

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062818\
 Data File : BF106954.D
 Acq On : 29 Jun 2018 6:42
 Operator : JU/SJ
 Sample : J3693-03
 Misc :
 ALS Vial : 29 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:\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	493	rBV	55404	62702	3.34%	0.505%
2	5.589	549	553	567	rBV	900694	787167	41.96%	6.340%
3	6.589	719	723	734	rBV	535145	481770	25.68%	3.880%
4	6.731	742	747	750	rBV	1438817	1361359	72.57%	10.964%
5	6.954	781	785	788	rBV	449825	390507	20.82%	3.145%
6	7.107	807	811	815	rBV	1363594	1254812	66.89%	10.106%
7	7.519	876	881	884	rBV	1136843	1025226	54.66%	8.257%
8	8.236	999	1003	1021	rBV	450677	431941	23.03%	3.479%
9	9.307	1181	1185	1188	rBV	1819740	1619281	86.32%	13.042%
10	9.701	1246	1252	1257	rBB	36731	37812	2.02%	0.305%
11	9.989	1298	1301	1305	rBV	404146	395005	21.06%	3.181%
12	10.024	1305	1307	1311	rVB	43811	35047	1.87%	0.282%
13	10.642	1409	1412	1417	rVB	101062	86662	4.62%	0.698%
14	10.783	1432	1436	1443	rBV	970635	930694	49.62%	7.496%
15	10.842	1443	1446	1450	rVV	88372	85668	4.57%	0.690%
16	11.483	1552	1555	1563	rVB	474145	385738	20.56%	3.107%
17	13.071	1820	1825	1828	rBV	1992429	1875813	100.00%	15.108%
18	13.677	1924	1928	1934	rBV	34492	37497	2.00%	0.302%
19	13.948	1970	1974	1983	rBV	55723	72846	3.88%	0.587%
20	14.136	2002	2006	2013	rBV	665294	572334	30.51%	4.610%
21	14.736	2105	2108	2115	rVB5	12966	21399	1.14%	0.172%
22	15.671	2261	2267	2275	rVB	352218	464833	24.78%	3.744%

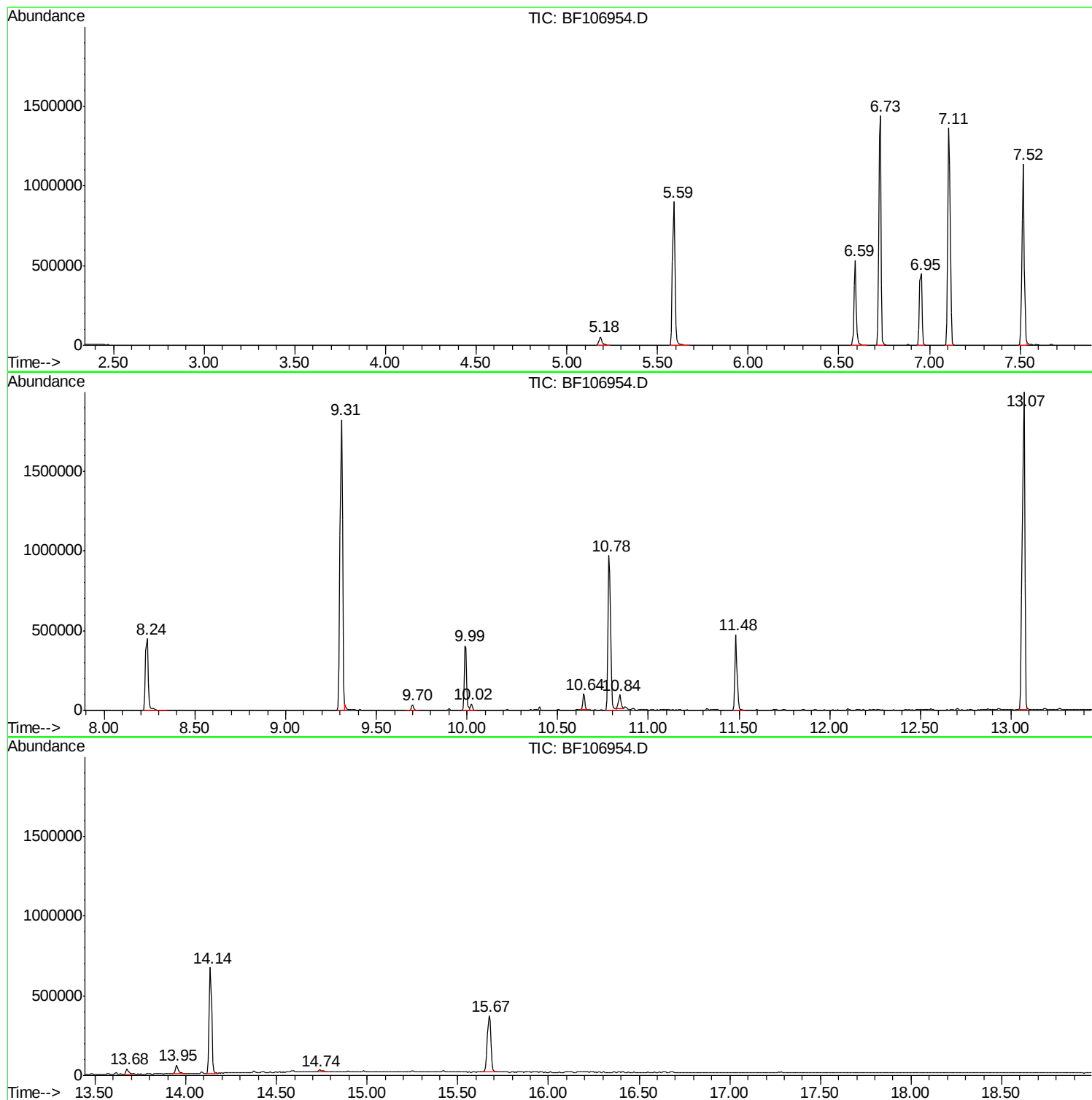
