	2.994	375	390	406	rBV	152379	332720	14.60%	0.533%
8	3.380	494	510	532	rBV	137933	302228	13.26%	0.484%
9	3.573	556	570	591	rVB	68583	161501	7.09%	0.259%
10	3.701	591	610	626	rVV3	275492	864779	37.94%	1.385%
11	3.785	627	636	655	rVV	122313	311559	13.67%	0.499%
12	3.907	659	674	689	rVV	87422	238161	10.45%	0.381%
13	4.004	690	704	729	rVB	149335	386386	16.95%	0.619%
14	4.277	757	789	825	rBV4	218691	672095	29.49%	1.076%
15	4.502	838	859	881	rBV2	155862	463962	20.36%	0.743%
16	4.769	923	942	970	rVB2	35003	129239	5.67%	0.207%
17	4.991	974	1011	1046	rBV5	350473	1823081	79.99%	2.920%
18	5.849	1241	1278	1290	rBV2	602503	2251306	98.78%	3.606%
19	6.785	1540	1569	1588	rBV3	475952	1548196	67.93%	2.480%
20	6.891	1589	1602	1647	rVB4	213061	835483	36.66%	1.338%
21	7.168	1656	1688	1716	rBV4	307756	1289098	56.56%	2.065%
22	7.328	1720	1738	1761	rVB	179454	468416	20.55%	0.750%
23	7.534	1779	1802	1814	rBV3	238354	739005	32.43%	1.184%
24	7.618	1815	1828	1843	rVV3	461962	1267332	55.61%	2.030%
25	7.743	1843	1867	1890	rVB4	359369	1505827	66.07%	2.412%
26	7.997	1926	1946	1962	rBV4	523670	1323327	58.06%	2.120%
27	8.087	1962	1974	1979	rVV	156737	335579	14.72%	0.537%
28	8.129	1981	1987	2009	rVB	216833	430311	18.88%	0.689%
29	8.547	2103	2117	2141	rVB	340369	710543	31.18%	1.138%
30	8.801	2180	2196	2215	rBV	302976	628997	27.60%	1.007%
31	9.045	2251	2272	2278	rBV	384700	825399	36.22%	1.322%
32	9.171	2298	2311	2322	rBV3	418123	845542	37.10%	1.354%
33	9.235	2322	2331	2348	rVB	201676	370258	16.25%	0.593%
34	9.367	2354	2372	2389	rVB	210745	425290	18.66%	0.681%
35	9.592	2428	2442	2451	rBV	50859	99547	4.37%	0.159%
36	9.663	2451	2464	2493	rVV	798072	1472282	64.60%	2.358%

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Integrator: RTE

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37	9.804	2493	2508	2528	rVV	313916	585183	25.68%	0.937%
38	9.952	2539	2554	2572	rBV	1011318	1830171	80.30%	2.931%
39	10.058	2574	2587	2597	rVV	471775	873394	38.32%	1.399%
40	10.122	2597	2607	2632	rVB	649350	1178557	51.71%	1.888%
41	10.351	2663	2678	2685	rBV	299505	534904	23.47%	0.857%
42	10.399	2685	2693	2713	rVB	321937	548904	24.08%	0.879%
43	10.531	2718	2734	2744	rVV	328547	584064	25.63%	0.935%
44	10.598	2744	2755	2767	rVV	458457	817170	35.86%	1.309%
45	10.675	2767	2779	2785	rVV	304041	538152	23.61%	0.862%
46	10.720	2785	2793	2813	rVV	739333	1263413	55.44%	2.024%
47	10.823	2813	2825	2833	rVV	307425	517133	22.69%	0.828%
48	10.872	2833	2840	2856	rVV	196058	348265	15.28%	0.558%
49	10.974	2859	2872	2888	rVB	145947	262501	11.52%	0.420%
50	11.383	2982	2999	3000	rBV	520796	754130	33.09%	1.208%
51	11.479	3017	3029	3048	rVB2	1062129	1808127	79.34%	2.896%
52	11.592	3048	3064	3096	rVB	1171661	2279049	100.00%	3.650%
53	11.923	3151	3167	3188	rBV3	974838	2151581	94.41%	3.446%
54	12.042	3192	3204	3213	rVV	404932	642680	28.20%	1.029%
55	12.097	3213	3221	3247	rVV	145681	270610	11.87%	0.433%
56	12.219	3247	3259	3268	rVV	709689	1169450	51.31%	1.873%
57	12.270	3268	3275	3295	rVV	205232	349156	15.32%	0.559%
58	12.373	3295	3307	3326	rVV	321061	541478	23.76%	0.867%
59	12.495	3326	3345	3358	rVV4	602219	1828593	80.23%	2.929%
60	12.560	3359	3365	3379	rVV	712685	1129854	49.58%	1.810%
61	12.643	3379	3391	3401	rVV	552322	948327	41.61%	1.519%
62	12.704	3401	3410	3416	rVV	730787	1167996	51.25%	1.871%
63	12.743	3416	3422	3442	rVB	558835	889166	39.01%	1.424%
64	12.965	3476	3491	3497	rBV	654449	1080055	47.39%	1.730%
65	13.007	3497	3504	3520	rVB	889258	1497375	65.70%	2.398%
66	13.142	3529	3546	3560	rBV	613755	979700	42.99%	1.569%
67	13.257	3568	3582	3591	rBV2	1073148	1790988	78.58%	2.869%
68	13.325	3591	3603	3623	rVB2	578332	1447968	63.53%	2.319%
69	13.425	3623	3634	3650	rBV	51319	93562	4.11%	0.150%
70	13.585	3671	3684	3690	rBV	601036	964232	42.31%	1.544%
71	13.624	3690	3696	3716	rVB	446386	727189	31.91%	1.165%
72	13.842	3752	3764	3777	rVB	302396	512296	22.48%	0.821%
73	14.238	3873	3887	3900	rVB2	99701	186730	8.19%	0.299%
74	14.550	3971	3984	3999	rBV	657328	1046257	45.91%	1.676%
75	14.878	4074	4086	4105	rVB	328889	543433	23.84%	0.870%
76	14.977	4105	4117	4131	rBV2	238832	394487	17.31%	0.632%

