

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062718\
 Data File : BF106893.D
 Acq On : 28 Jun 2018 1:36
 Operator : JU/SJ
 Sample : J3693-04
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-12

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-BF061918.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	5.184	481	484	494	rBB	27643	32058	2.86%	0.360%
2	5.590	550	553	566	rVB	525660	488758	43.53%	5.485%
3	6.590	720	723	734	rBB	342622	314683	28.03%	3.532%
4	6.731	743	747	750	rBV	976378	853297	76.00%	9.576%
5	6.954	781	785	788	rBV	299139	234436	20.88%	2.631%
6	7.113	807	812	815	rBV	809980	733751	65.35%	8.235%
7	7.519	876	881	884	rBV	652696	640722	57.06%	7.191%
8	8.236	999	1003	1009	rBV	329878	267335	23.81%	3.000%
9	9.313	1181	1186	1189	rBV	1164102	1045189	93.09%	11.730%
10	9.701	1247	1252	1257	rBV	47238	39389	3.51%	0.442%
11	9.995	1298	1302	1311	rVB2	312644	262952	23.42%	2.951%
12	10.401	1369	1371	1376	rVB	14394	11761	1.05%	0.132%
13	10.666	1410	1416	1419	rBV	526878	667460	59.45%	7.491%
14	10.789	1433	1437	1443	rBV	689269	653454	58.20%	7.334%
15	10.872	1443	1451	1453	rBV	546243	706936	62.96%	7.934%
16	11.489	1552	1556	1559	rBV	315316	255386	22.75%	2.866%
17	12.960	1803	1806	1810	rVB	25538	23374	2.08%	0.262%
18	13.077	1821	1826	1829	rBV	1168874	1122815	100.00%	12.601%
19	13.954	1972	1975	1977	rVB2	20295	19656	1.75%	0.221%
20	14.142	2003	2007	2011	rBV	353075	326760	29.10%	3.667%
21	15.677	2263	2268	2275	rVB	166033	210208	18.72%	2.359%

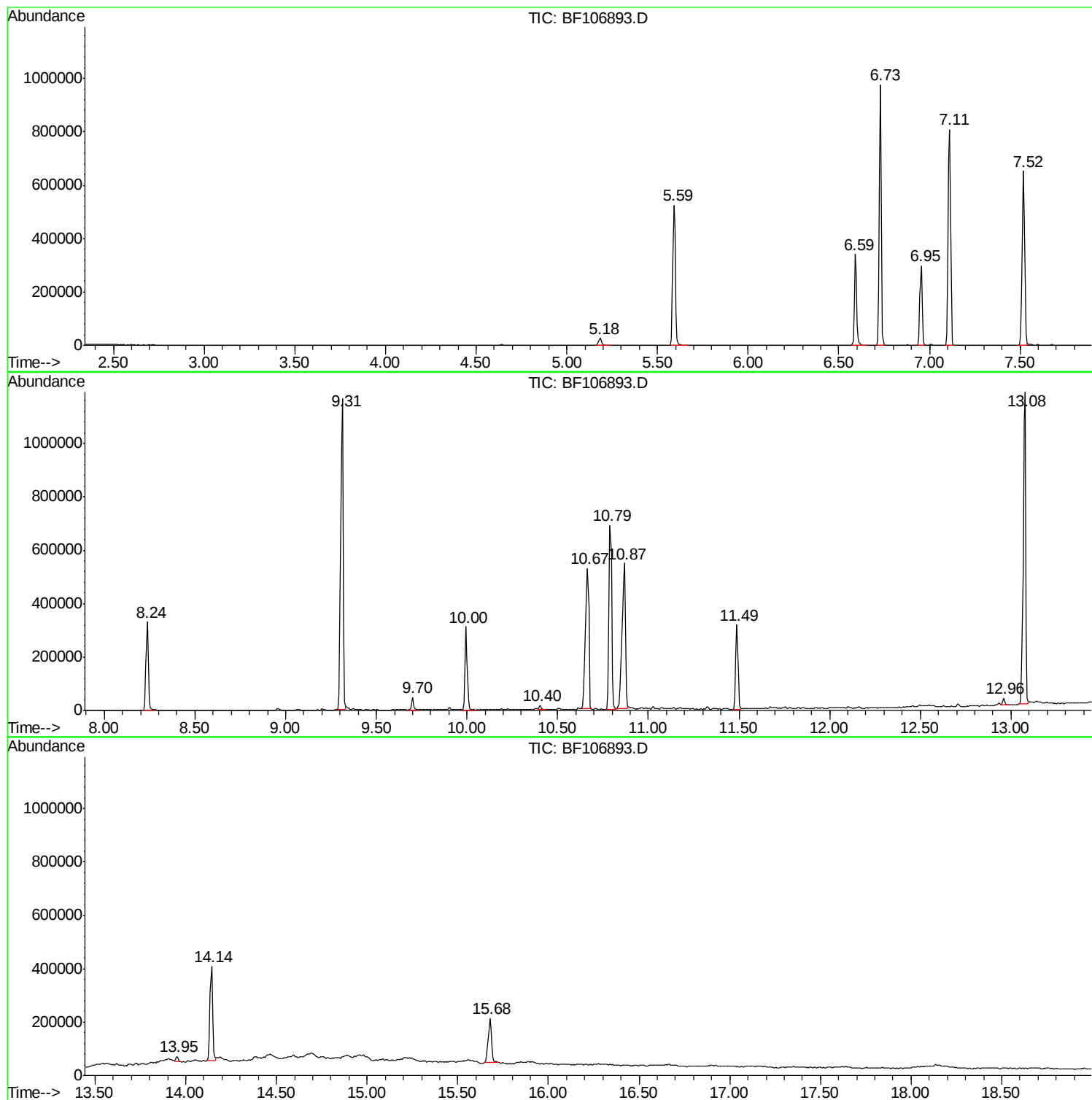
