

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
 Data File : BF091981.D
 Acq On : 27 Dec 2016 21:32
 Operator : UM/SJ
 Sample : H6245-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-4

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:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.876	242	244	254	rBV	735143	1048926	13.54%	1.944%
2	5.344	283	285	288	rBV	2611941	3485892	45.00%	6.459%
3	6.396	376	377	384	rVB	1468269	2248384	29.02%	4.166%
4	6.510	384	387	389	rBV	6420108	6429703	83.00%	11.914%
5	6.727	404	406	408	rBV	1732425	1556419	20.09%	2.884%
6	6.887	417	420	422	rBV	5686342	5844419	75.44%	10.829%
7	7.299	453	456	459	rBV	3838900	4621482	59.65%	8.563%
8	8.019	516	519	521	rBV	2268933	2237964	28.89%	4.147%
9	9.105	610	614	616	rBV	5639352	7747023	100.00%	14.355%
10	9.493	646	648	650	rBV	205771	165761	2.14%	0.307%
11	9.768	670	672	674	rBV	2206889	2015268	26.01%	3.734%
12	10.568	739	742	744	rBV	3947569	4407918	56.90%	8.168%
13	10.682	750	752	757	rVB	65524	86559	1.12%	0.160%
14	11.254	799	802	804	rBV	2143181	1912879	24.69%	3.544%
15	11.608	831	833	835	rBV	106954	123729	1.60%	0.229%
16	12.842	938	941	944	rBV	5020154	6374076	82.28%	11.811%
17	13.437	990	993	995	rVB	927395	886737	11.45%	1.643%
18	13.894	1030	1033	1035	rBV	1223740	1579777	20.39%	2.927%
19	15.288	1152	1155	1157	rBV	1014660	1195567	15.43%	2.215%

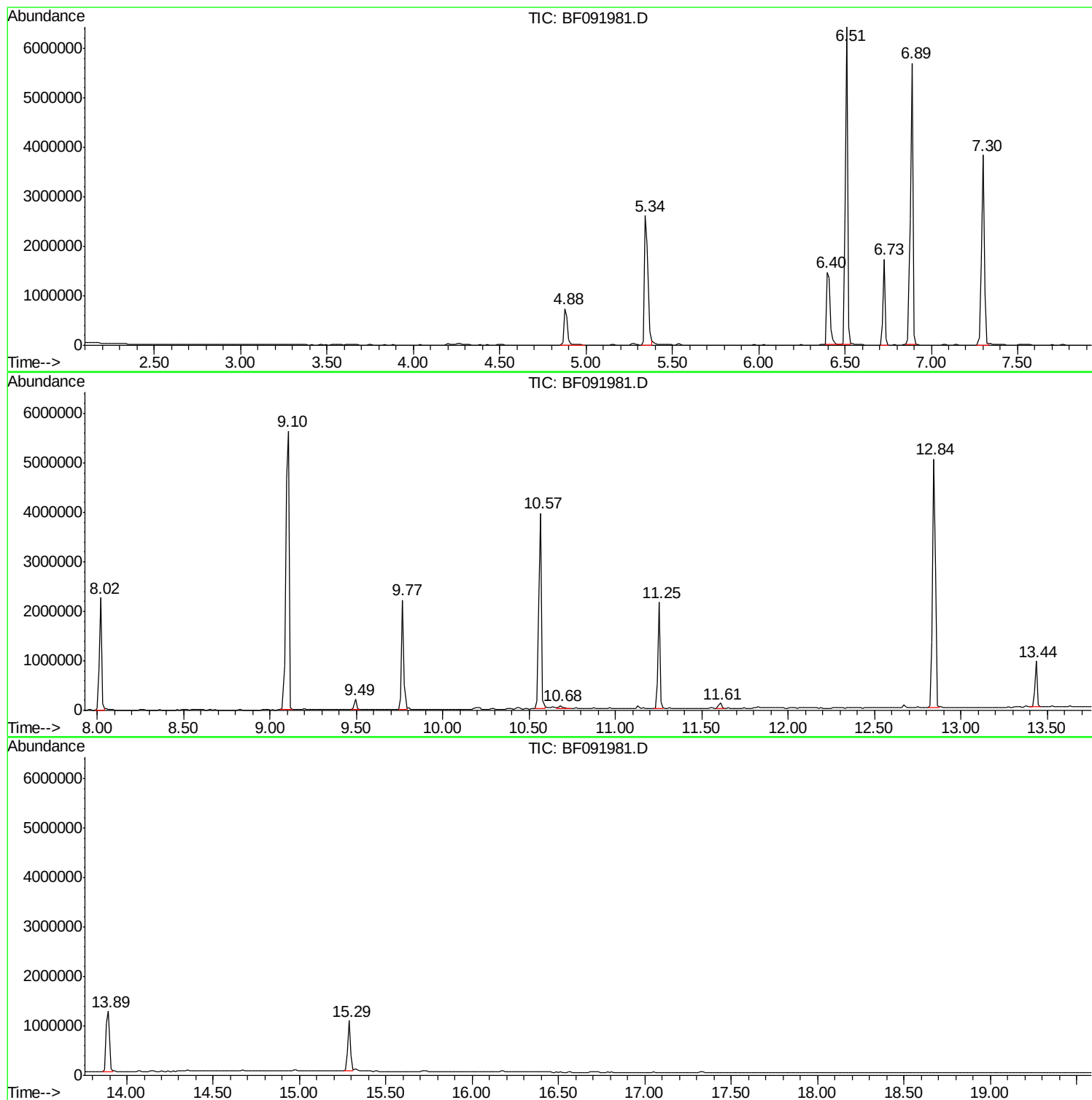
Sum of corrected areas: 53968483

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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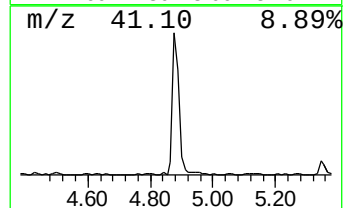
