

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
 Data File : VN065578.D
 Acq On : 25 Jan 2021 15:41
 Operator : JC/MD
 Sample : VN0125WBS01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VN0125WBS01

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: VN065578.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	22	30	43	rVB	47659	61772	5.67%	0.240%
2	2.036	82	92	108	rBV	62161	91520	8.41%	0.356%
3	2.168	124	133	143	rBV	55991	81253	7.46%	0.316%
4	2.544	238	250	266	rBV	46628	86491	7.95%	0.336%
5	2.682	282	293	307	rVB	33393	62575	5.75%	0.243%
6	2.994	377	390	409	rVB	56238	123315	11.33%	0.479%
7	3.377	497	509	524	rBV	48369	105606	9.70%	0.410%
8	3.570	559	569	589	rVB	27233	64565	5.93%	0.251%
9	3.705	595	611	625	rBV5	97064	300762	27.63%	1.168%
10	3.782	628	635	656	rVV	48051	113371	10.41%	0.440%
11	3.907	659	674	689	rVV2	31526	87926	8.08%	0.342%
12	4.004	691	704	724	rVB	58823	154343	14.18%	0.600%
13	4.277	765	789	809	rBV3	78647	229238	21.06%	0.891%
14	4.499	835	858	881	rBV2	57013	169694	15.59%	0.659%
15	4.759	918	939	966	rBV2	17085	62027	5.70%	0.241%
16	4.987	975	1010	1043	rBV6	130302	661382	60.76%	2.569%
17	5.843	1240	1276	1289	rBV2	216479	813939	74.77%	3.162%
18	6.782	1543	1568	1587	rBV4	174277	576206	52.93%	2.238%
19	6.888	1588	1601	1639	rVB3	79996	312108	28.67%	1.212%
20	7.164	1657	1687	1720	rBV6	116041	479766	44.07%	1.864%
21	7.325	1720	1737	1757	rVB	64589	164516	15.11%	0.639%
22	7.540	1780	1804	1815	rBV3	142120	436497	40.10%	1.696%
23	7.618	1816	1828	1844	rVV4	290200	765802	70.35%	2.975%
24	7.740	1844	1866	1888	rVB4	130291	548658	50.40%	2.131%
25	7.991	1926	1944	1961	rBV4	255678	661016	60.72%	2.568%
26	8.084	1961	1973	1978	rVV	55999	119626	10.99%	0.465%
27	8.126	1980	1986	2005	rVB2	77909	159069	14.61%	0.618%
28	8.547	2098	2117	2141	rBV	327583	686924	63.10%	2.669%
29	8.798	2178	2195	2215	rBV	111288	228884	21.03%	0.889%
30	9.042	2254	2271	2278	rBV	150474	332337	30.53%	1.291%
31	9.167	2297	2310	2322	rBV3	151741	310268	28.50%	1.205%
32	9.235	2322	2331	2349	rVB	74190	135631	12.46%	0.527%
33	9.367	2355	2372	2389	rVB	76031	150626	13.84%	0.585%
34	9.592	2428	2442	2451	rBV2	18907	36881	3.39%	0.143%
35	9.659	2451	2463	2491	rVV	305964	554834	50.97%	2.155%
36	9.804	2495	2508	2524	rBV	111556	207631	19.07%	0.807%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
 Data File : VN065578.D
 Acq On : 25 Jan 2021 15:41
 Operator : JC/MD
 Sample : VN0125WBS01
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VN0125WBS01

