

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
 Data File : BF088163.D
 Acq On : 19 Jun 2016 5:42
 Operator : UM/SJ
 Sample : H3628-08
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-25

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-BF060716.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	1.667	6	7	15	rVB	49207	79550	3.48%	0.465%
2	1.781	15	17	57	rVB	629663	1164494	50.88%	6.808%
3	4.833	281	284	290	rBV	56362	76184	3.33%	0.445%
4	5.279	321	323	326	rBV	1083110	1023129	44.71%	5.981%
5	6.341	413	416	418	rBV	534599	690552	30.17%	4.037%
6	6.456	424	426	428	rBV	1930136	1760706	76.94%	10.293%
7	6.524	431	432	439	rVB	13278	24783	1.08%	0.145%
8	6.684	444	446	448	rBV	626571	521701	22.80%	3.050%
9	6.844	457	460	462	rVB	1732676	1870196	81.72%	10.933%
10	7.256	493	496	498	rBV	1357339	1375631	60.11%	8.042%
11	7.976	556	559	561	rBV	483685	616387	26.93%	3.603%
12	9.050	650	653	656	rBV	2416587	2288559	100.00%	13.379%
13	9.450	686	688	690	rBV	87516	89165	3.90%	0.521%
14	9.725	709	712	713	rBV	495296	589754	25.77%	3.448%
15	9.748	713	714	717	rVB	47782	50977	2.23%	0.298%
16	10.159	748	750	752	rVB	35362	31780	1.39%	0.186%
17	10.376	766	769	773	rBV	97532	94671	4.14%	0.553%
18	10.513	778	781	783	rBV	926812	1113868	48.67%	6.512%
19	10.570	785	786	788	rVV	96047	82968	3.63%	0.485%
20	10.628	790	791	795	rVB	32570	45719	2.00%	0.267%
21	11.073	828	830	836	rVB2	13487	25751	1.13%	0.151%
22	11.199	838	841	843	rBV	620516	519961	22.72%	3.040%
23	12.571	959	961	963	rBV	21066	24642	1.08%	0.144%
24	12.616	963	965	968	rVB2	24724	30212	1.32%	0.177%
25	12.788	977	980	982	rBV	1626698	1960806	85.68%	11.463%
26	13.382	1031	1032	1038	rBV5	15712	23024	1.01%	0.135%
27	13.702	1057	1060	1063	rBV	20004	32907	1.44%	0.192%
28	13.828	1068	1071	1074	rBV	539818	492915	21.54%	2.882%
29	14.457	1124	1126	1131	rBV3	11515	24367	1.06%	0.142%
30	15.211	1189	1192	1197	rVB	324906	380046	16.61%	2.222%

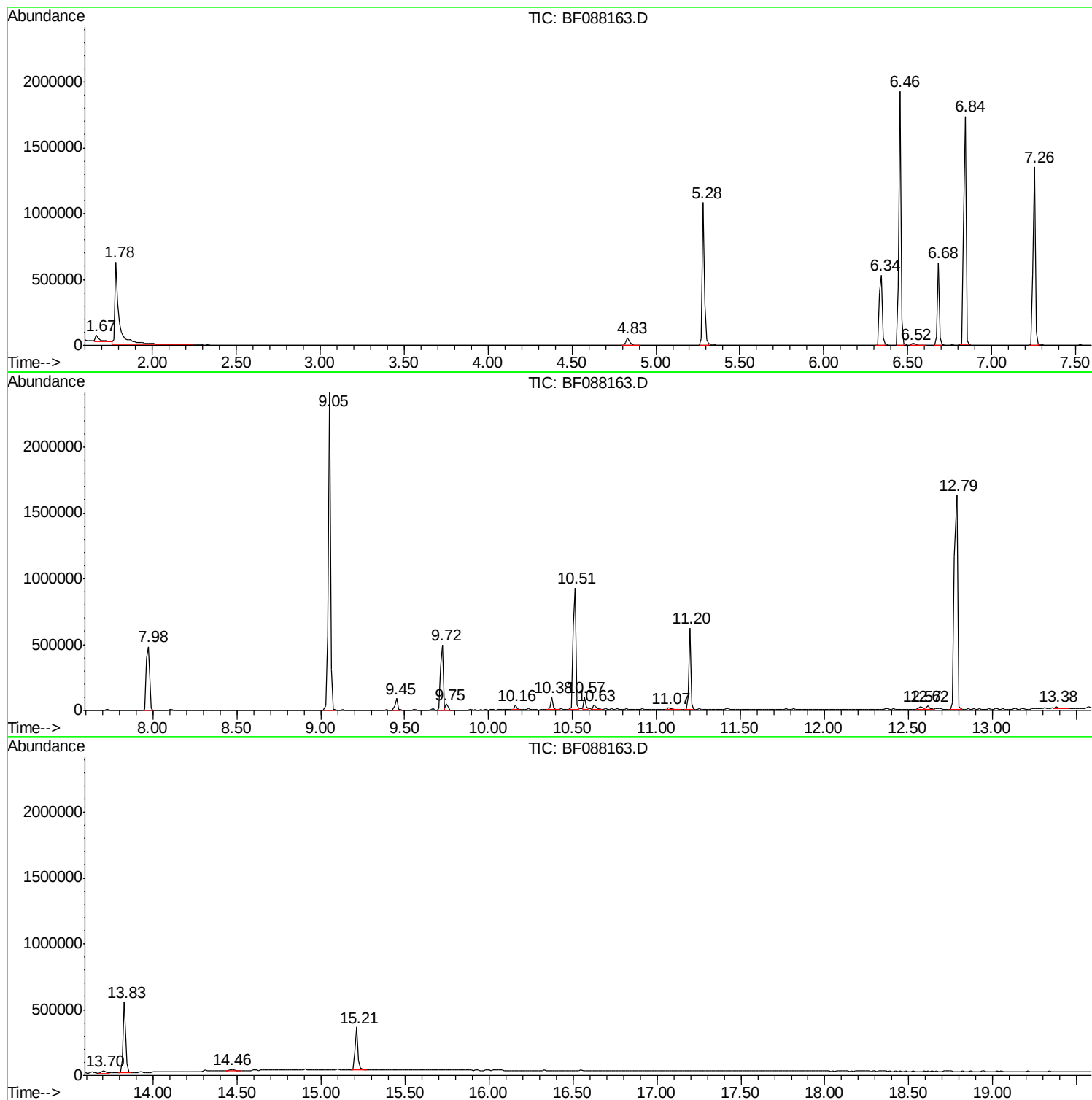