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Instrument :
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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

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Title : SW846 8260

77	15.100	4142	4155	4174	rVB	395725	700015	30.72%	1.121%
78	15.277	4193	4210	4227	rBV	301536	551683	24.21%	0.884%

Sum of corrected areas: 62434388

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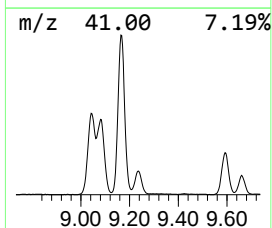
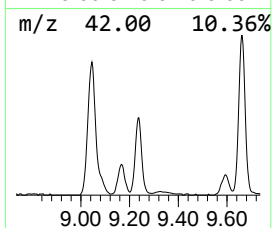
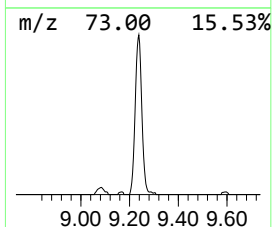
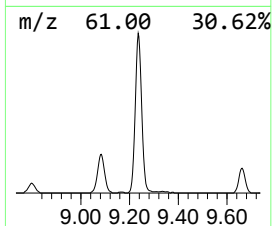
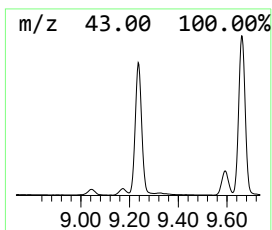
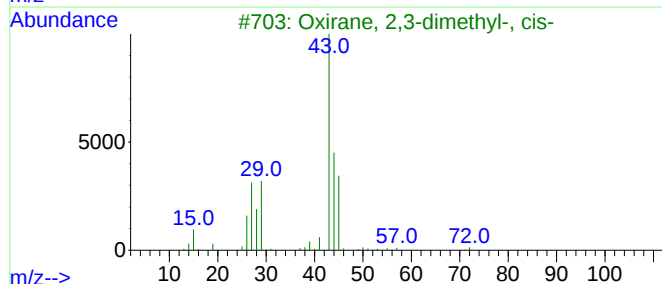
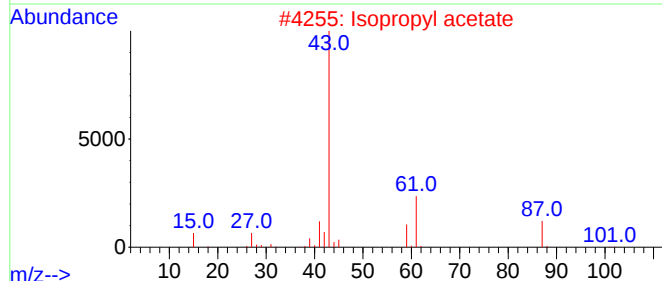
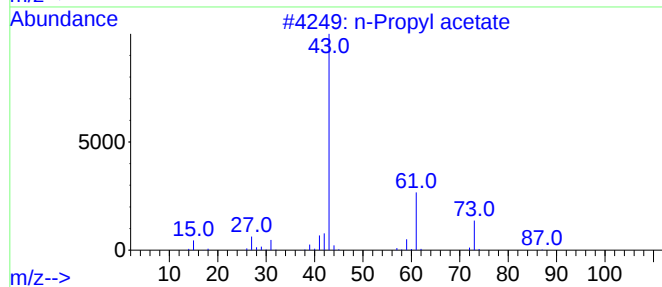
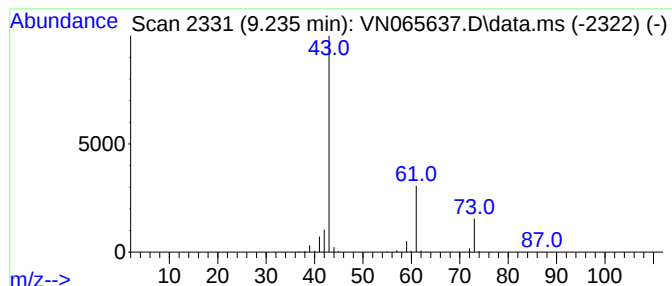
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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	26.05 ug/l	370258	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			Isopropyl acetate	102	C5H10O2	000108-21-4	9
3			Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4			1-Butanamine	73	C4H11N	000109-73-9	5
5			Isobutylamine	73	C4H11N	000078-81-9	4