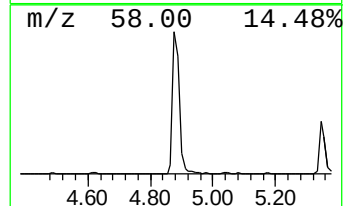
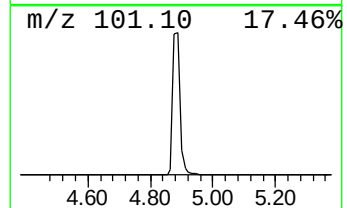
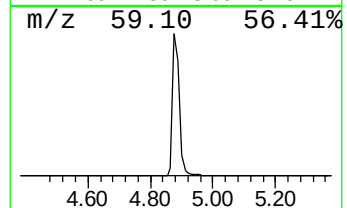
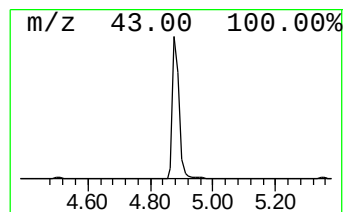
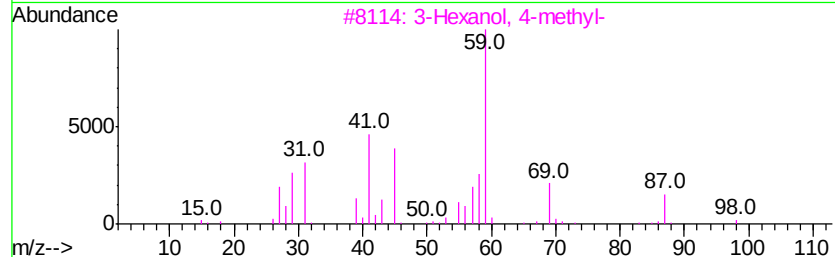
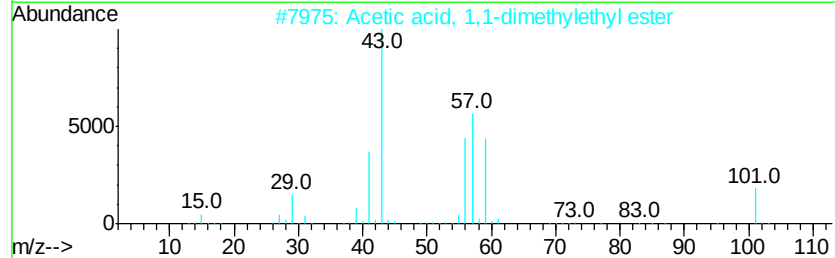
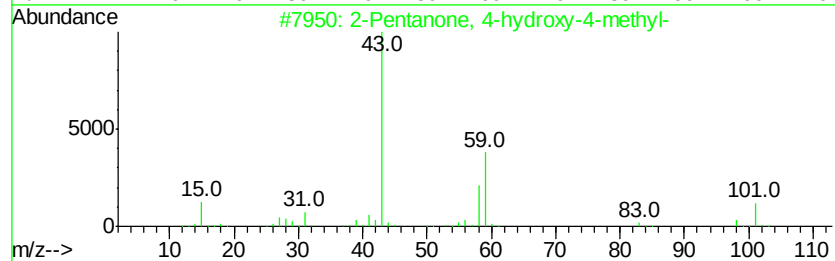
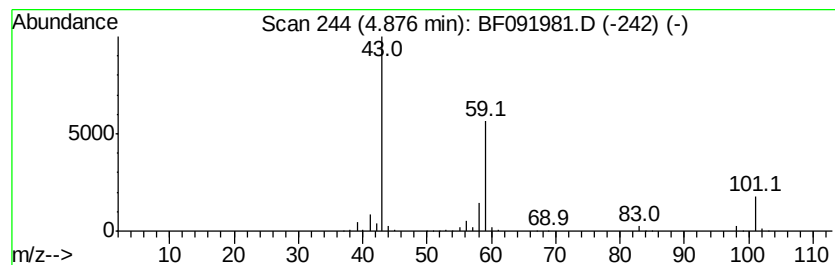
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	13.48 ng	1048930	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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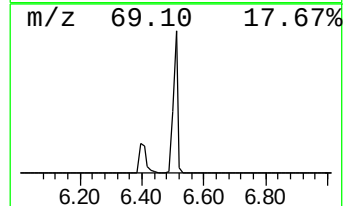
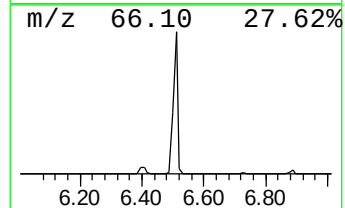
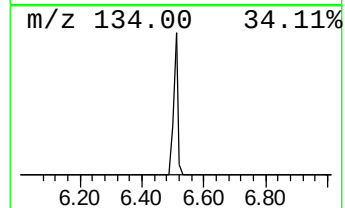
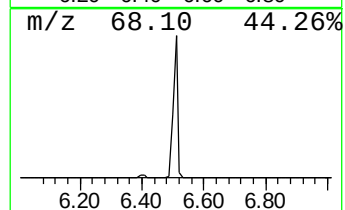
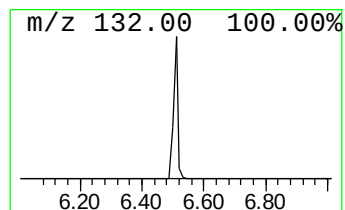
