

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092421\
 Data File : BF125630.D
 Acq On : 24 Sep 2021 20:17
 Operator : JU/CG
 Sample : M3911-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-CB-04-(0.5)

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125630.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	14	22	27	rBV	4425290	6189335	91.62%	14.574%
2	5.204	526	530	534	rBV	166291	151734	2.25%	0.357%
3	5.504	576	581	584	rBV	2815740	2582452	38.23%	6.081%
4	6.498	745	750	753	rBV	1889476	1621799	24.01%	3.819%
5	6.539	754	757	761	rVB	91304	77568	1.15%	0.183%
6	6.886	812	816	822	rBV	1361249	1185118	17.54%	2.791%
7	7.445	905	911	914	rBV	3470747	3529254	52.25%	8.310%
8	8.063	1013	1016	1021	rVB	175229	145797	2.16%	0.343%
9	8.169	1029	1034	1037	rBV	1609693	1591605	23.56%	3.748%
10	9.057	1179	1185	1188	rVB	141645	112321	1.66%	0.264%
11	9.245	1211	1217	1220	rBV	6829084	6755153	100.00%	15.906%
12	9.457	1247	1253	1258	rBV	90585	91319	1.35%	0.215%
13	9.922	1327	1332	1335	rVB	2362280	1890501	27.99%	4.452%
14	10.551	1433	1439	1442	rBV	328204	284764	4.22%	0.671%
15	10.710	1459	1466	1469	rBV	4340696	4082068	60.43%	9.612%
16	10.821	1477	1485	1488	rBV	1491140	2207486	32.68%	5.198%
17	11.404	1580	1584	1587	rBV	2154500	1786433	26.45%	4.207%
18	11.927	1670	1673	1678	rBV	157392	155830	2.31%	0.367%
19	12.710	1803	1806	1815	rBV2	54279	71615	1.06%	0.169%
20	12.992	1849	1854	1857	rBV	5936901	5767453	85.38%	13.581%
21	13.886	2001	2006	2008	rBV2	41859	68247	1.01%	0.161%
22	14.039	2028	2032	2035	rBV	1257801	1023120	15.15%	2.409%
23	15.515	2277	2283	2287	rBV	914754	1097117	16.24%	2.583%

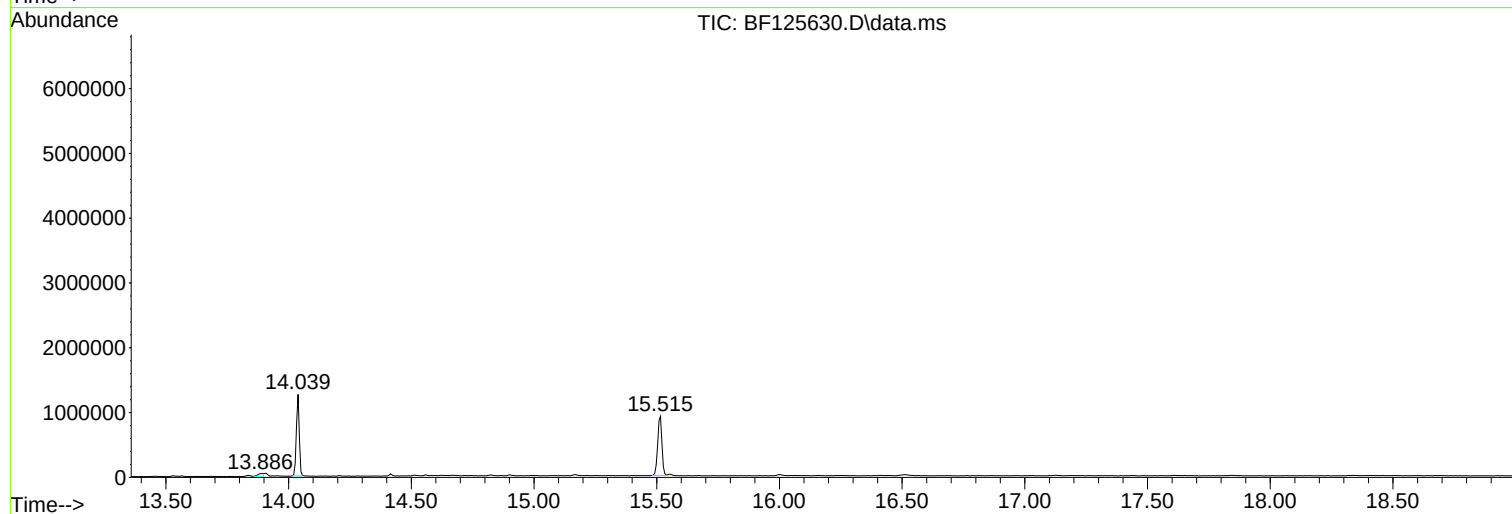
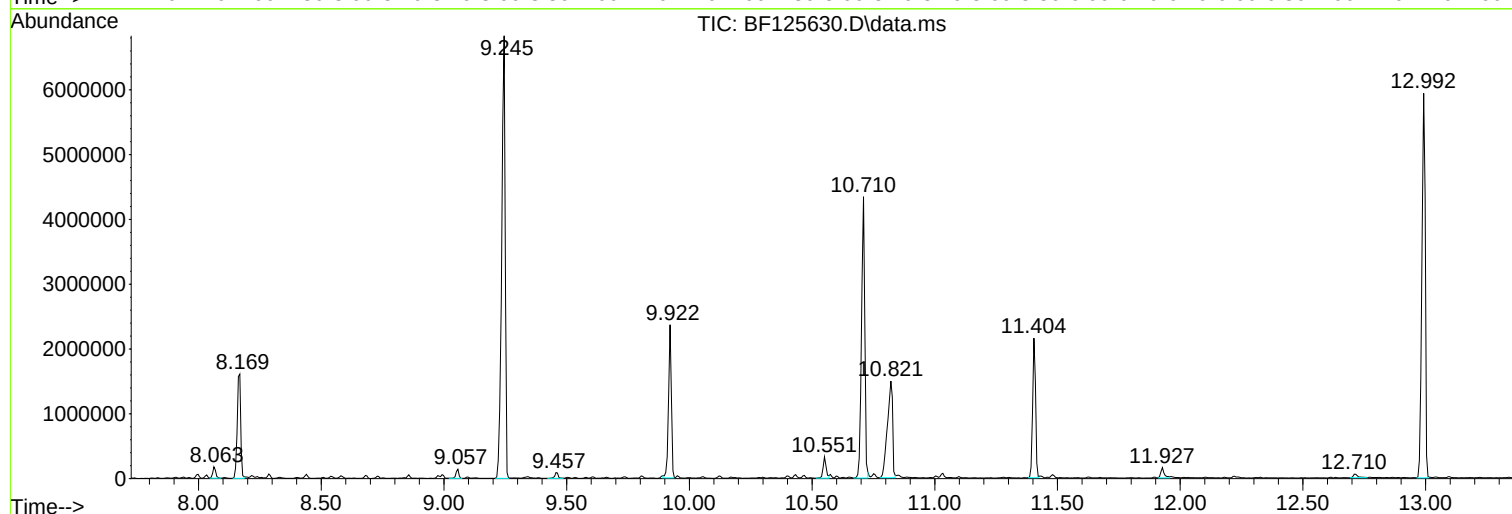
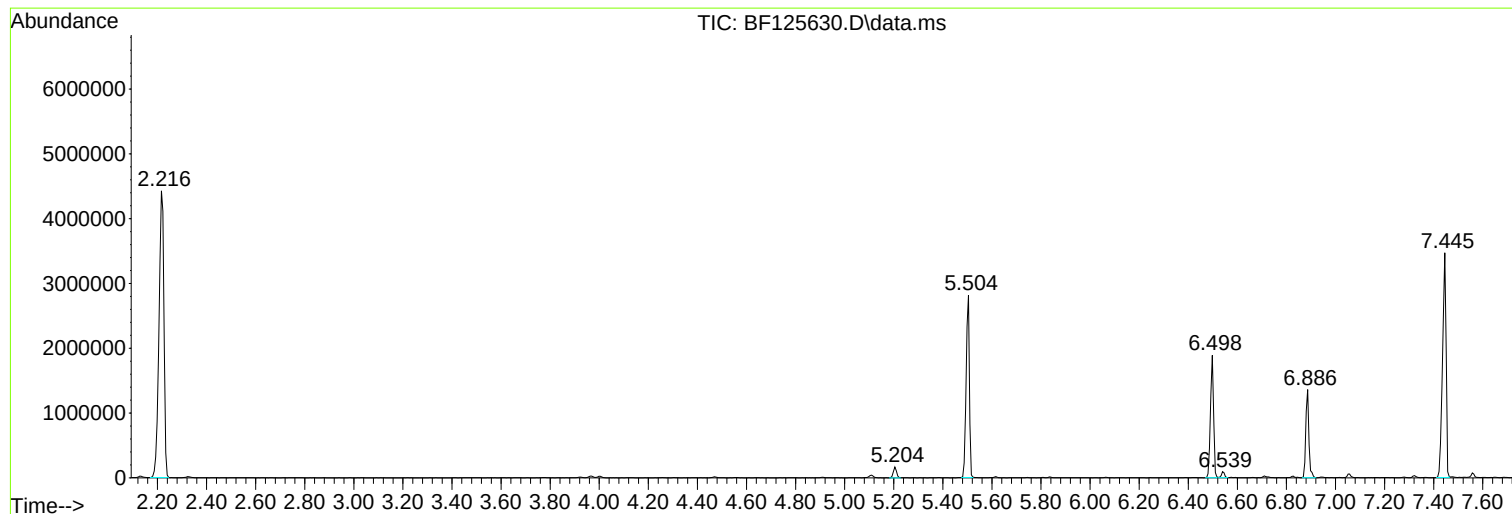