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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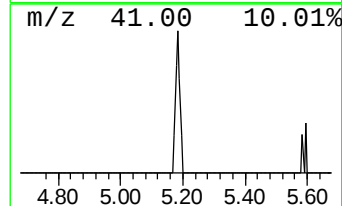
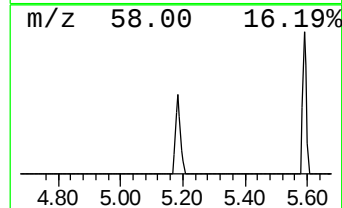
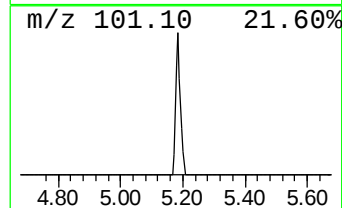
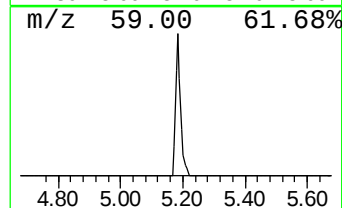
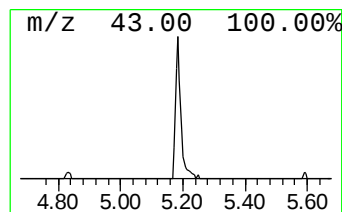
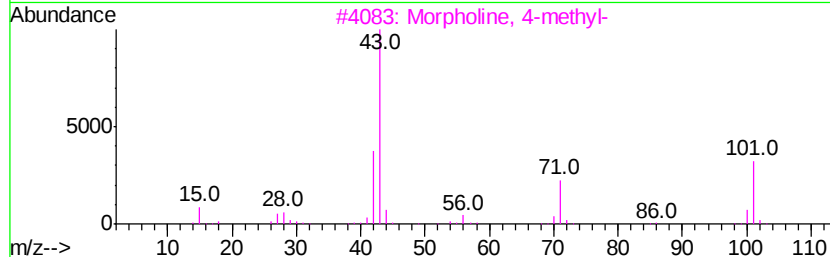
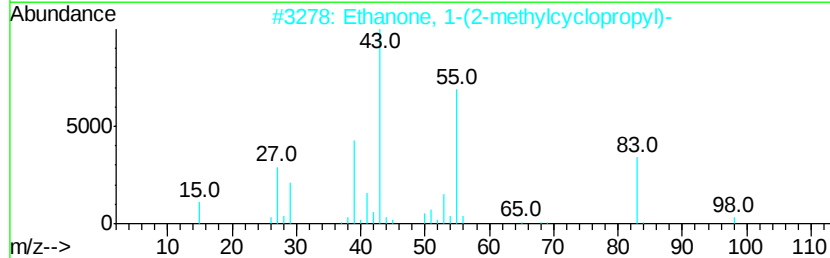
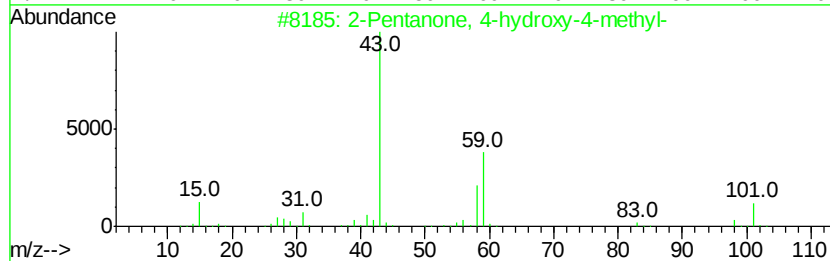
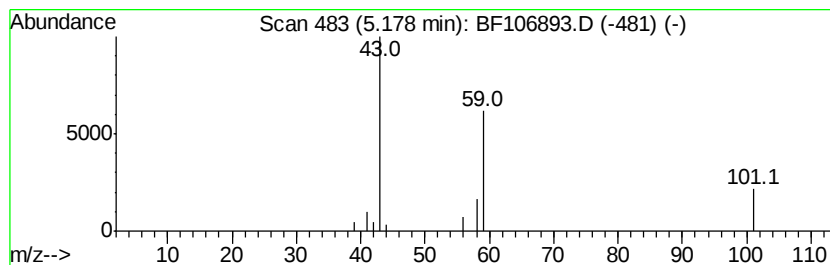
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	2.73 ng	32058	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	5
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	4
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	4



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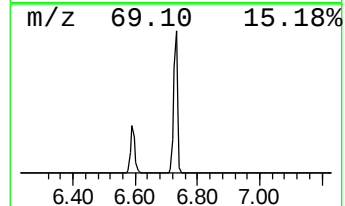
