

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN021820\
 Data File : VN060138.D
 Acq On : 18 Feb 2020 15:32
 Operator : JC/MD
 Sample : VN0218MBSD01
 Misc : 5.00µL/100µL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VN0218MBSD01

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N021220W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.834	10	19	35	rBV	48662	64386	5.39%	0.238%
2	2.037	73	82	95	rBV	55193	74210	6.22%	0.274%
3	2.166	111	122	135	rBV	56093	85676	7.18%	0.317%
4	2.294	152	162	172	rBV	8204	13415	1.12%	0.050%
5	2.548	229	241	261	rVB2	44710	89525	7.50%	0.331%
6	2.686	272	284	303	rBV	25986	51775	4.34%	0.191%
7	3.005	367	383	403	rBV	65957	144715	12.12%	0.535%
8	3.387	488	502	524	rVB2	41653	92821	7.78%	0.343%
9	3.580	548	562	583	rBV	23108	56479	4.73%	0.209%
10	3.725	588	607	618	rBV2	102131	322727	27.03%	1.193%
11	3.931	654	671	688	rBV	28310	77508	6.49%	0.286%
12	4.034	688	703	729	rVB	49595	130632	10.94%	0.483%
13	4.294	768	784	811	rVB4	76638	220727	18.49%	0.816%
14	4.522	833	855	881	rBV	50389	157693	13.21%	0.583%
15	4.728	897	919	941	rBV3	16952	60326	5.05%	0.223%
16	4.953	968	989	992	rBV	68710	176608	14.79%	0.653%
17	5.857	1237	1270	1283	rBV2	194888	738172	61.84%	2.728%
18	6.799	1540	1563	1581	rBV3	200728	608467	50.97%	2.249%
19	6.899	1581	1594	1607	rBV2	67428	185221	15.52%	0.685%
20	7.175	1653	1680	1716	rVV4	138368	495360	41.50%	1.831%
21	7.345	1716	1733	1756	rVB	68770	182755	15.31%	0.675%
22	7.561	1775	1800	1811	rBV4	176971	515951	43.22%	1.907%
23	7.638	1812	1824	1840	rVV3	319112	811581	67.99%	2.999%
24	7.760	1840	1862	1885	rVB5	145841	585819	49.07%	2.165%
25	8.011	1919	1940	1957	rBV3	253881	681252	57.07%	2.518%
26	8.104	1957	1969	1973	rBV	54165	107818	9.03%	0.398%
27	8.567	2096	2113	2141	rBV	338286	694909	58.21%	2.568%
28	8.818	2176	2191	2208	rBB2	117364	241274	20.21%	0.892%
29	9.066	2253	2268	2274	rBV	151611	328721	27.54%	1.215%
30	9.185	2292	2305	2317	rBV4	150034	315290	26.41%	1.165%
31	9.252	2317	2326	2340	rVB	66394	123794	10.37%	0.458%
32	9.387	2354	2368	2383	rVB	83452	164176	13.75%	0.607%
33	9.609	2424	2437	2447	rBV2	22787	44605	3.74%	0.165%
34	9.680	2447	2459	2480	rVB	284772	513006	42.97%	1.896%