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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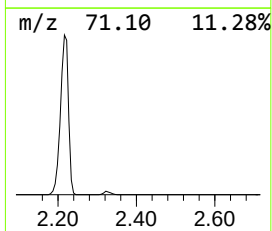
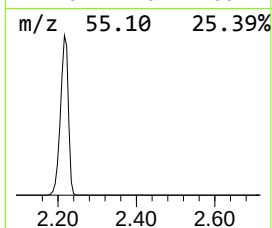
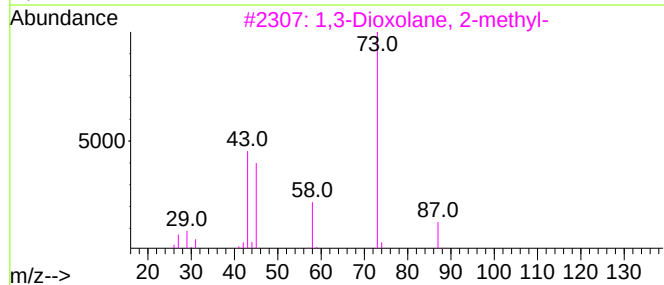
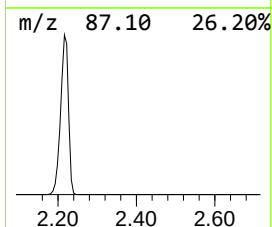
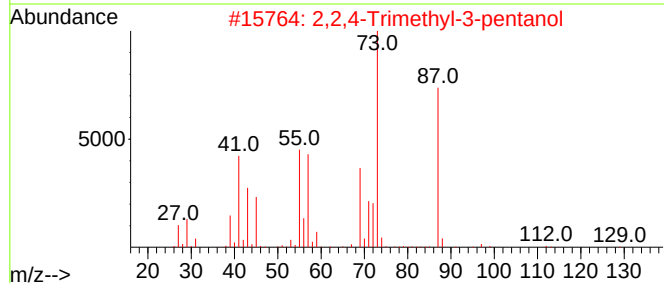
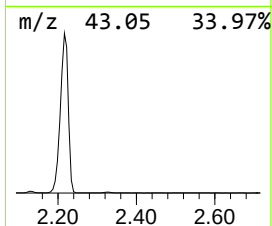
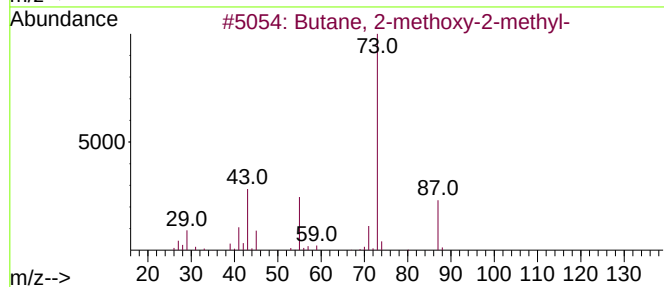
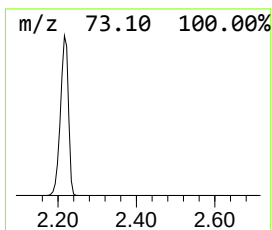
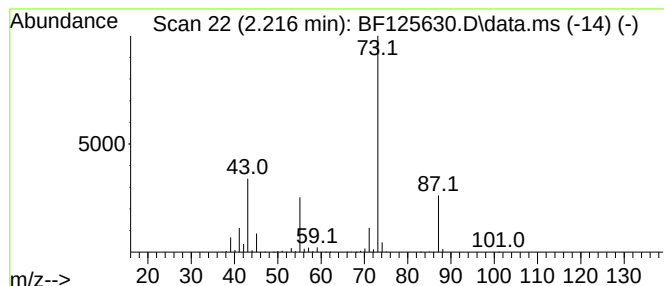
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	104.45 ng	6189340	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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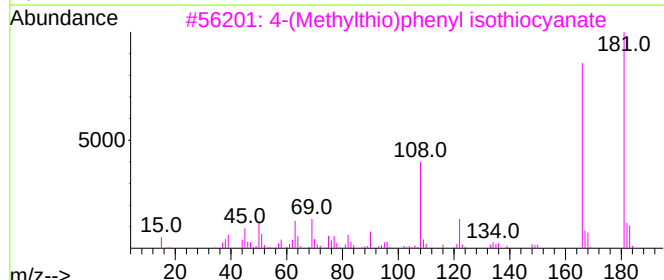
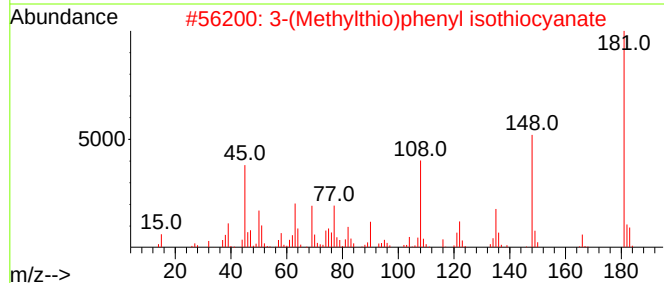
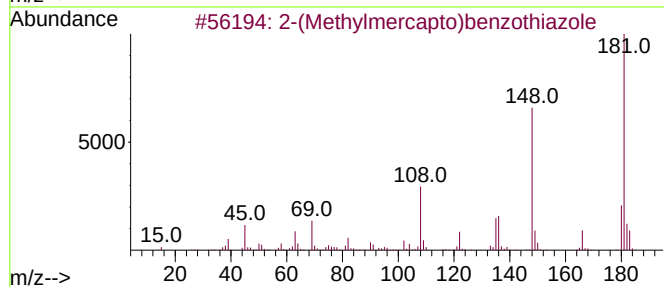
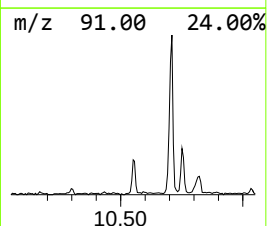
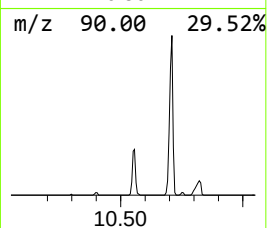
