

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061820\
 Data File : VU038969.D
 Acq On : 18 Jun 2020 14:55
 Operator : SY/MD
 Sample : L3058-03
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9L30

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\SOMUTR061720WMA.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	1.630	80	90	102	rBV	126956	168388	11.96%	1.598%
2	1.787	129	139	140	rBV6	11829	17305	1.23%	0.164%
3	1.954	184	191	202	rBV	147916	191641	13.61%	1.819%
4	2.604	383	393	409	rVB	289883	465687	33.07%	4.419%
5	4.790	1042	1073	1106	rBV	98939	456588	32.43%	4.333%
6	5.137	1167	1181	1204	rVB	201786	447881	31.81%	4.250%
7	5.793	1365	1385	1408	rBV2	435380	1022295	72.60%	9.702%
8	6.308	1530	1545	1566	rBV	361545	658932	46.80%	6.253%
9	6.591	1625	1633	1644	rVB	6760	14099	1.00%	0.134%
10	6.745	1668	1681	1699	rVB	252005	483442	34.33%	4.588%
11	7.227	1820	1831	1847	rVB4	16377	32960	2.34%	0.313%
12	7.607	1935	1949	1966	rBV	123420	214195	15.21%	2.033%
13	7.935	2039	2051	2066	rVB	452651	758516	53.87%	7.198%
14	8.215	2125	2138	2152	rBV	83301	138199	9.81%	1.312%
15	8.674	2265	2281	2319	rBV	712249	1408091	100.00%	13.363%
16	9.443	2502	2520	2542	rBV	504567	839443	59.62%	7.966%
17	10.774	2922	2934	2946	rBV	212517	345138	24.51%	3.275%
18	11.825	3248	3261	3277	rBV	520261	819794	58.22%	7.780%
19	12.076	3327	3339	3356	rBV2	34240	74321	5.28%	0.705%
20	12.205	3366	3379	3393	rBV	502082	792392	56.27%	7.520%
21	14.227	3997	4008	4020	rBV3	59587	95184	6.76%	0.903%
22	14.353	4037	4047	4058	rBV6	9723	16804	1.19%	0.159%
23	15.745	4469	4480	4491	rBV7	34280	58268	4.14%	0.553%
24	16.195	4611	4620	4630	rVB4	25141	40635	2.89%	0.386%
25	16.838	4809	4820	4833	rBV2	170123	276029	19.60%	2.620%
26	16.967	4847	4860	4879	rBV	406667	701041	49.79%	6.653%

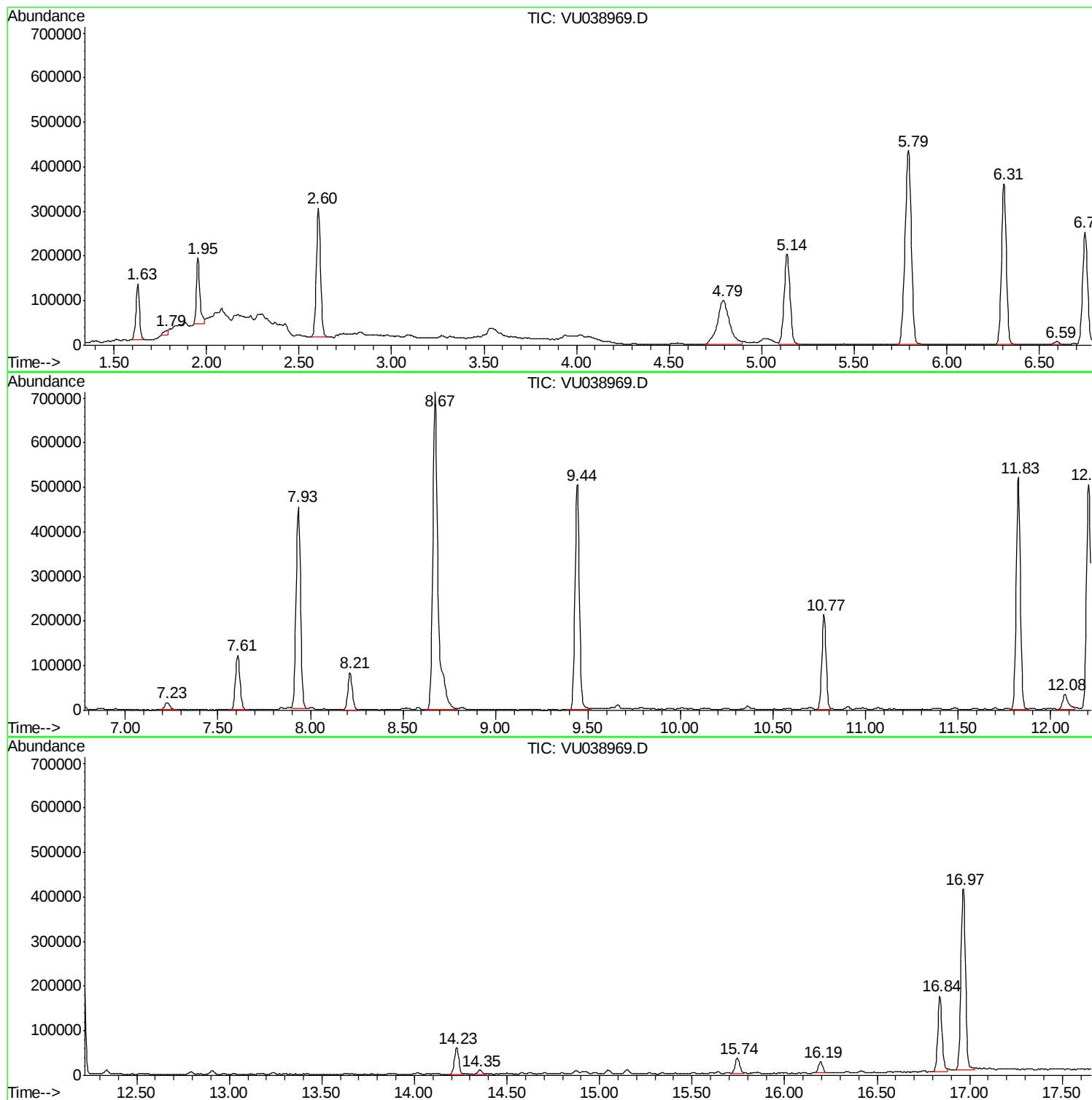
Sum of corrected areas: 10537268

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ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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ClientSampleId :