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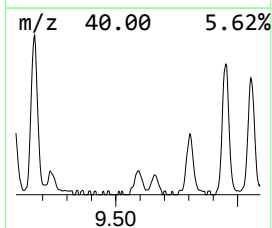
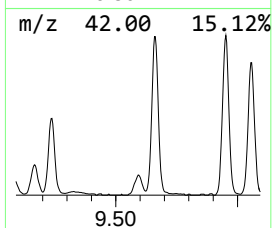
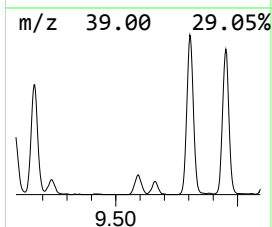
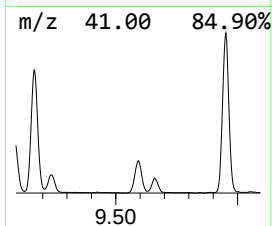
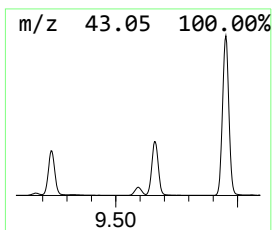
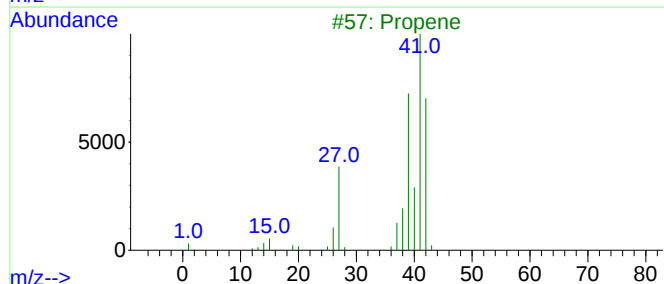
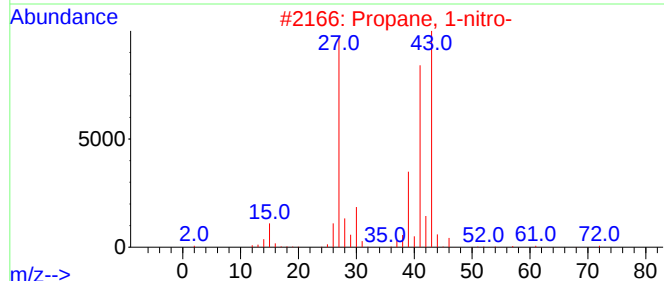
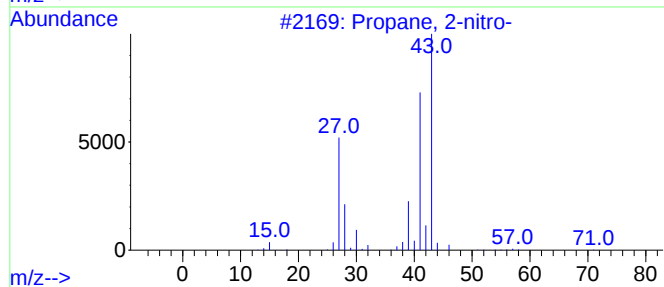
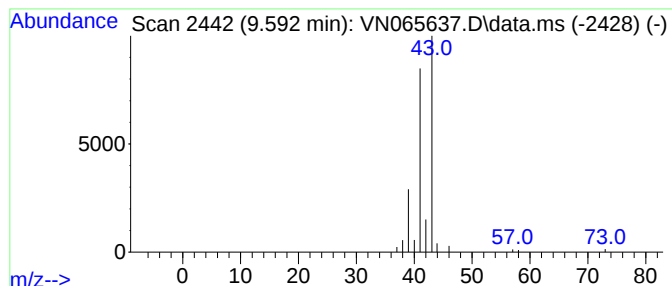
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	7.00 ug/l	99547	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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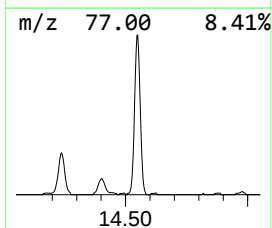
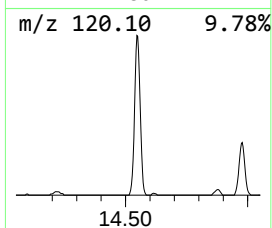
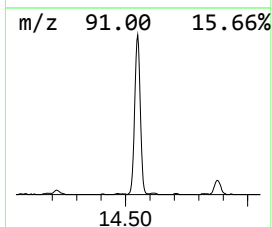