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ClientSampled :
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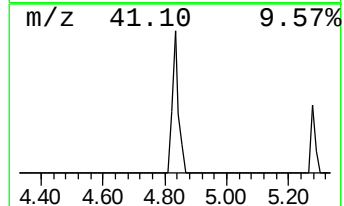
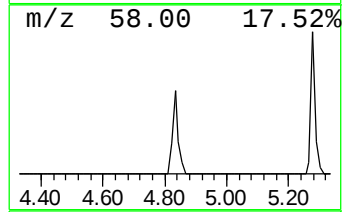
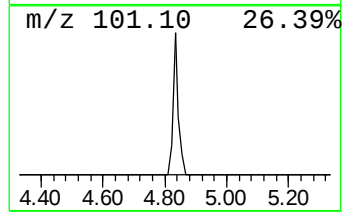
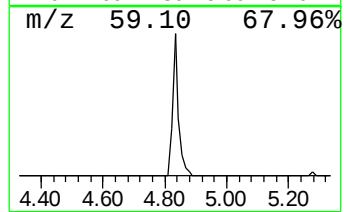
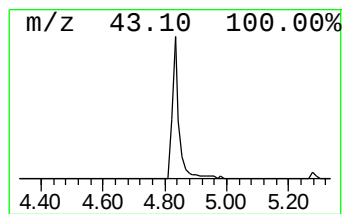
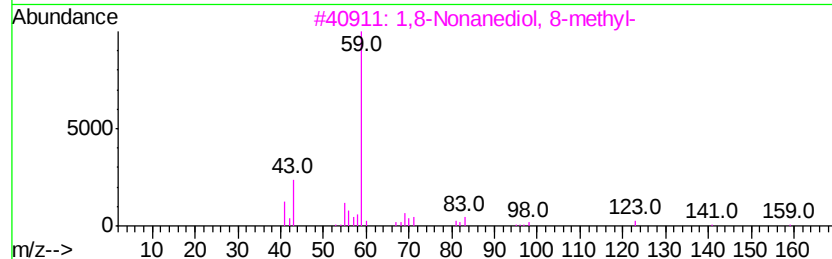
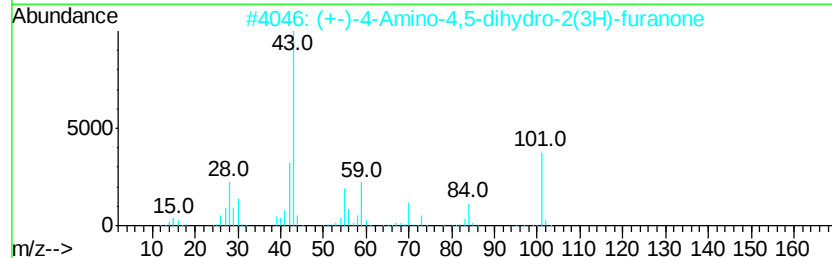
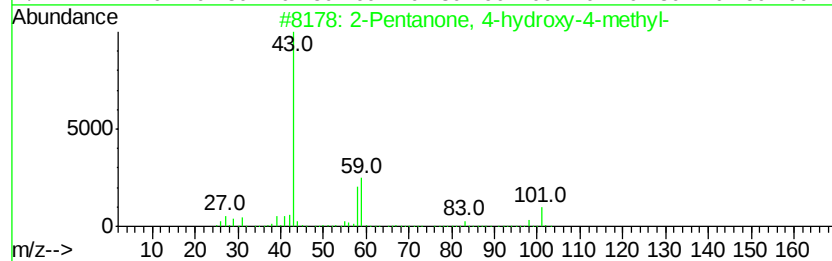
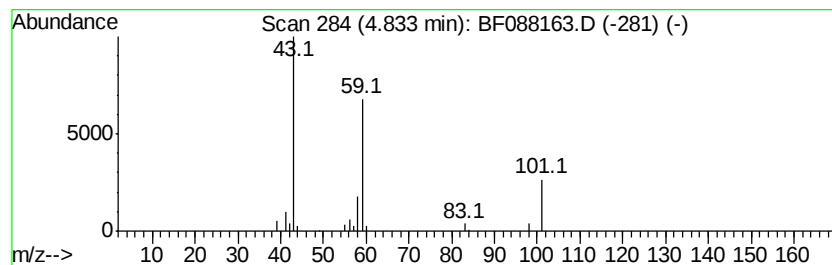
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	2.92 ng	76184	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	25
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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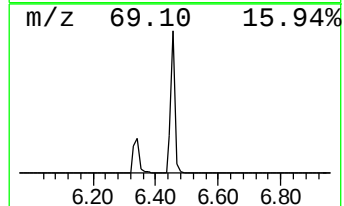
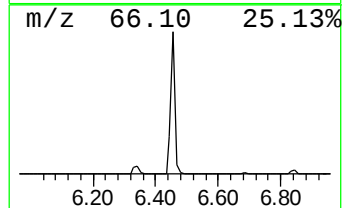
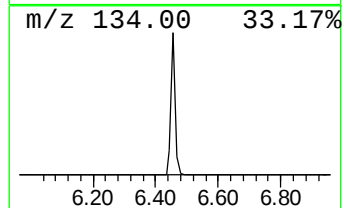
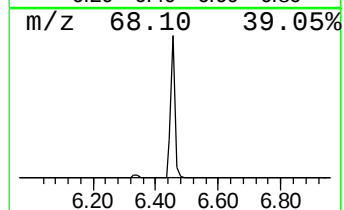
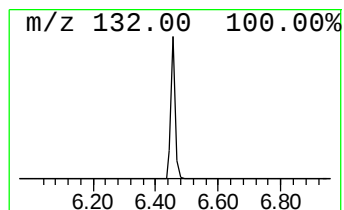
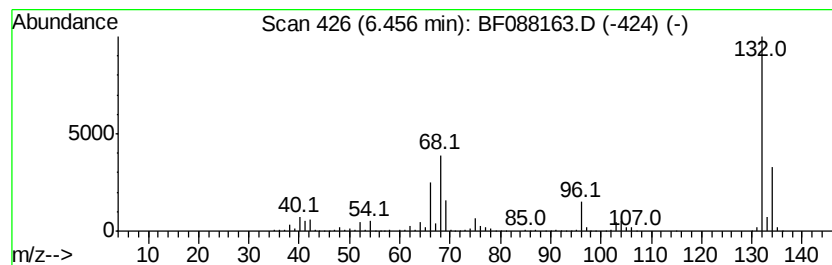