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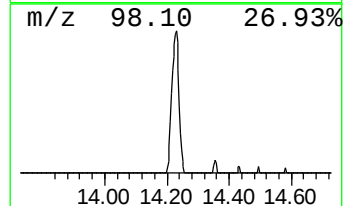
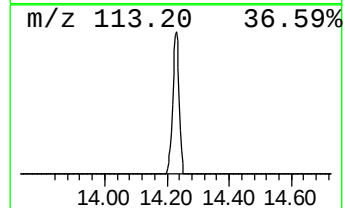
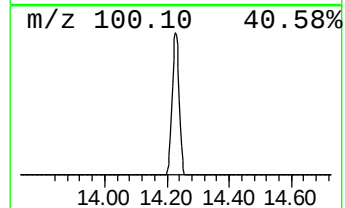
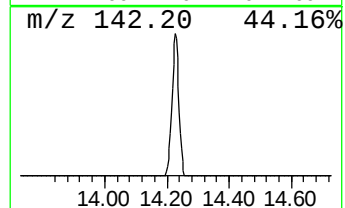
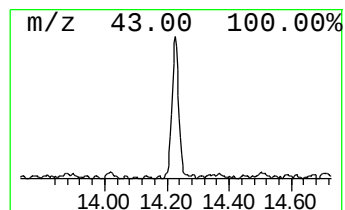
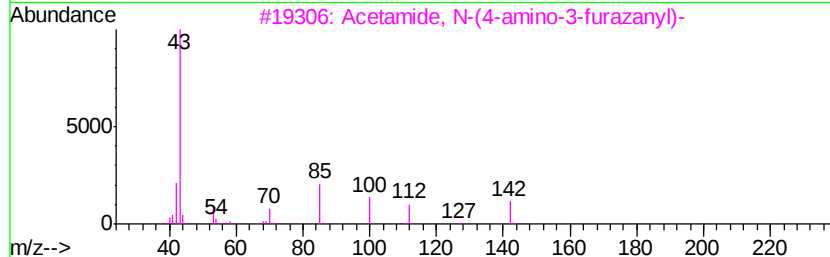
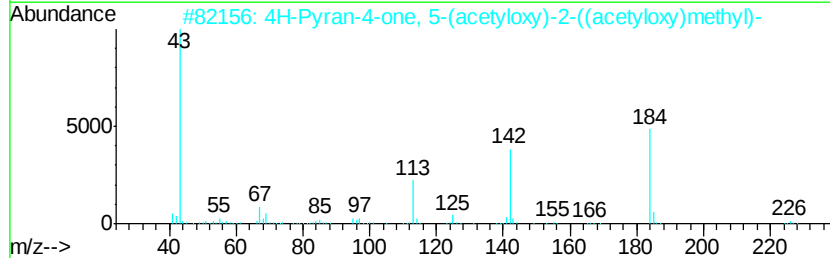
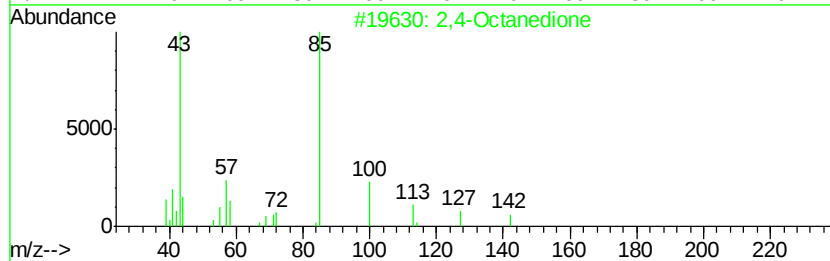
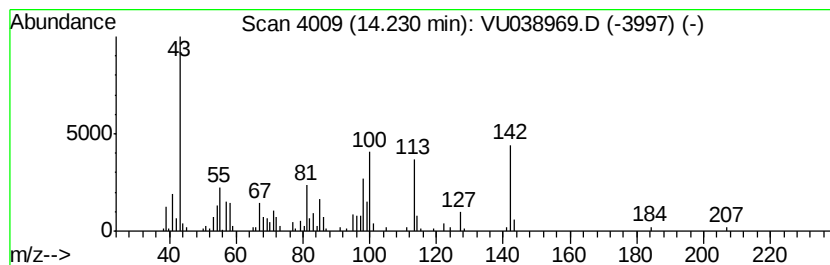
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 2,4-Octanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	0.58 ug/L	95184	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Octanedione	142	C8H14O2	014090-87-0	50
2		4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	35
3		Acetamide, N-(4-amino-3-furazanyl)-	142	C4H6N4O2	140706-47-4	23
4		6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	16
5		3-t-Butylhexan-2-one	156	C10H20O	1000202-22-9	12