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

37	9.949	2538	2553	2572	rBV	375071	680663	62.53%	2.644%
38	10.055	2572	2586	2597	rVV	462996	848629	77.96%	3.297%
39	10.119	2597	2606	2630	rVB	228810	418021	38.40%	1.624%
40	10.347	2664	2677	2685	rBV	105092	189885	17.44%	0.738%
41	10.396	2685	2692	2710	rVB	113169	193310	17.76%	0.751%
42	10.527	2721	2733	2744	rBV	114894	205877	18.91%	0.800%
43	10.598	2744	2755	2768	rVV	172183	305559	28.07%	1.187%
44	10.675	2768	2779	2785	rVV	110692	191994	17.64%	0.746%
45	10.720	2785	2793	2814	rVV	266181	464682	42.69%	1.805%
46	10.823	2814	2825	2832	rVV	106875	180675	16.60%	0.702%
47	10.868	2832	2839	2855	rVB	71731	129947	11.94%	0.505%
48	10.974	2860	2872	2889	rBV	50698	91667	8.42%	0.356%
49	11.376	2983	2997	3017	rBV2	463715	1088553	100.00%	4.229%
50	11.479	3017	3029	3044	rVB2	376403	644952	59.25%	2.505%
51	11.589	3047	3063	3080	rBV	412508	806389	74.08%	3.133%
52	11.923	3150	3167	3192	rBV4	335573	765079	70.28%	2.972%
53	12.039	3192	3203	3213	rVV	129951	208905	19.19%	0.812%
54	12.097	3213	3221	3234	rVB2	51341	91876	8.44%	0.357%
55	12.219	3243	3259	3268	rBV	264051	431588	39.65%	1.677%
56	12.270	3268	3275	3294	rVV	71762	124919	11.48%	0.485%
57	12.370	3294	3306	3327	rVV	303439	518150	47.60%	2.013%
58	12.495	3327	3345	3358	rVV5	206419	650008	59.71%	2.525%
59	12.560	3359	3365	3379	rVV	256323	409708	37.64%	1.592%
60	12.643	3379	3391	3400	rVV	204043	339983	31.23%	1.321%
61	12.701	3400	3409	3416	rVV	268865	436273	40.08%	1.695%
62	12.743	3416	3422	3441	rVB	194753	313919	28.84%	1.219%
63	12.965	3477	3491	3497	rBV	246111	407336	37.42%	1.582%
64	13.006	3497	3504	3524	rVB	314336	532851	48.95%	2.070%
65	13.142	3534	3546	3563	rVB	233710	373276	34.29%	1.450%
66	13.257	3569	3582	3591	rBV2	391387	665976	61.18%	2.587%
67	13.315	3591	3600	3630	rVB3	430011	926465	85.11%	3.599%
68	13.585	3670	3684	3690	rBV	219789	357877	32.88%	1.390%
69	13.624	3690	3696	3710	rVB	155922	258340	23.73%	1.004%
70	13.842	3751	3764	3776	rBV	113114	192957	17.73%	0.750%
71	14.238	3873	3887	3903	rVB3	32819	62703	5.76%	0.244%
72	14.550	3972	3984	4000	rBV	243190	385051	35.37%	1.496%
73	14.878	4075	4086	4098	rBV	103632	171306	15.74%	0.665%
74	14.977	4106	4117	4128	rBV	90804	145622	13.38%	0.566%
75	15.100	4143	4155	4171	rBV	117740	210565	19.34%	0.818%
76	15.280	4191	4211	4229	rVB	97306	183291	16.84%	0.712%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
Data File : VN065578.D
Acq On : 25 Jan 2021 15:41
Operator : JC/MD
Sample : VN0125WBS01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0125WBS01