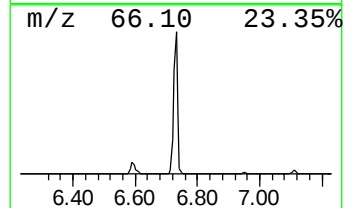
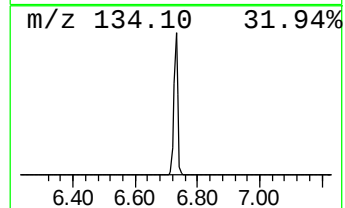
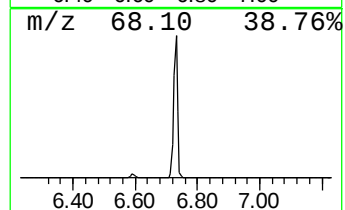
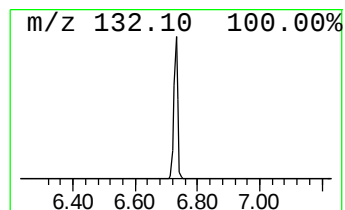
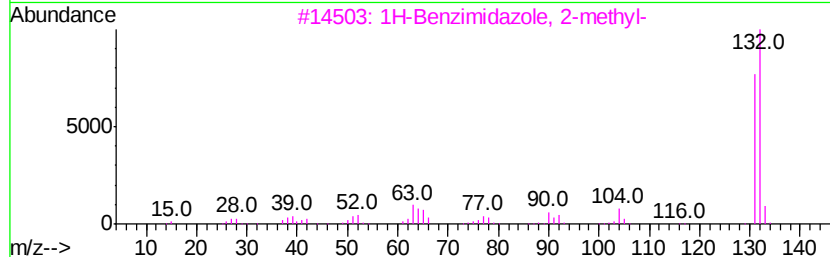
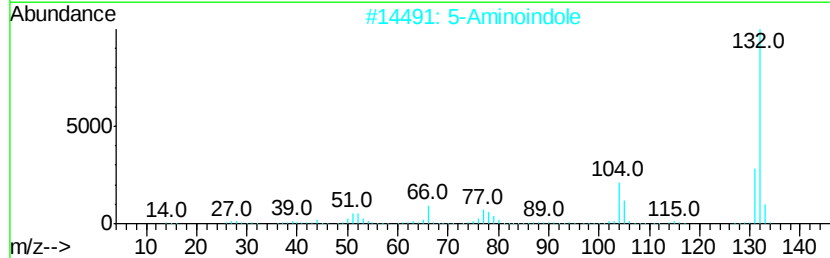
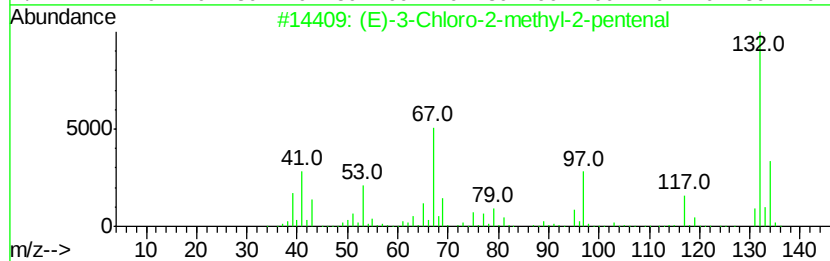
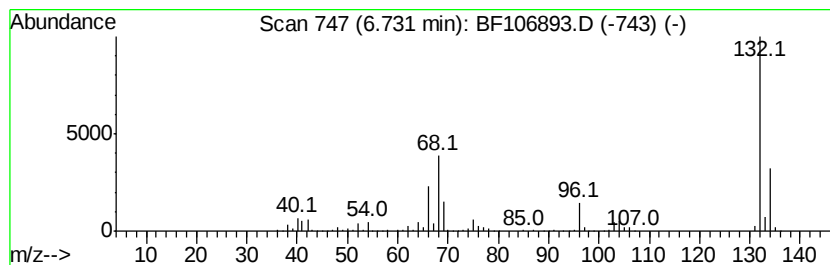
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	72.80 ng	853297	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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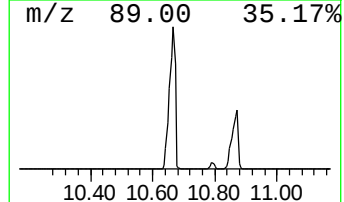
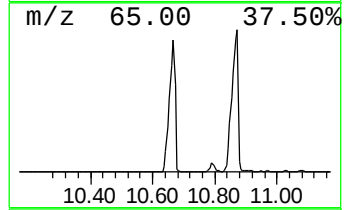
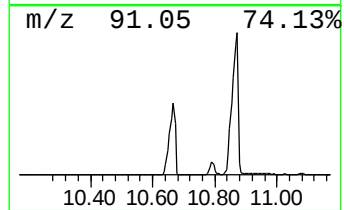
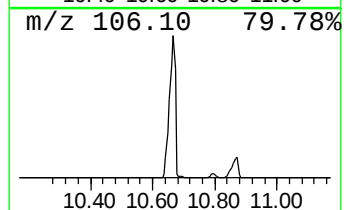
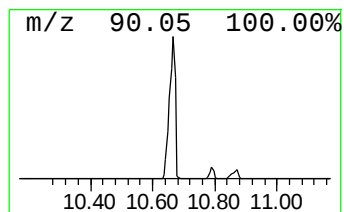
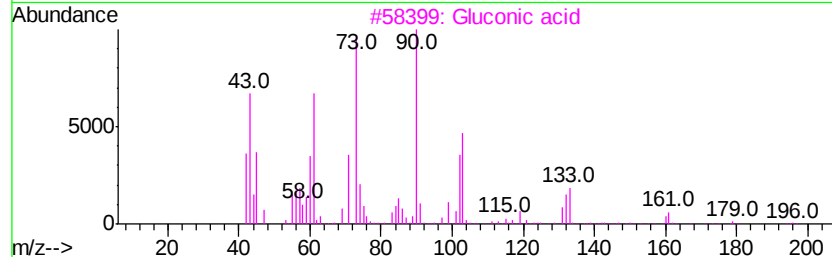