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	67.50 ng	1760710	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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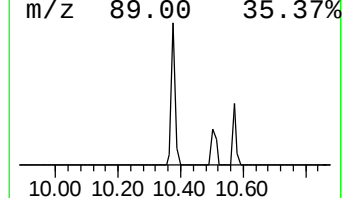
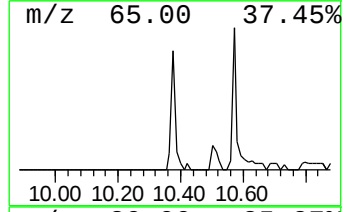
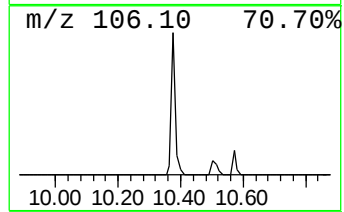
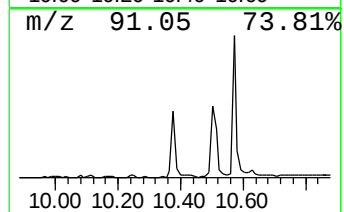
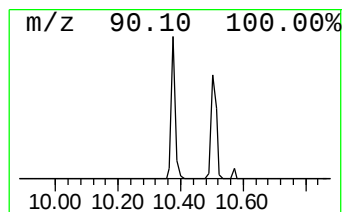
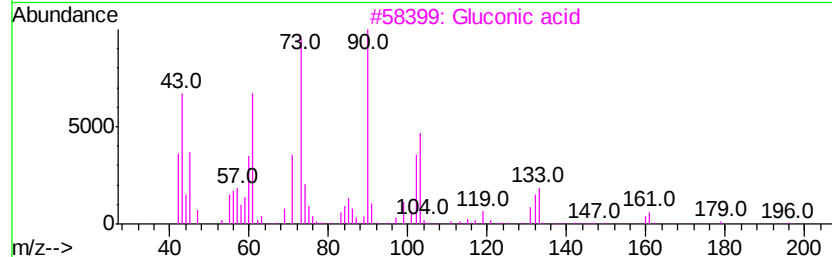
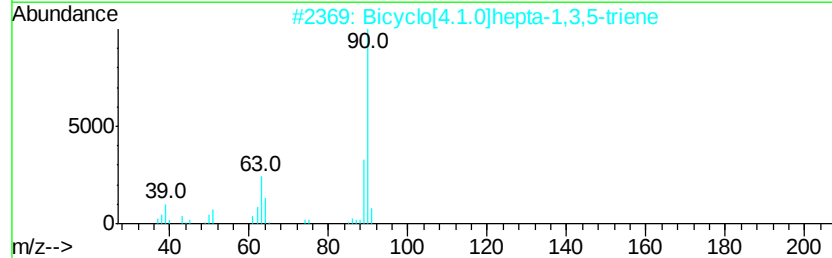
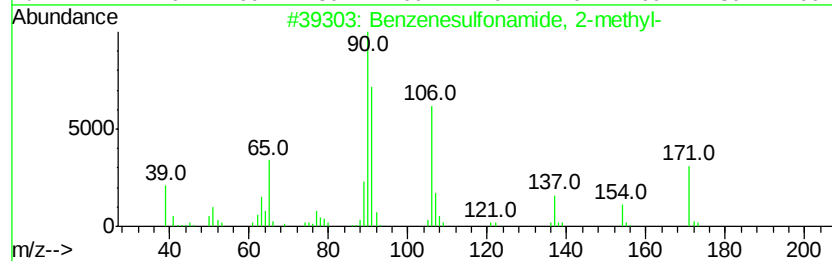
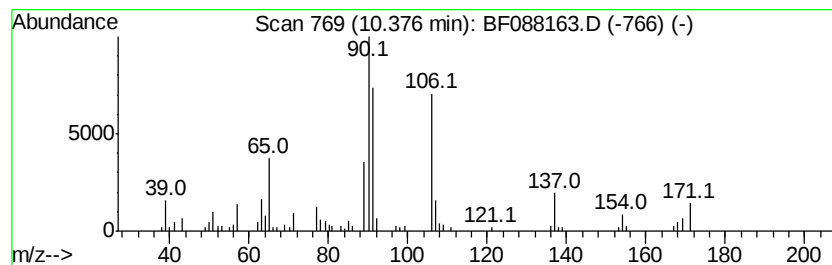
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Peak Number 6 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	3.21 ng	94671	Acenaphthene-d10	9.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	93
2		Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	53
3		Gluconic acid	196	C6H12O7	000526-95-4	50
4		4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	38
5		Formic acid, phenylmethyl ester	136	C8H8O2	000104-57-4	9



