

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
 Data File : VU038422.D
 Acq On : 30 May 2020 18:43
 Operator : JC/MD
 Sample : L2787-01
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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_U\METHOD\SOMUTR053120WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

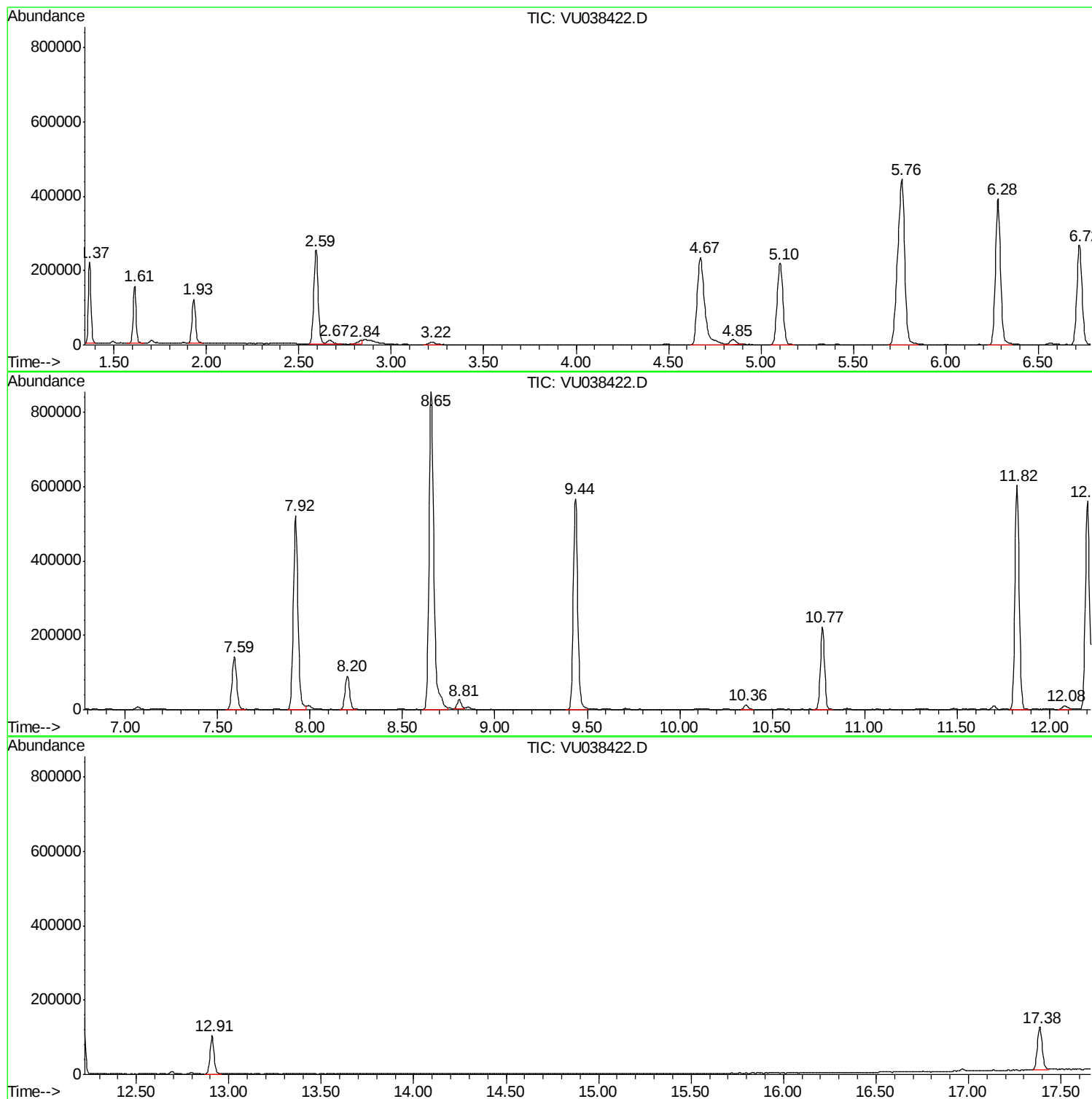
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.369	3	9	19	rBV	216926	213410	13.77%	1.918%
2	1.613	71	85	100	rBV	154049	176850	11.41%	1.590%
3	1.932	175	184	198	rVB	118084	154189	9.95%	1.386%
4	2.594	377	390	404	rBV	253192	417302	26.93%	3.751%
5	2.668	404	413	432	rVB	11773	28396	1.83%	0.255%
6	2.835	448	465	467	rBV7	10512	19138	1.24%	0.172%
7	3.218	571	584	601	rBV2	7240	16450	1.06%	0.148%
8	4.671	1019	1036	1079	rBV	235179	661197	42.67%	5.943%
9	4.848	1081	1091	1108	rVB3	13275	31419	2.03%	0.282%
10	5.102	1154	1170	1193	rVB	219206	470695	30.38%	4.231%