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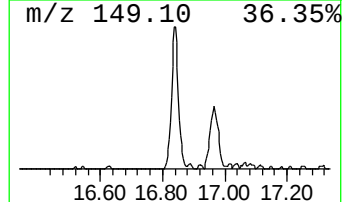
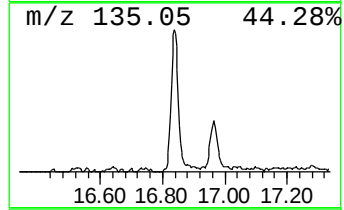
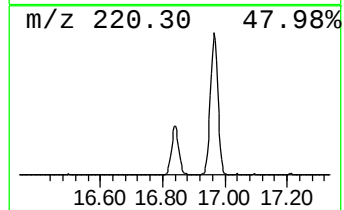
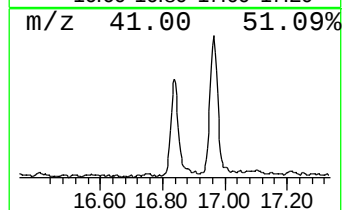
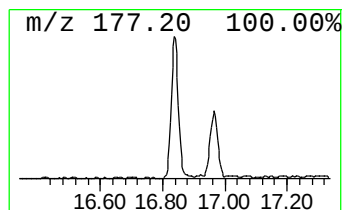
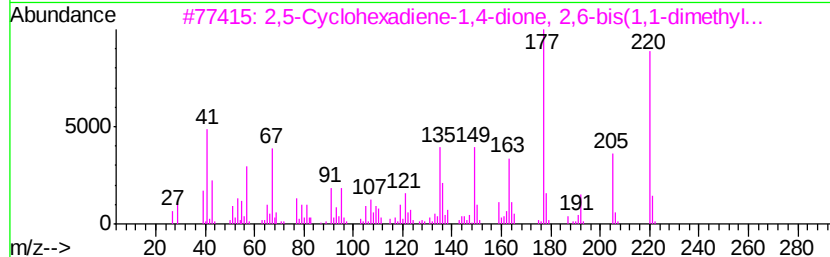
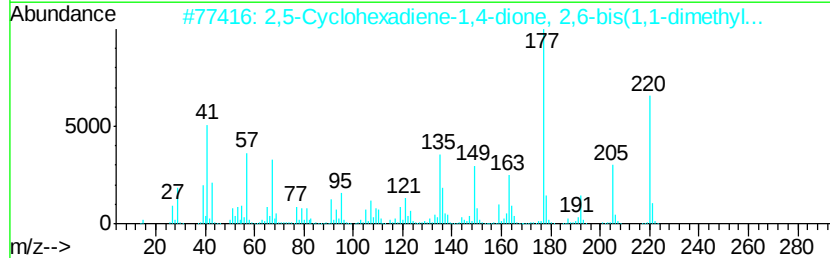
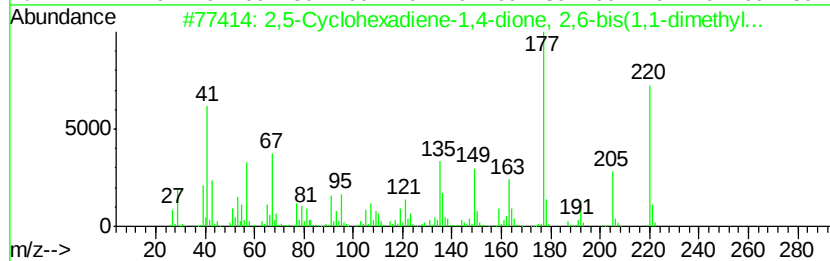
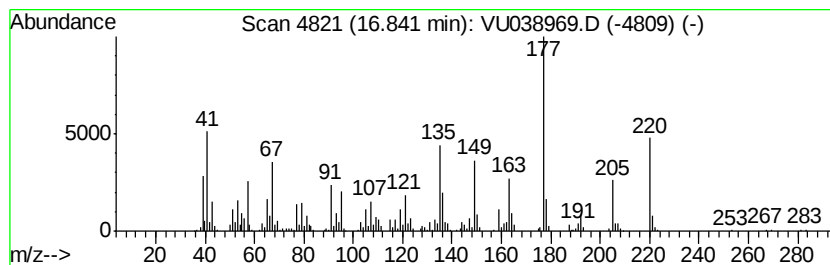
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Peak Number 3 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	1.68 ug/L	276029	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
2		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
3		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	64
4		2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	60
5		trans-.beta.-Ionone	192	C13H20O	000079-77-6	42



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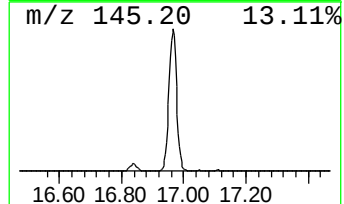
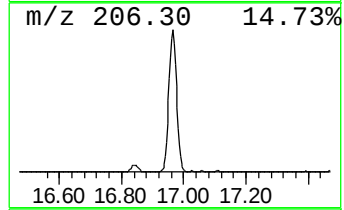