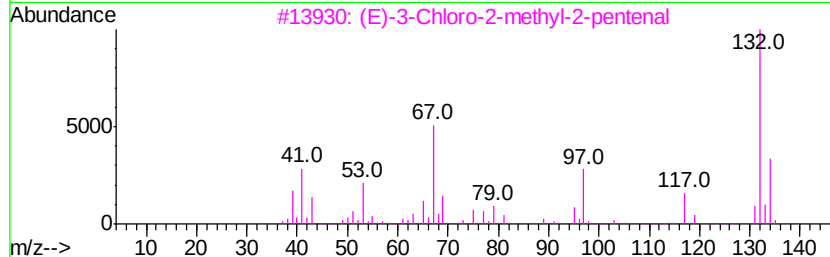
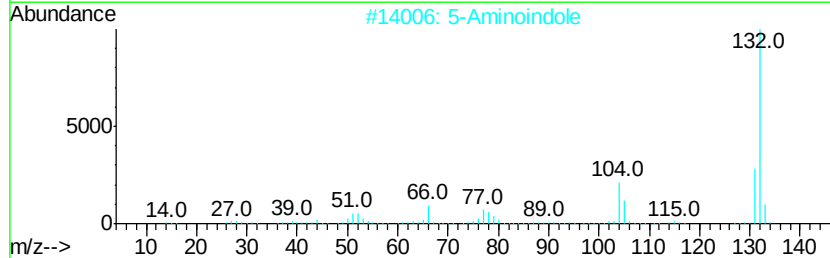
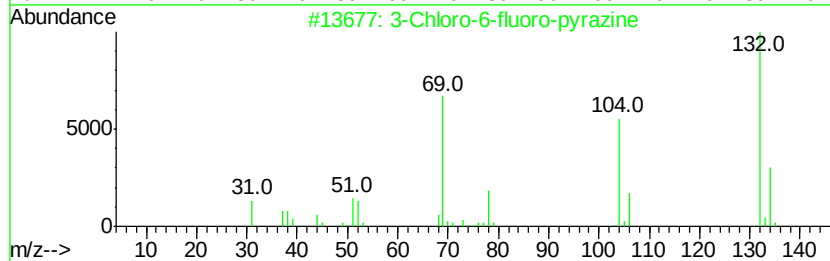
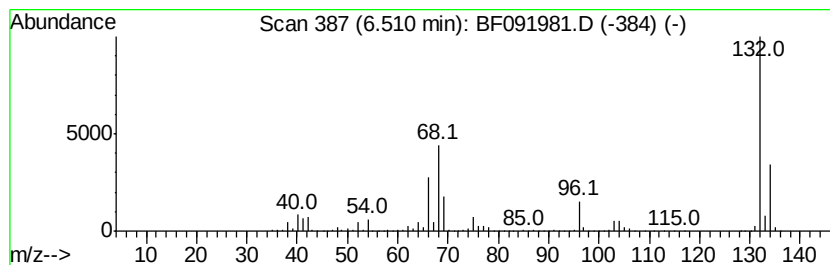
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Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	82.62 ng	6429700	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	9
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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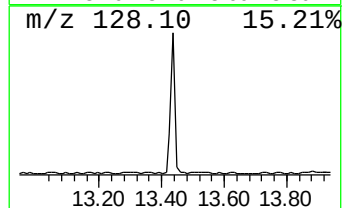
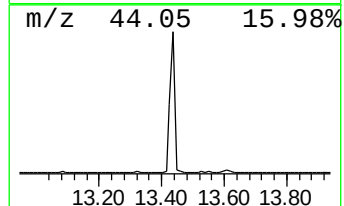
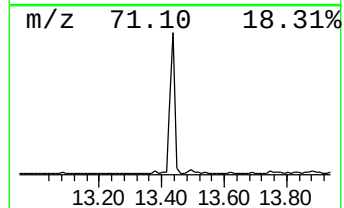
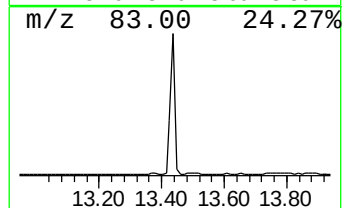
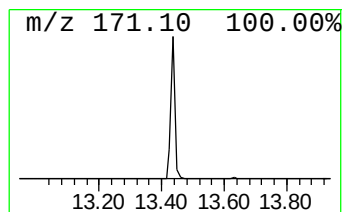
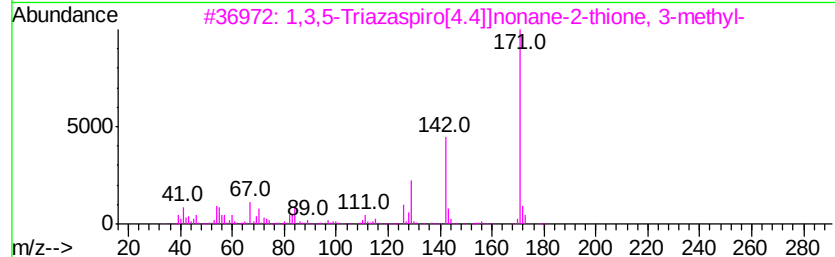
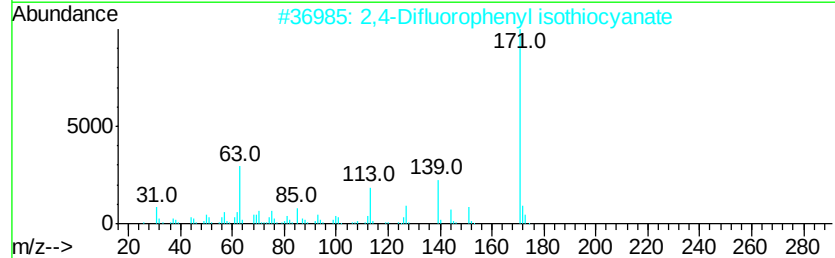