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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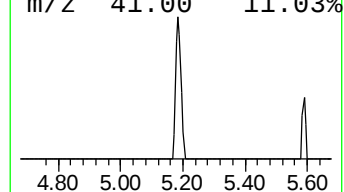
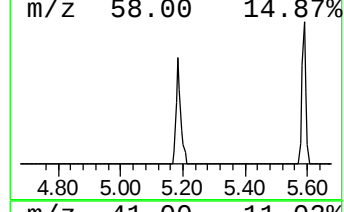
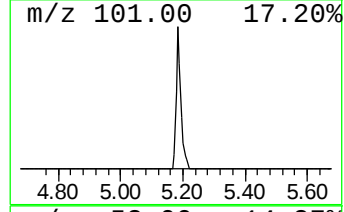
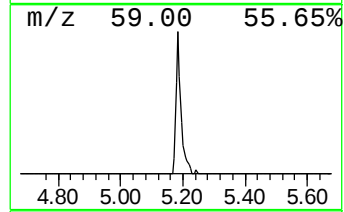
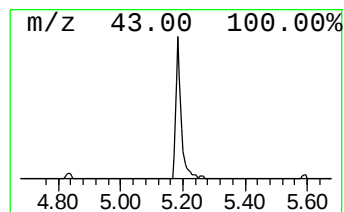
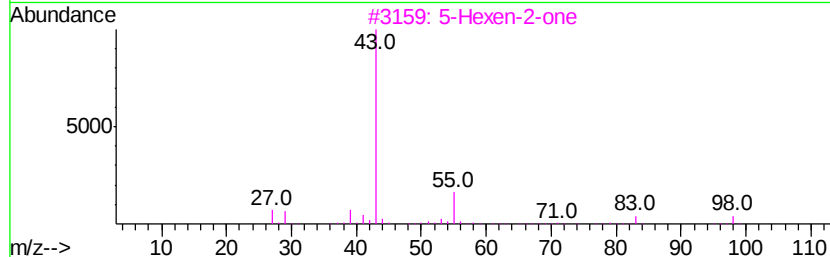
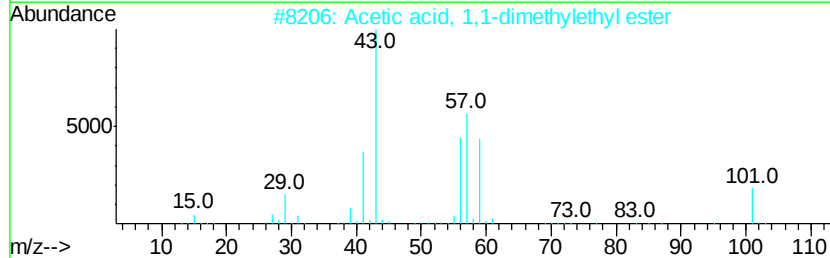
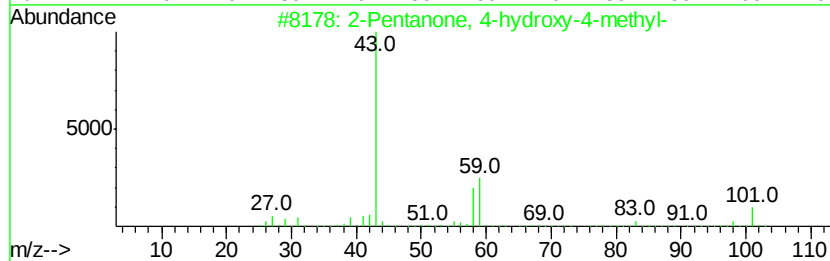
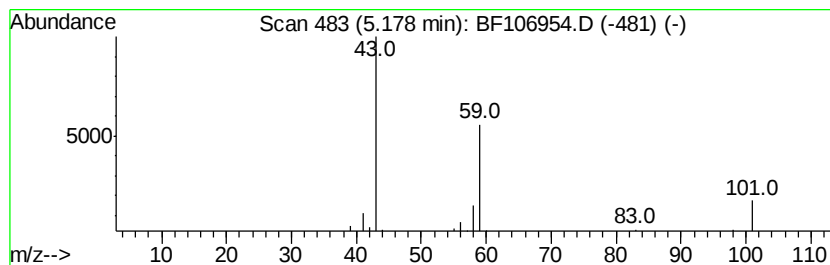
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.21 ng	62702	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	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Acetone	58	C3H6O	000067-64-1	9
5			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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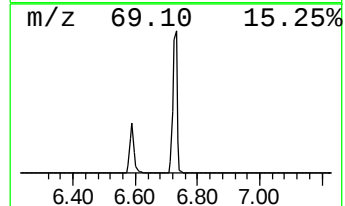