11	5.761	1352	1375	1403	rBV2	445264	1161190	74.94%	10.437%
12	6.282	1520	1537	1561	rBV	392266	761124	49.12%	6.841%
13	6.722	1658	1674	1693	rBV	267174	524508	33.85%	4.715%
14	7.591	1929	1944	1962	rBV	142830	249831	16.12%	2.246%
15	7.922	2033	2047	2064	rBV	521137	917603	59.22%	8.248%
16	8.201	2121	2134	2150	rBV2	90527	155182	10.01%	1.395%
17	8.655	2260	2275	2303	rBV	854251	1549565	100.00%	13.928%
18	8.806	2312	2322	2331	rBV3	23902	37300	2.41%	0.335%
19	9.436	2501	2518	2539	rBV	566569	961492	62.05%	8.642%
20	10.359	2796	2805	2816	rBV3	12770	18831	1.22%	0.169%
21	10.771	2917	2933	2950	rBV2	223170	353168	22.79%	3.174%
22	11.822	3247	3260	3280	rVB	603140	964558	62.25%	8.670%
23	12.079	3330	3340	3351	rBV3	8986	18708	1.21%	0.168%
24	12.205	3364	3379	3396	rVB	559388	890528	57.47%	8.005%
25	12.909	3587	3598	3614	rBV2	103240	156178	10.08%	1.404%
26	17.384	4979	4990	5005	rBV	115475	216492	13.97%	1.946%

Sum of corrected areas: 11125304