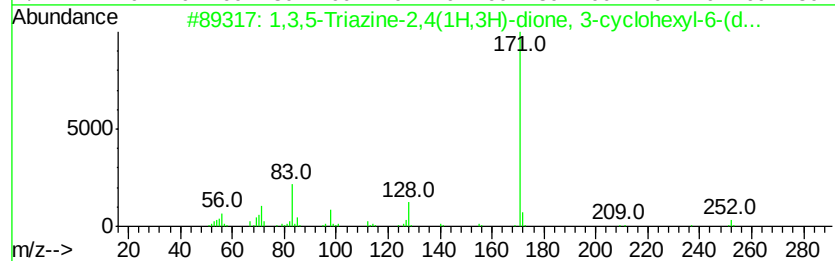
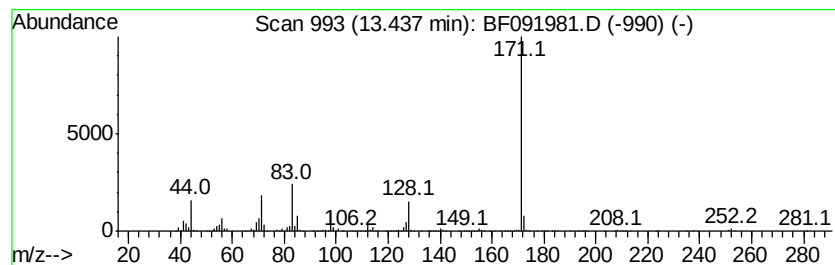
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Peak Number 4 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.44	11.23 ng	886737	Chrysene-d12	13.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	94
2	2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	40
3	1,3,5-Triazaspiro[4.4]nonane-2-...	171	C7H13N3S	1000277-58-6	38
4	Thiazolo[5,4-d]pyrimidine, 5-chl...	171	C5H2ClN3S	013316-08-0	38
5	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FN02	1000116-43-3	28



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	13.5	ng	1048930	1	6.73	1556420	20.0
unknown6.51	6.51	82.6	ng	6429700	1	6.73	1556420	20.0
1,3,5-Triazine-2,...	13.44	11.2	ng	886737	5	13.89	1579780	20.0