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

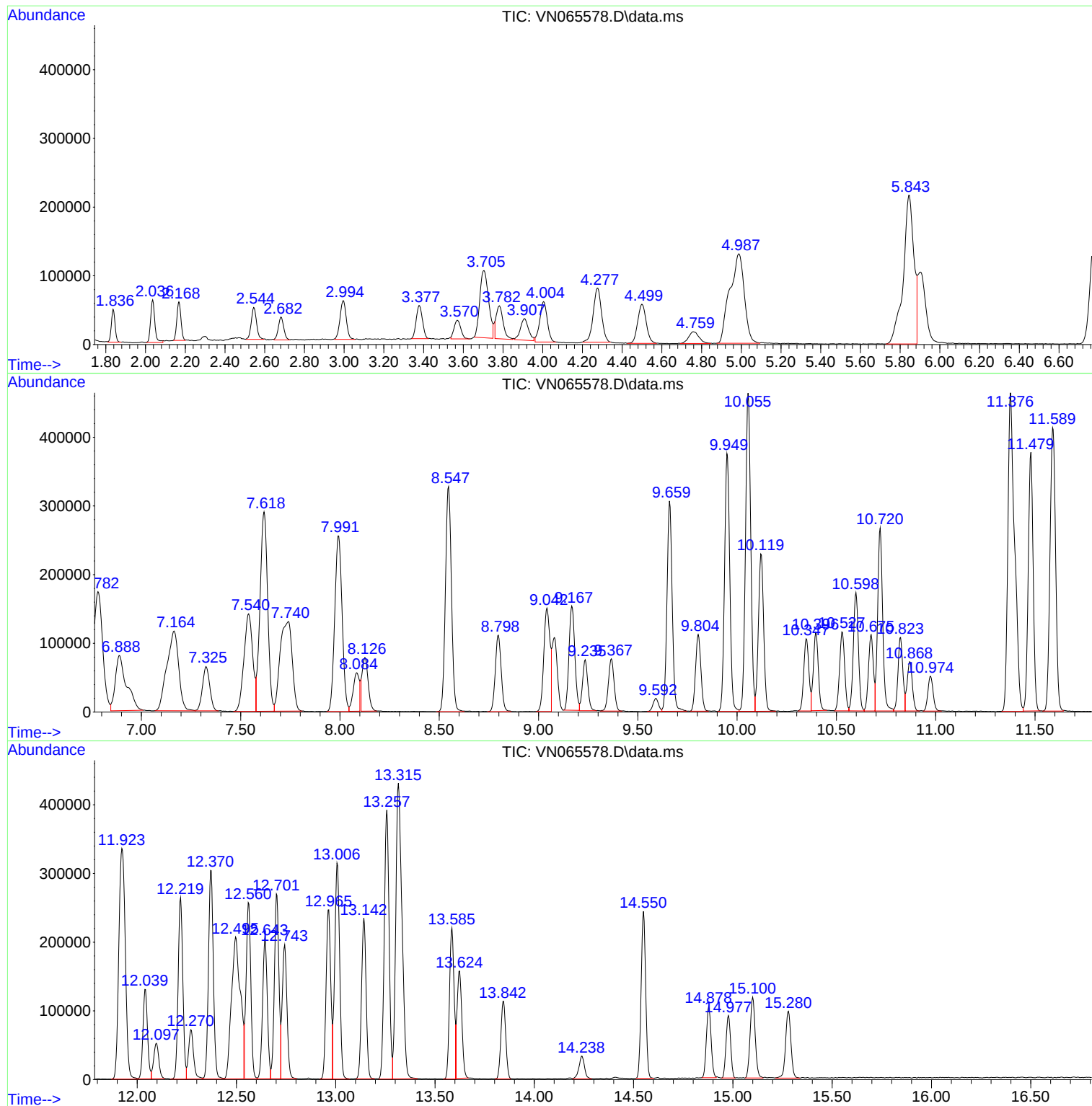
Sum of corrected areas: 25741886

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
Data File : VN065578.D
Acq On : 25 Jan 2021 15:41
Operator : JC/MD
Sample : VN0125WBS01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0125WBS01

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
Data File : VN065578.D
Acq On : 25 Jan 2021 15:41
Operator : JC/MD
Sample : VN0125WBS01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0125WBS01