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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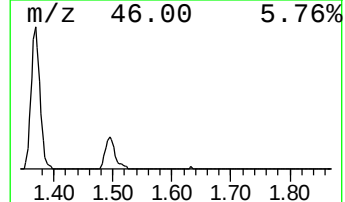
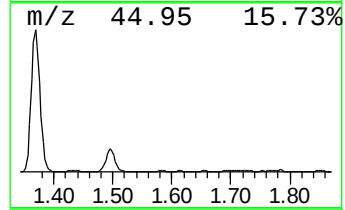
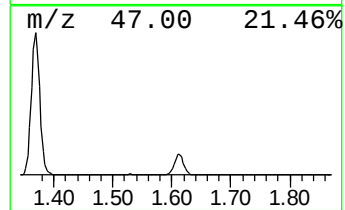
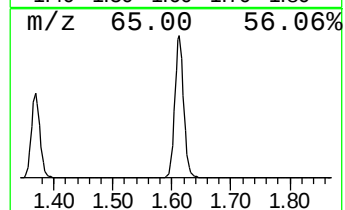
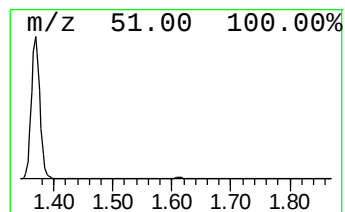
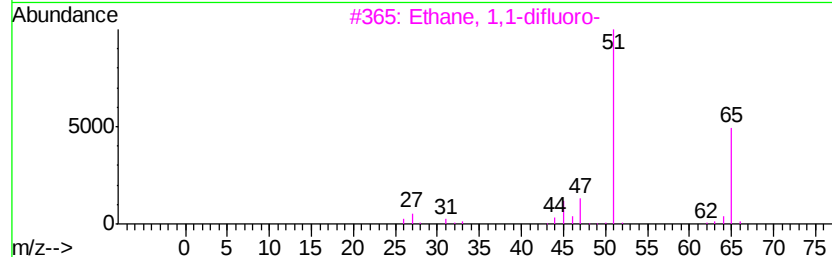
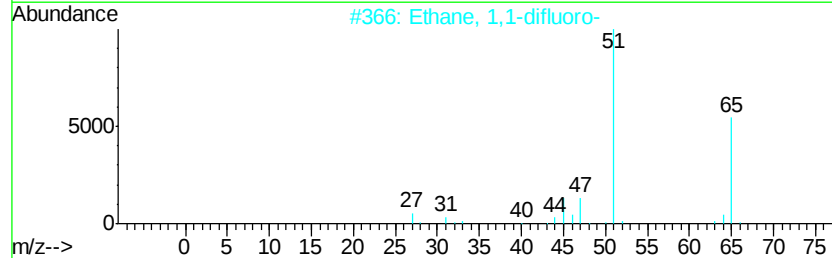
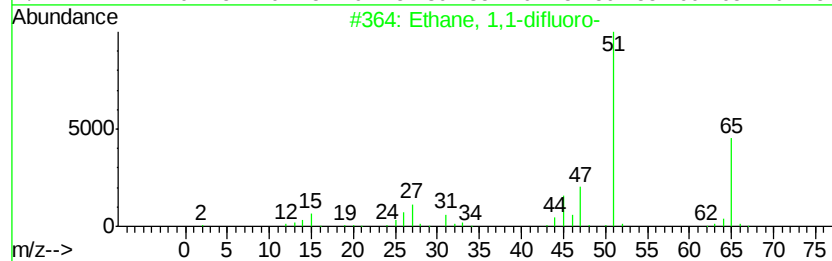
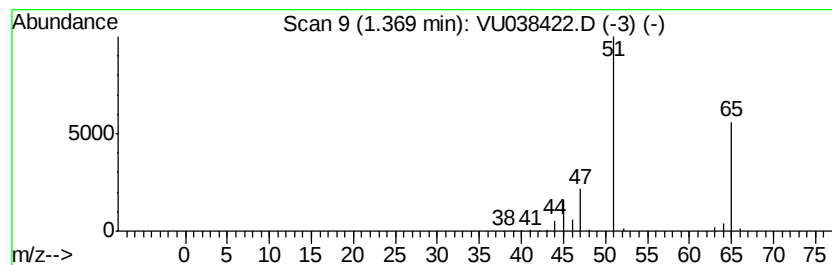
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	1.40 ug/L	213410	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
2			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90
3			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90
4			Propiolonitrile	51	C3HN	001070-71-9	3
5			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2



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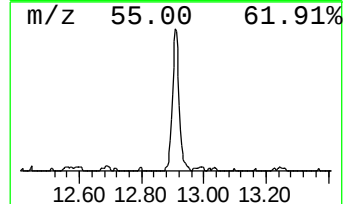