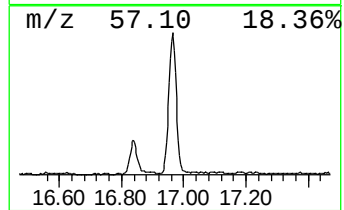
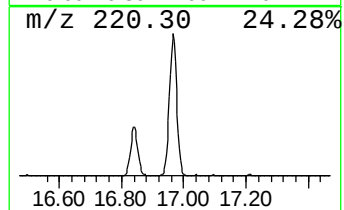
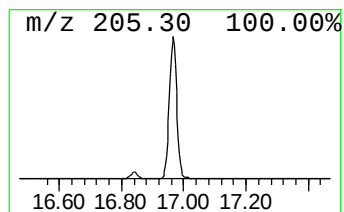
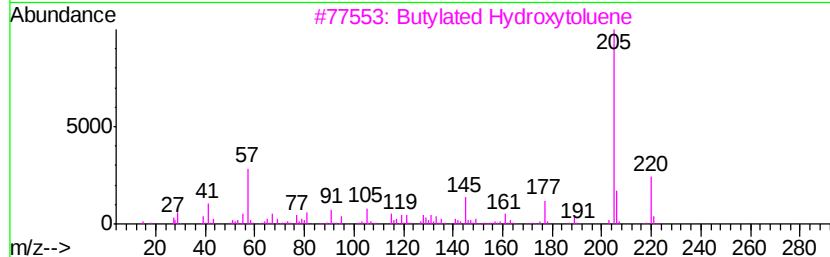
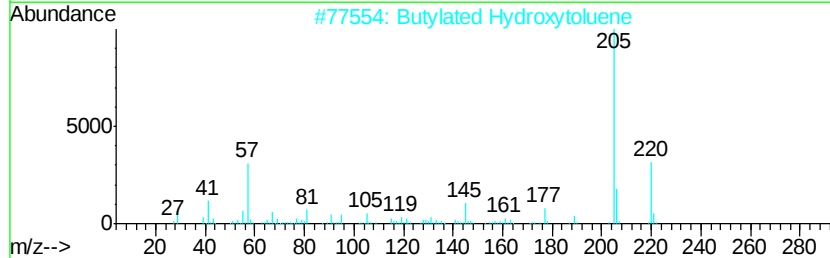
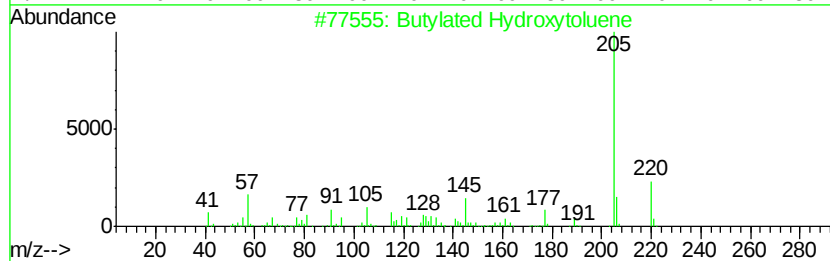
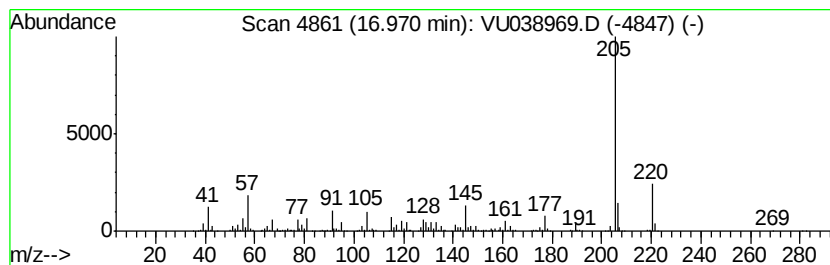
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Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	4.28 ug/L	701041	1,4-Dichlorobenzene-d4	11.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	99
2	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	96
3	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	96
4	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 2,4,6-tris(1-methylethyl)-			220	C15H24O	002934-07-8	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4-Octanedione	14.23	0.6	ug/L	95184	3	11.83	819794	5.0
2,5-Cyclohexadien...	16.84	1.7	ug/L	276029	3	11.83	819794	5.0
Butylated Hydroxy...	16.97	4.3	ug/L	701041	3	11.83	819794	5.0