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 Title : SW846 8260

35	9.824	2490	2504	2524	rVB	117737	219067	18.35%	0.810%
36	9.969	2533	2549	2568	rBV	379468	689150	57.73%	2.547%
37	10.075	2568	2582	2593	rVV	526681	966382	80.95%	3.572%
38	10.143	2593	2603	2621	rVB	234471	426368	35.72%	1.576%
39	10.368	2661	2673	2681	rBV	117490	209766	17.57%	0.775%
40	10.416	2681	2688	2702	rVB	109560	183584	15.38%	0.679%
41	10.551	2717	2730	2740	rBV	126695	222564	18.64%	0.823%
42	10.622	2740	2752	2764	rVV	172803	310588	26.02%	1.148%
43	10.696	2764	2775	2781	rVV	113910	200554	16.80%	0.741%
44	10.741	2781	2789	2809	rVV	289973	490177	41.06%	1.812%
45	10.844	2809	2821	2828	rVV	105858	175313	14.69%	0.648%
46	10.892	2828	2836	2850	rVB	88141	155358	13.01%	0.574%
47	10.995	2856	2868	2884	rVB	60957	110772	9.28%	0.409%
48	11.400	2980	2994	3014	rBV2	505687	1193744	100.00%	4.412%
49	11.503	3014	3026	3043	rVB2	417085	713098	59.74%	2.636%
50	11.612	3043	3060	3080	rBV	435087	857224	71.81%	3.168%
51	11.947	3148	3164	3181	rBV5	359606	783775	65.66%	2.897%
52	12.062	3189	3200	3210	rBV	129759	205888	17.25%	0.761%
53	12.120	3210	3218	3233	rVB	71350	122649	10.27%	0.453%
54	12.242	3243	3256	3265	rBV	286384	471880	39.53%	1.744%
55	12.294	3265	3272	3286	rVB	86028	141671	11.87%	0.524%
56	12.397	3291	3304	3320	rVV	394220	658711	55.18%	2.435%
57	12.522	3324	3343	3356	rVV5	246736	793241	66.45%	2.932%
58	12.586	3356	3363	3376	rVV	275745	444243	37.21%	1.642%
59	12.670	3376	3389	3398	rVV	225334	375308	31.44%	1.387%
60	12.728	3398	3407	3414	rVV	290789	482643	40.43%	1.784%
61	12.770	3414	3420	3434	rVB	215737	345010	28.90%	1.275%
62	12.988	3475	3488	3494	rBV	277168	452617	37.92%	1.673%
63	13.033	3494	3502	3518	rVB2	390869	674795	56.53%	2.494%
64	13.168	3530	3544	3556	rBV	266345	426824	35.76%	1.577%
65	13.281	3566	3579	3588	rBV2	464276	778509	65.22%	2.877%
66	13.339	3588	3597	3619	rVB3	537139	1139544	95.46%	4.212%
67	13.609	3670	3681	3688	rBV	258415	418828	35.09%	1.548%
68	13.647	3688	3693	3709	rVB	193825	306377	25.67%	1.132%
69	13.869	3751	3762	3774	rBV	157093	268039	22.45%	0.991%
70	14.265	3875	3885	3897	rVB3	45481	83306	6.98%	0.308%
71	14.577	3971	3982	3994	rBV	279474	438571	36.74%	1.621%

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Instrument :
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ClientSampleId :
VN0218MBSD01

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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72	14.905	4075	4084	4097	rBV	143115	238120	19.95%	0.880%
73	15.008	4106	4116	4128	rBV	144068	238652	19.99%	0.882%
74	15.130	4144	4154	4170	rVB	147334	256523	21.49%	0.948%
75	15.310	4201	4210	4221	rVB	134460	230431	19.30%	0.852%