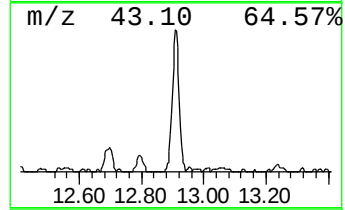
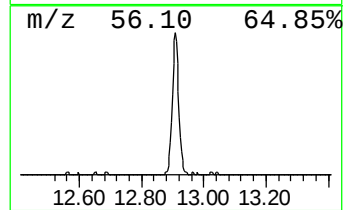
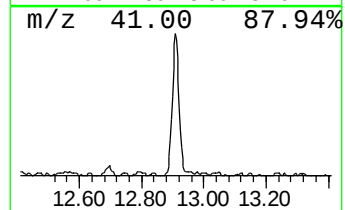
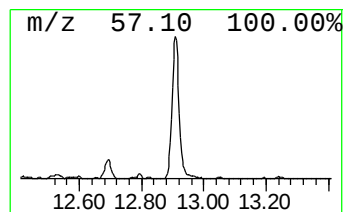
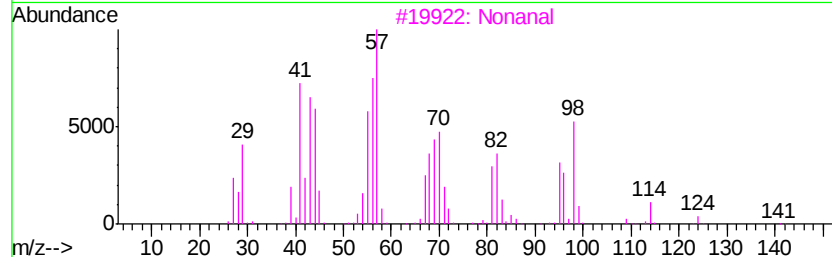
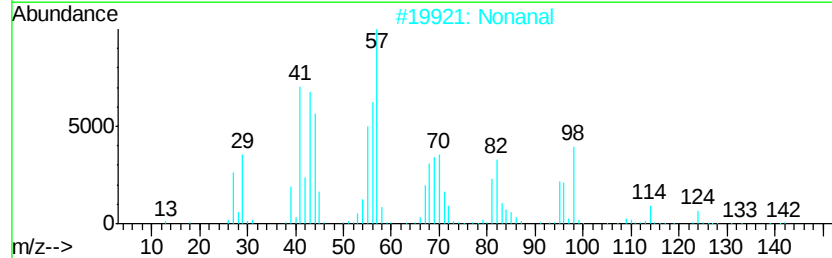
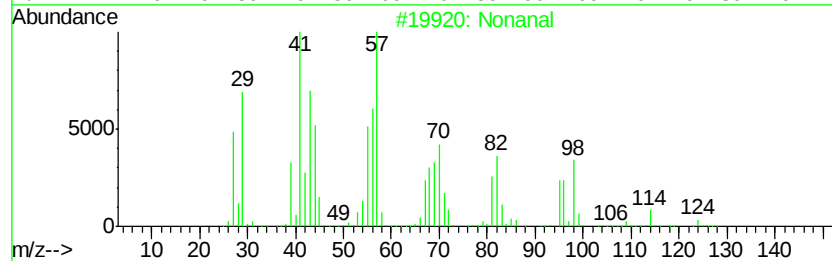
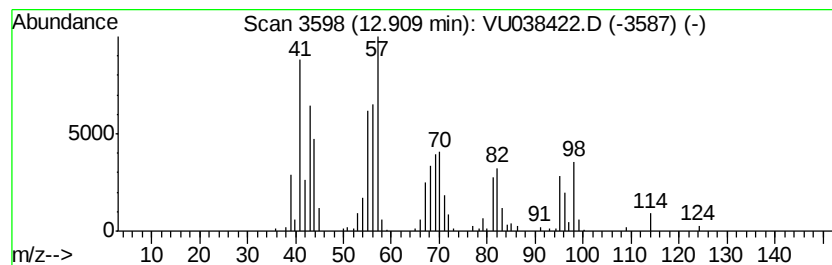
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Peak Number 3 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	0.81 ug/L	156178	1,4-Dichlorobenzene-d4	11.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal		142	C9H18O	000124-19-6	91
2	Nonanal		142	C9H18O	000124-19-6	91
3	Nonanal		142	C9H18O	000124-19-6	90
4	Nonanal		142	C9H18O	000124-19-6	90
5	Heptane, 4-chloro-		134	C7H15Cl	000998-95-8	27



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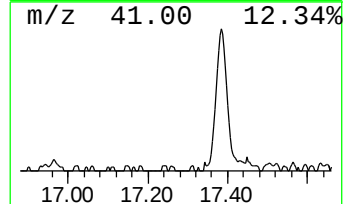
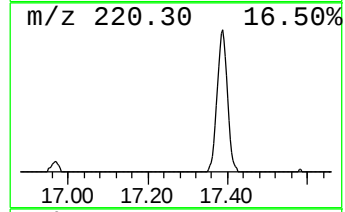
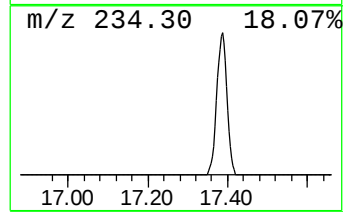
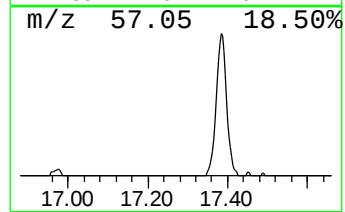