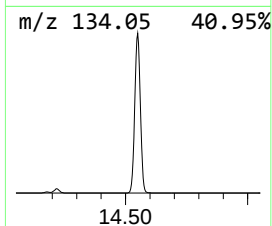
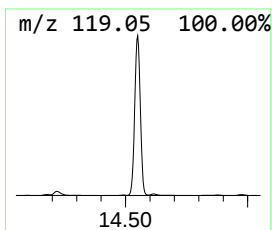
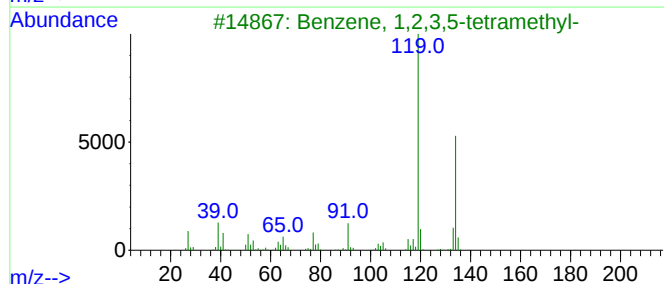
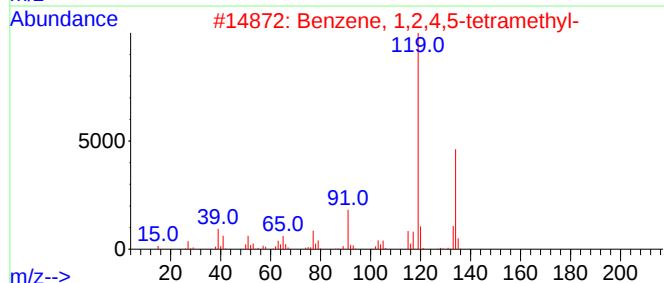
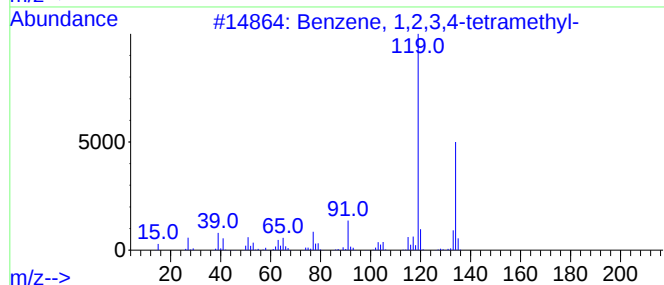
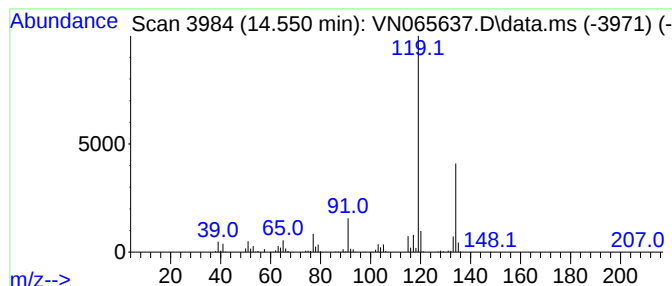
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.550	36.13 ug/l	1046260	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			p-Cymene	134	C10H14	000099-87-6	95



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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
n-Propyl acetate	9.235	26.1	ug/l	370258	2	8.547	710543	50.0
Propane, 2-nitro-	9.592	7.0	ug/l	99547	2	8.547	710543	50.0
Benzene, 1,2,3,...	14.550	36.1	ug/l	1046260	4	13.315	1447970	50.0