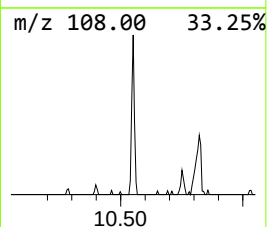
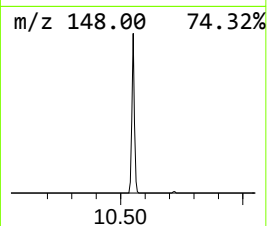
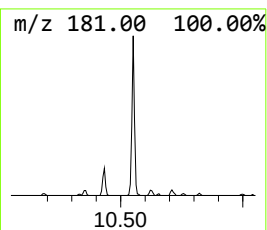
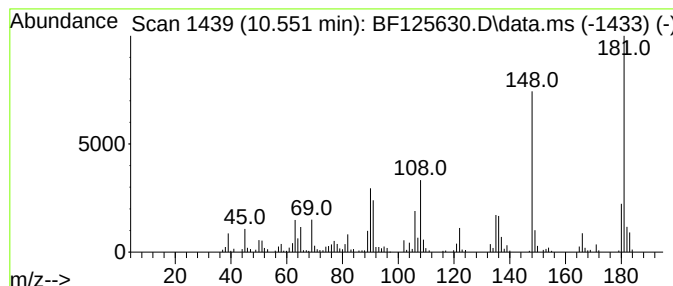
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Peak Number 3 2-(Methylmercapto)benzothia... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.551	3.01 ng	284764	Acenaphthene-d10	9.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	98
2		3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	70
3		4-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	015863-41-9	62
4		5-Aminoisophthalic acid	181	C8H7NO4	000099-31-0	35
5		2-Fluorenamine	181	C13H11N	000153-78-6	30



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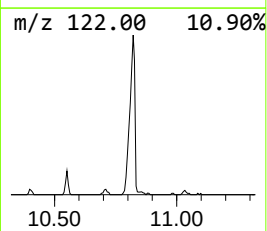
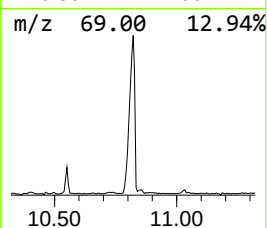
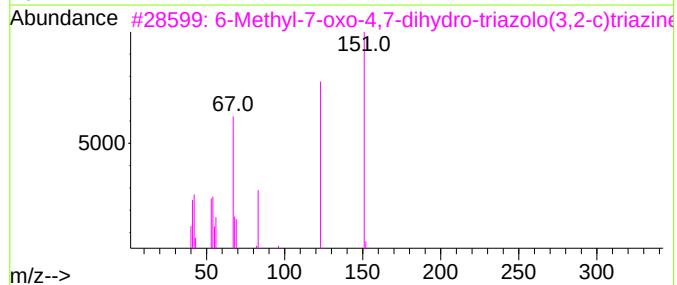
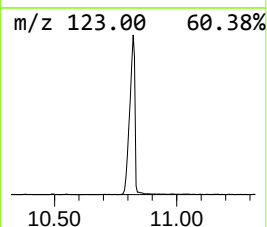