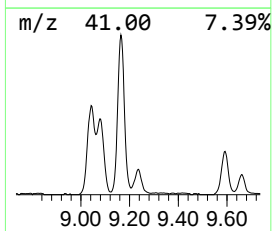
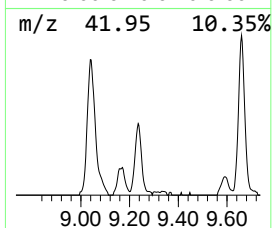
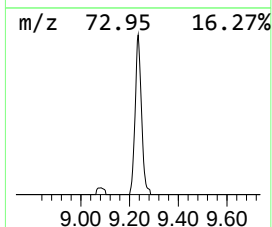
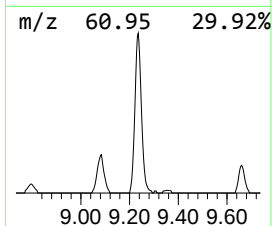
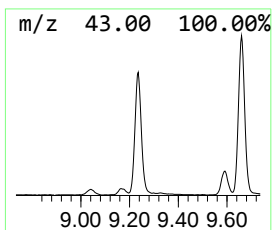
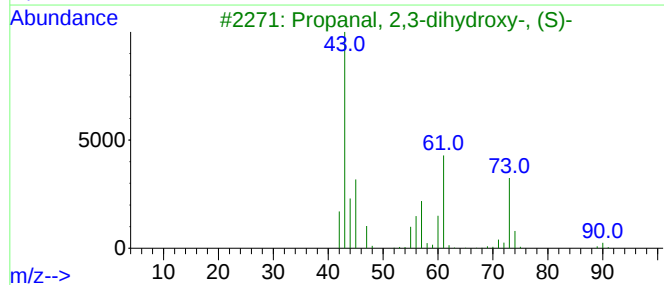
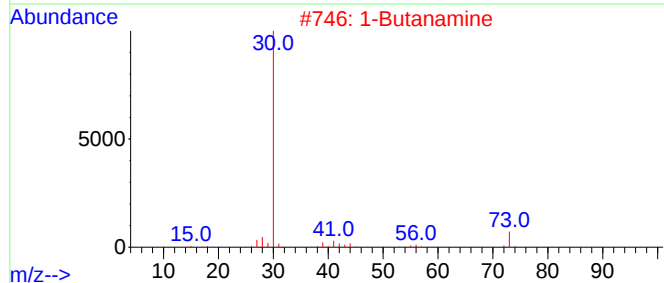
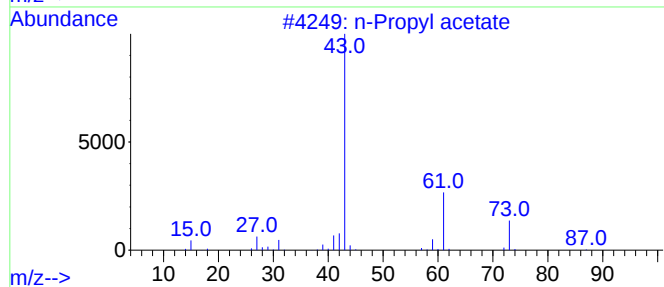
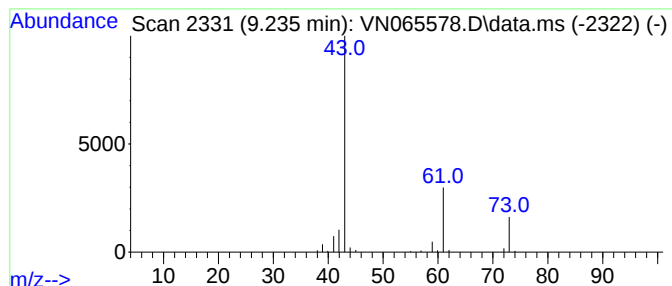
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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	9.87 ug/l	135631	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	9
3			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4			Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
5			Isobutylamine	73	C4H11N	000078-81-9	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
Data File : VN065578.D
Acq On : 25 Jan 2021 15:41
Operator : JC/MD
Sample : VN0125WBS01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0125WBS01