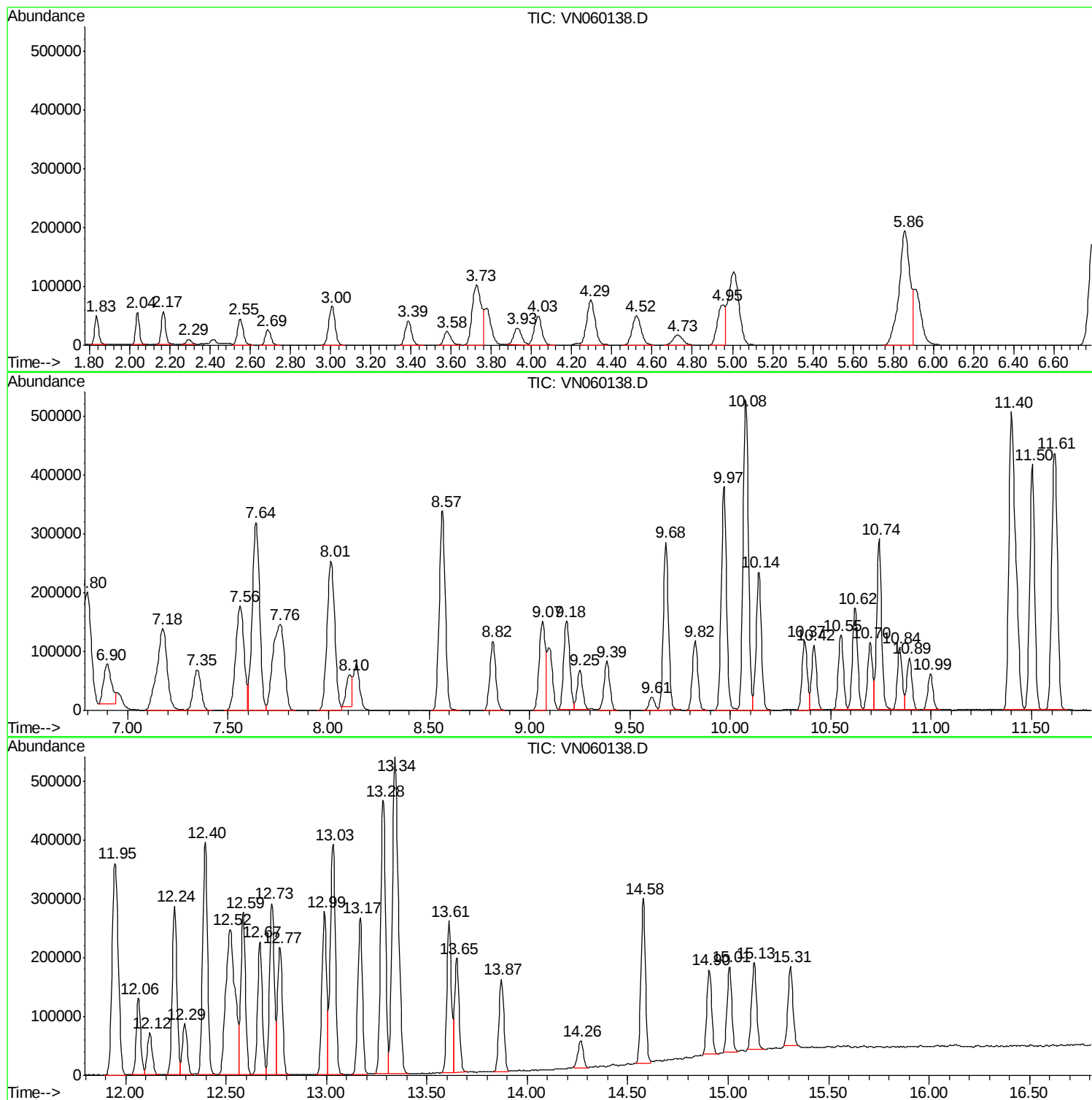
Sum of corrected areas: 27057258

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Instrument :
MSVOA_N
ClientSampleId :
VN0218MBSD01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N021220W.M
Quant Title : SW846 8260

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



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Misc : 5.00µl/10mL/100µL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleID :
VN0218MBS01