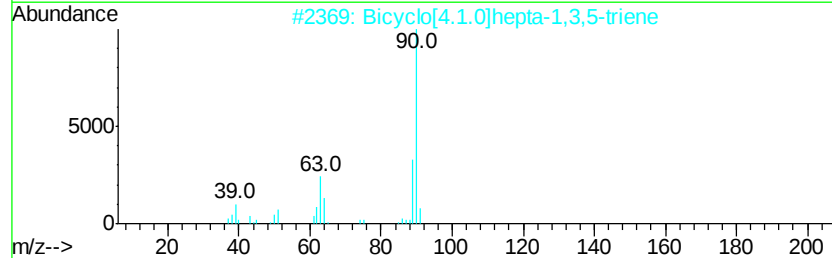
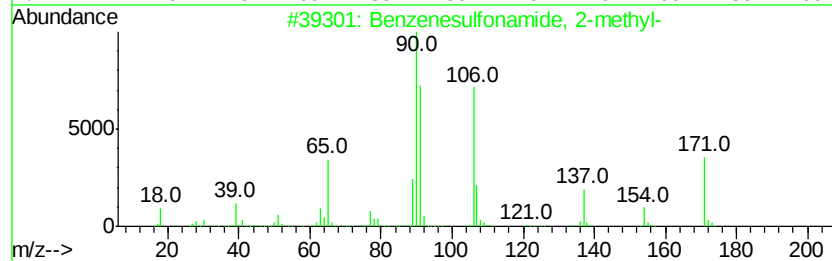
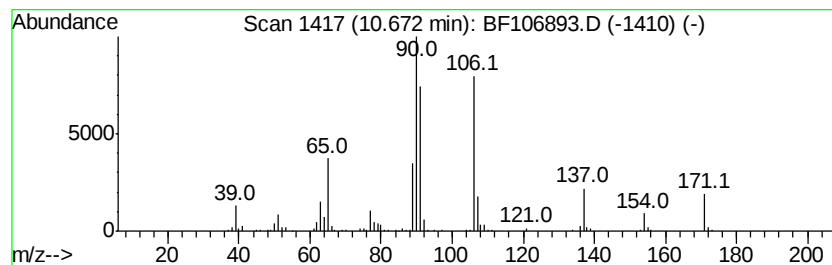
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Peak Number 4 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	50.77 ng	667460	Acenaphthene-d10	10.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	95
2		Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	46
3		Gluconic acid	196	C6H12O7	000526-95-4	38
4		4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	37
5		3,5-Octadiyne	106	C8H10	016387-70-5	27



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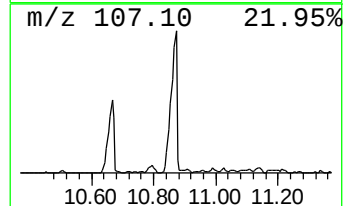
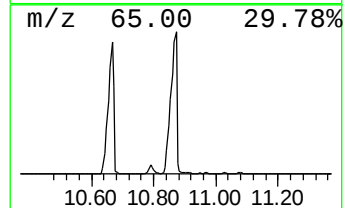
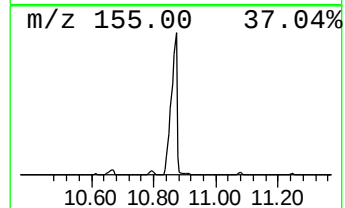
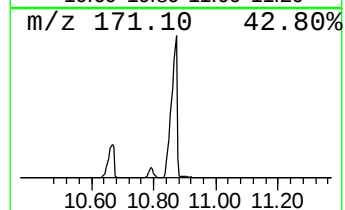