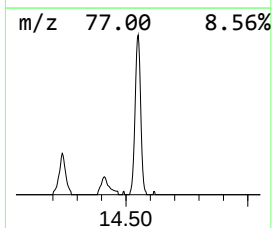
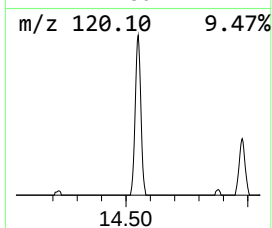
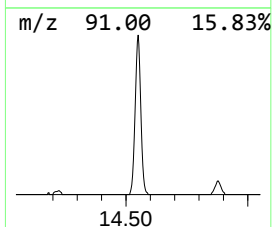
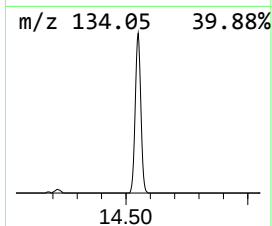
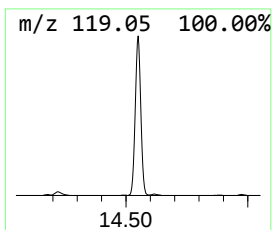
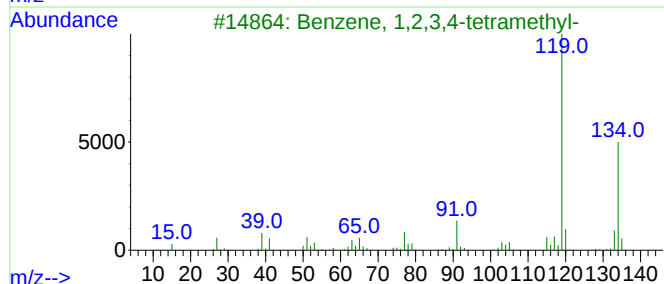
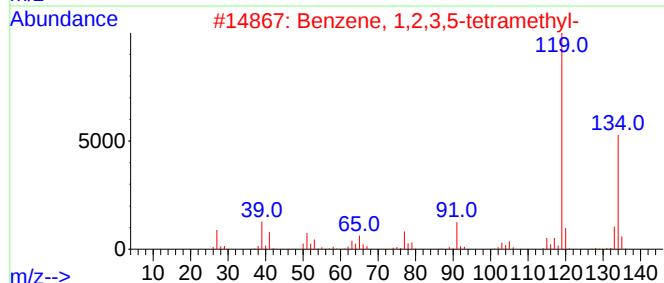
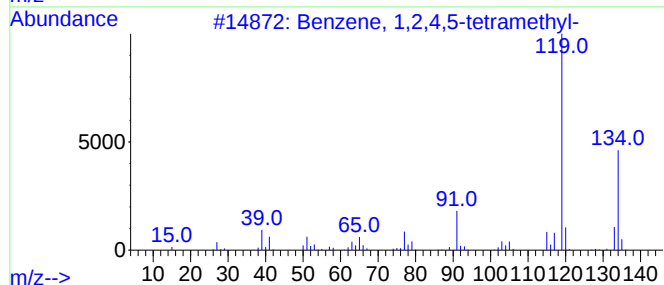
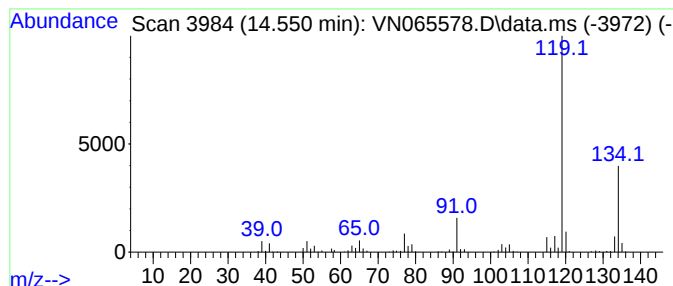
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.550	20.78 ug/l	385051	1,4-Dichlorobenzene-d4	13.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012521\
Data File : VN065578.D
Acq On : 25 Jan 2021 15:41
Operator : JC/MD
Sample : VN0125WBS01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VN0125WBS01

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	9.235	9.9	ug/l	135631	2	8.547	686924	50.0
Benzene, 1,2,4,...	14.550	20.8	ug/l	385051	4	13.315	926465	50.0