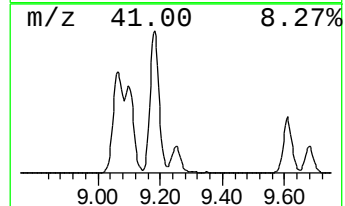
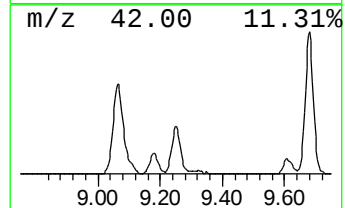
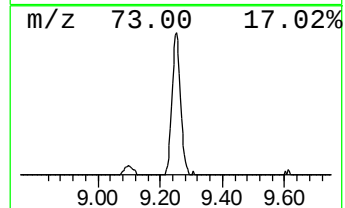
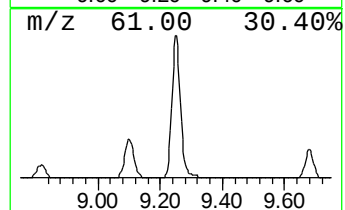
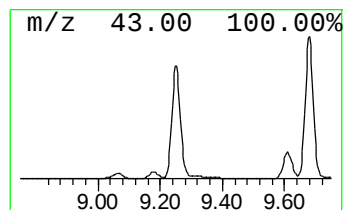
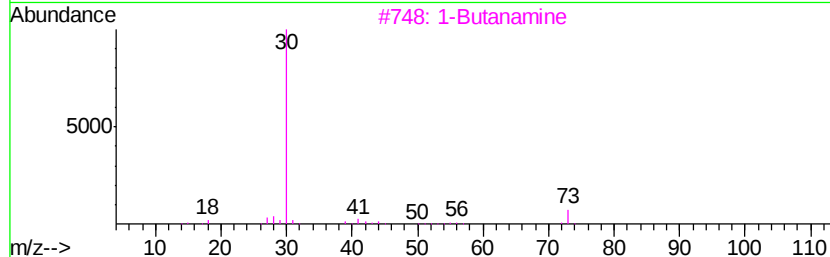
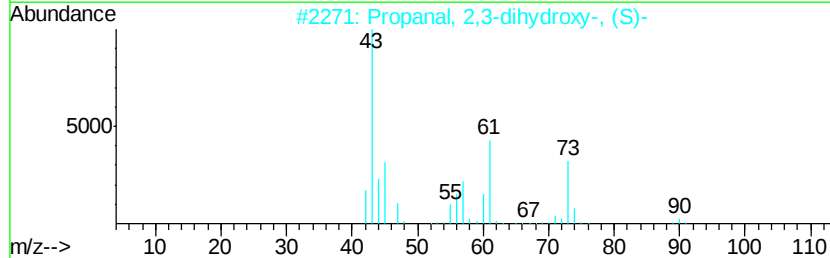
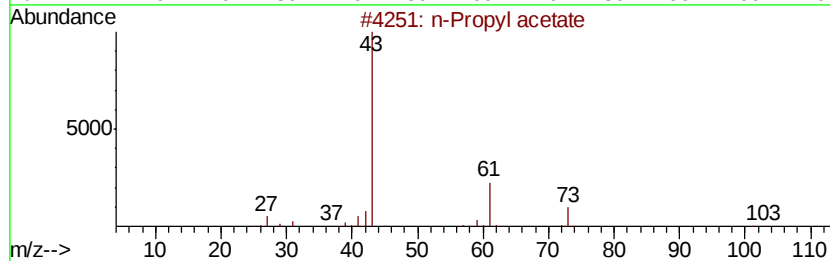
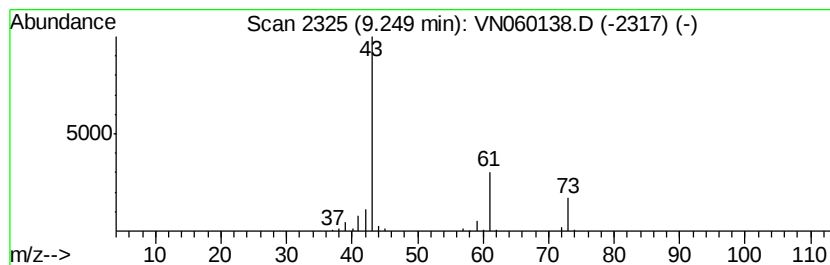
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N021220W.M
Quant Title : SW846 8260

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.
9.25	8.91 ug/l	123794	1,4-Difluorobenzene	8.57

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	36
3			1-Butanamine	73	C4H11N	000109-73-9	7
4			Isobutylamine	73	C4H11N	000078-81-9	7
5			Pentane	72	C5H12	000109-66-0	4