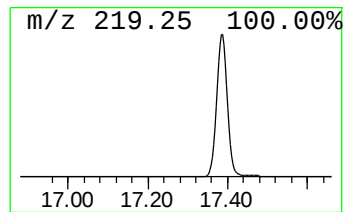
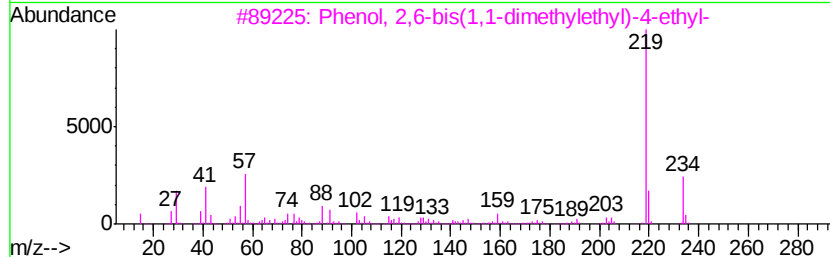
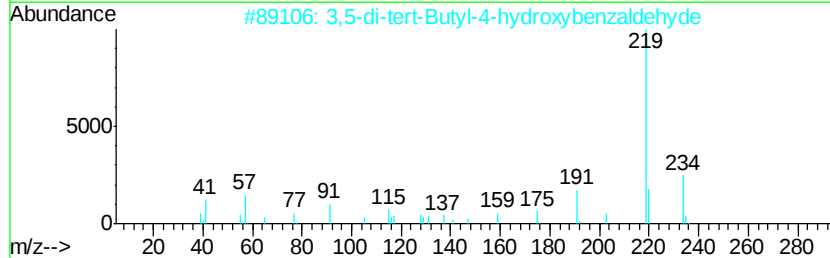
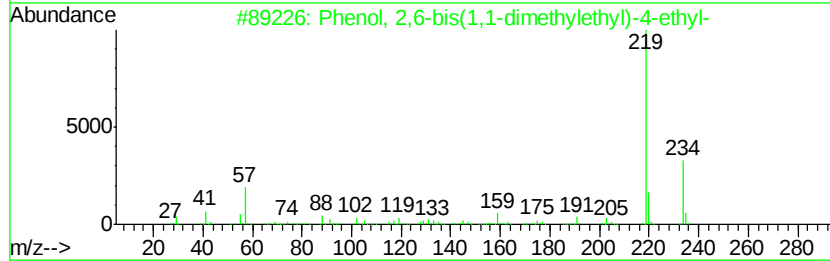
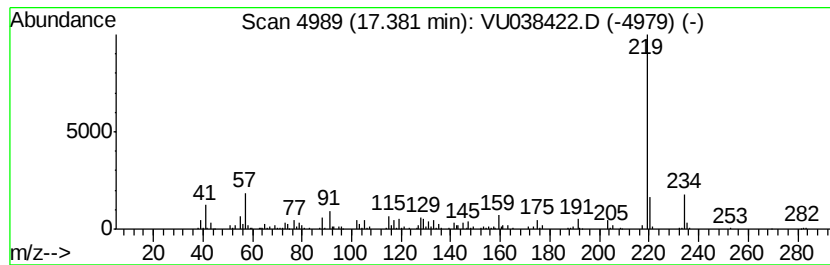
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Peak Number 4 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	1.12 ug/L	216492	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2,6-bis(1,1-dimethylethyl)...	234	C16H26O	004130-42-1	95
2		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	93
3		Phenol, 2,6-bis(1,1-dimethylethyl)...	234	C16H26O	004130-42-1	93
4		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	90
5		4-tert-Butyl-2,6-diisopropylphenol	234	C16H26O	057354-65-1	83



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethane, 1,1-diflu...	1.37	1.4	ug/L	213410	1	6.28	761124	5.0
Nonanal	12.91	0.8	ug/L	156178	3	11.82	964558	5.0
Phenol, 2,6-bis(1...	17.38	1.1	ug/L	216492	3	11.82	964558	5.0