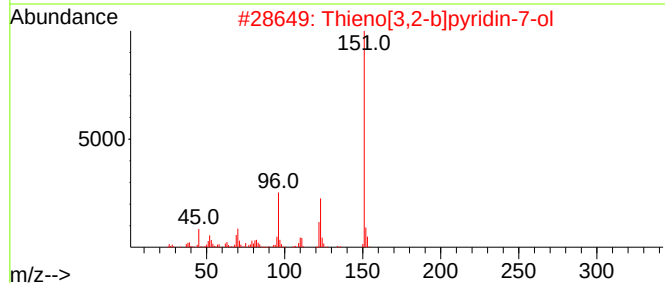
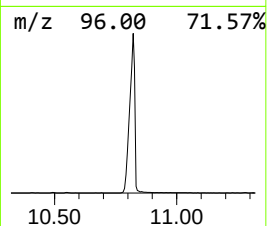
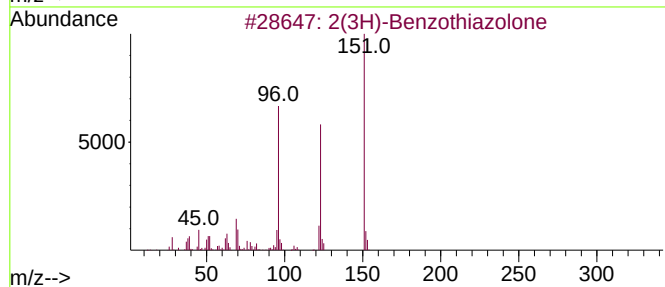
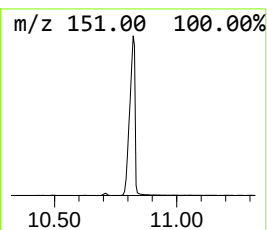
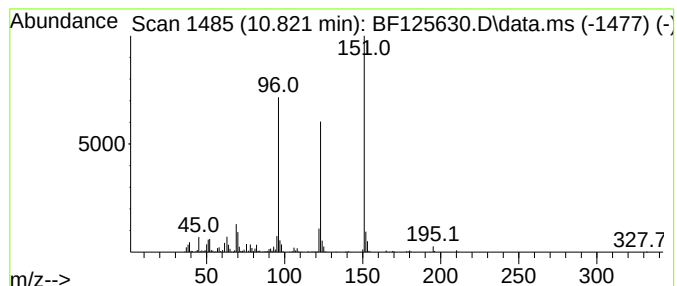
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Peak Number 4 2(3H)-Benzothiazolone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	24.71 ng	2207490	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
2			Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	64
3			6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50
4			t-Butylhydroquinone	166	C10H14O2	001948-33-0	40
5			4-Amino-2,1,3-benzothiadiazole	151	C6H5N3S	000767-64-6	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.216	104.5	ng	6189340	1	6.886	1185120	20.0
2-(Methylmercap...	10.551	3.0	ng	284764	3	9.922	1890500	20.0
2(3H)-Benzothia...	10.822	24.7	ng	2207490	4	11.404	1786430	20.0