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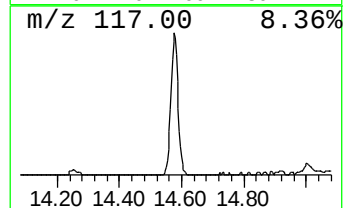
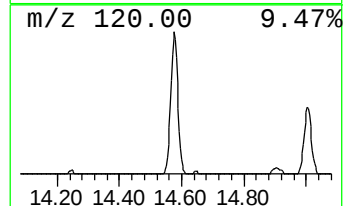
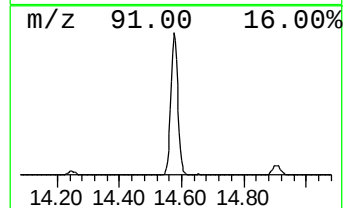
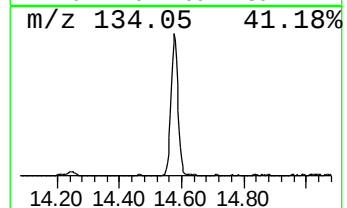
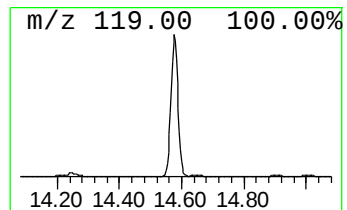
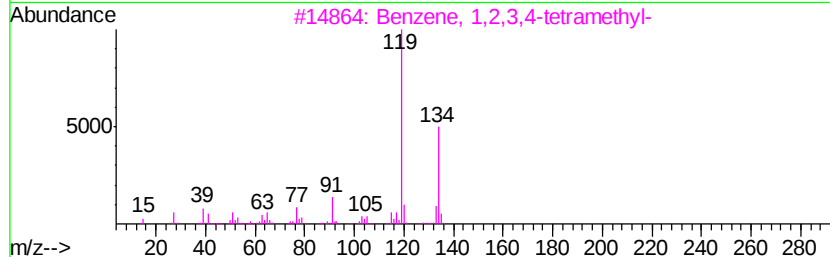
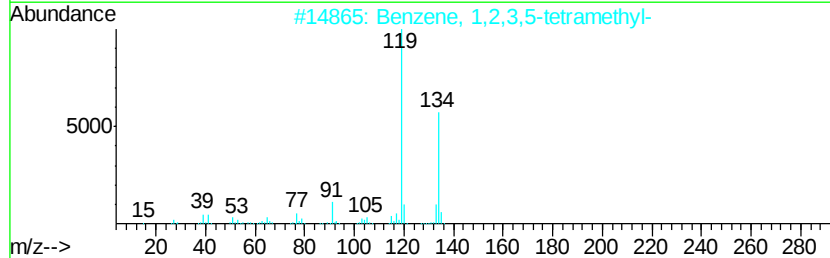
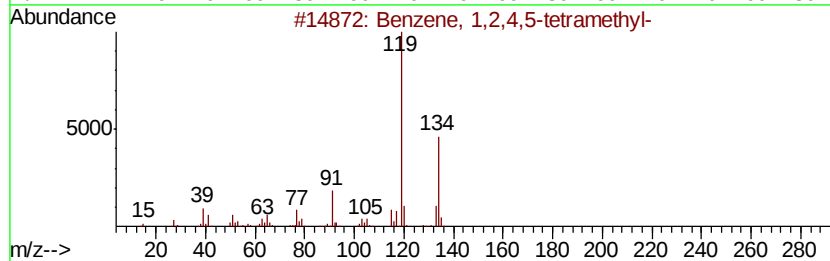
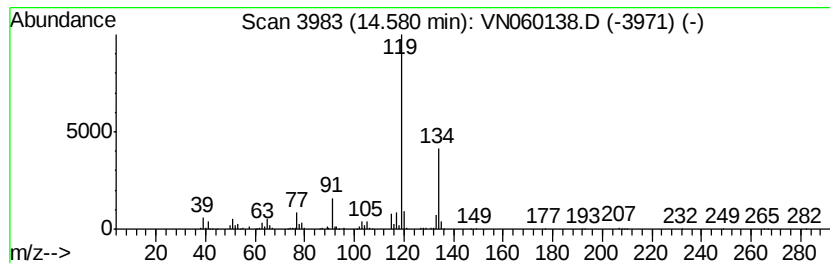
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Peak Number 2 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	19.24 ug/l	438571	1,4-Dichlorobenzene-d4	13.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	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	9.25	8.9	ug/l	123794	2	8.57	694909	50.0
Benzene, 1,2,4,5-...	14.58	19.2	ug/l	438571	4	13.34	1139540	50.0