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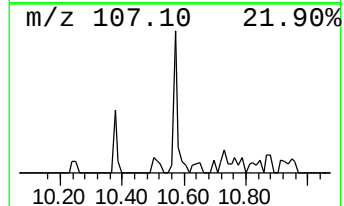
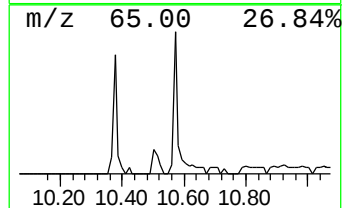
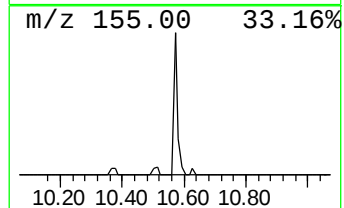
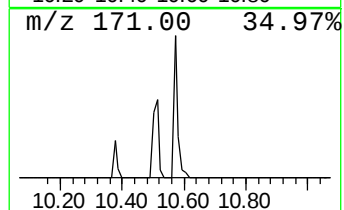
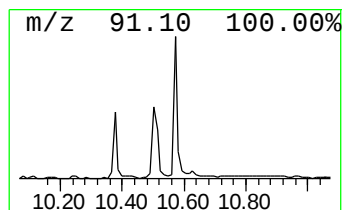
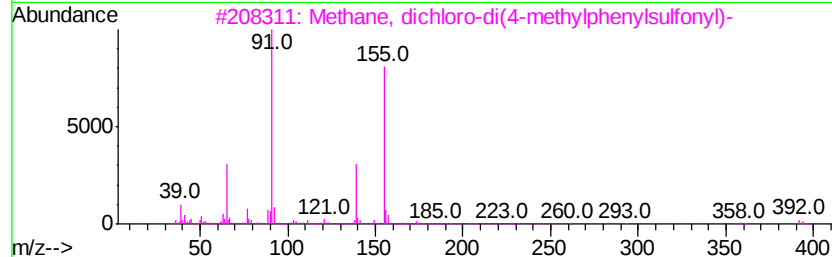
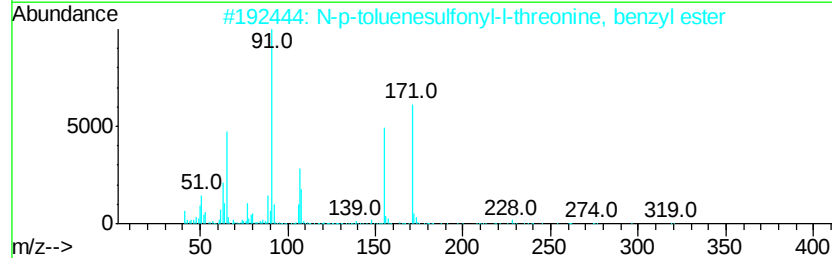
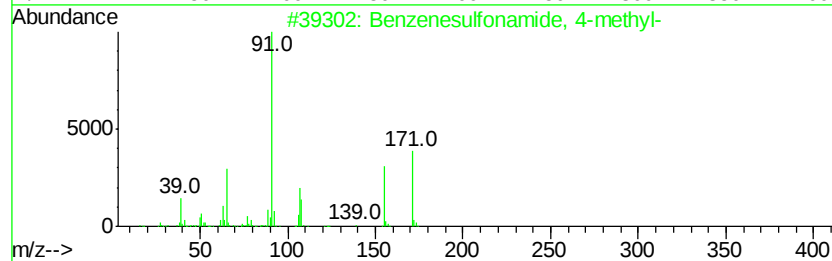
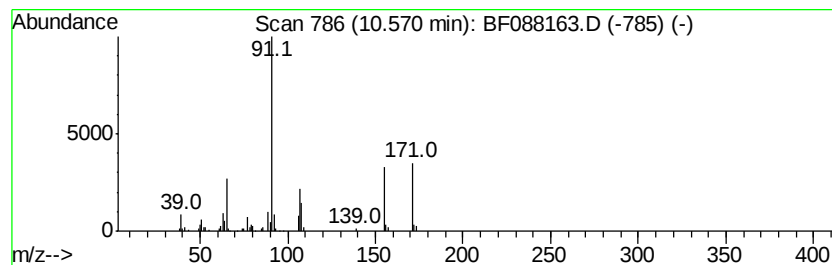
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Peak Number 7 Benzenesulfonamide, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	3.19 ng	82968	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	68
3		Methane, dichloro-di(4-methylphe...	392	C15H14Cl2O4S2	018087-01-9	43
4		(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	43
5		4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	2.9	ng	76184	1	6.68	521701	20.0
unknown6.46	6.46	67.5	ng	1760710	1	6.68	521701	20.0
Benzenesulfonamid...	10.38	3.2	ng	94671	3	9.72	589754	20.0
Benzenesulfonamid...	10.57	3.2	ng	82968	4	11.20	519961	20.0