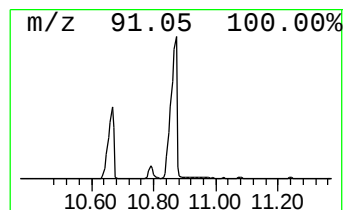
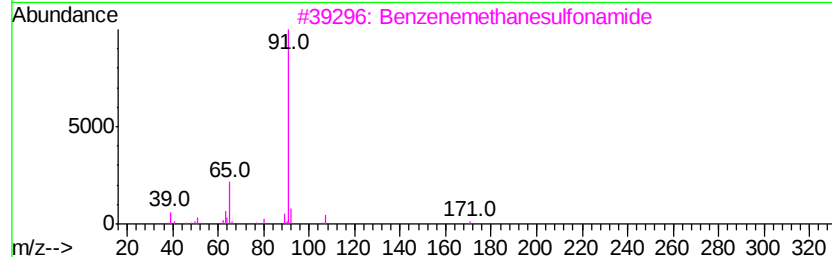
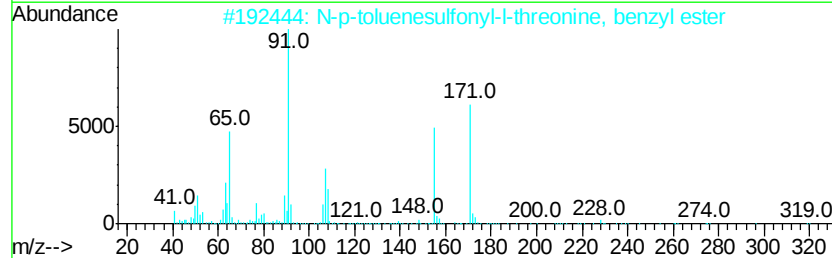
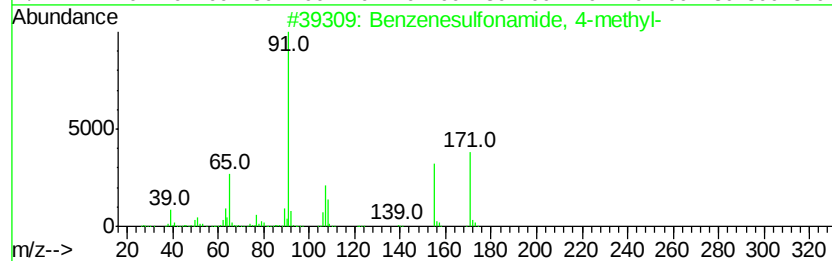
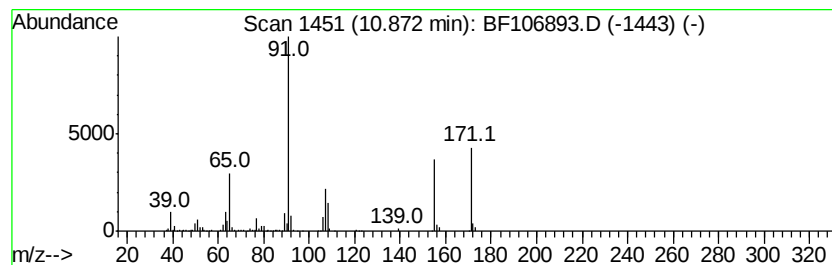
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Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	55.36 ng	706936	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	72
3		Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	50
4		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	35
5		4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	2.7	ng	32058	1	6.95	234436	20.0
unknown6.73	6.73	72.8	ng	853297	1	6.95	234436	20.0
Benzenesulfonamid...	10.67	50.8	ng	667460	3	10.00	262952	20.0
Benzenesulfonamid...	10.87	55.4	ng	706936	4	11.49	255386	20.0