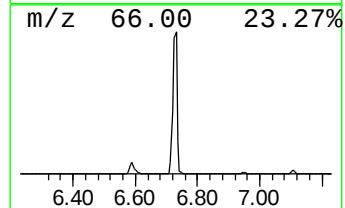
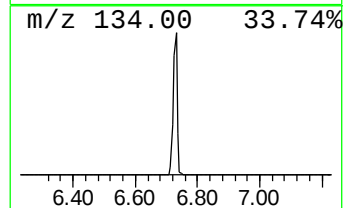
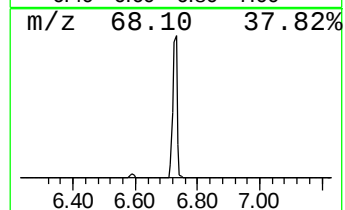
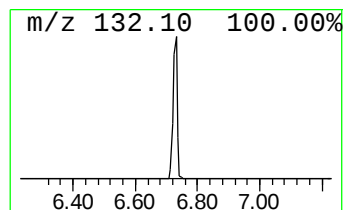
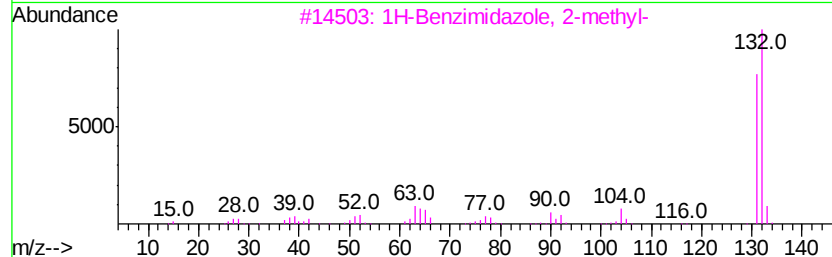
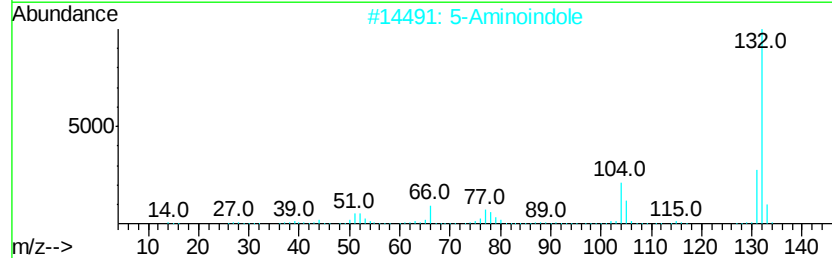
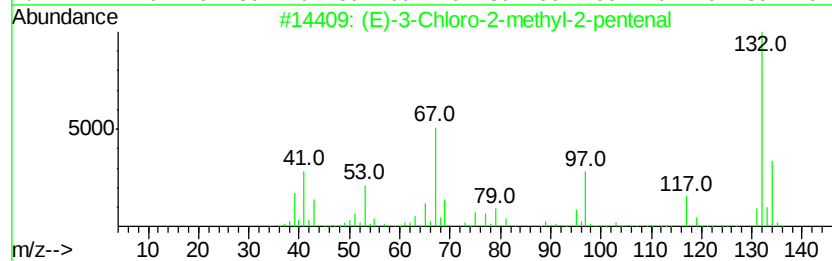
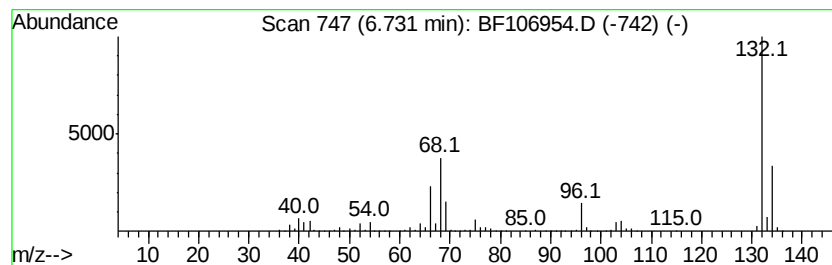
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	69.72 ng	1361360	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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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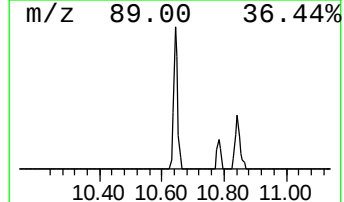
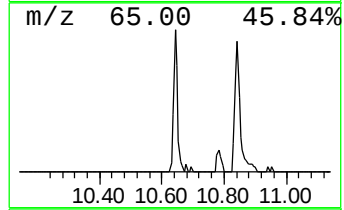
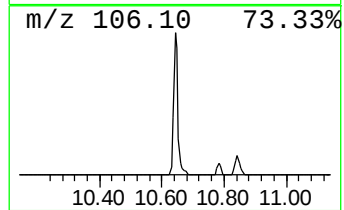
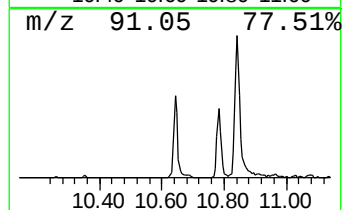
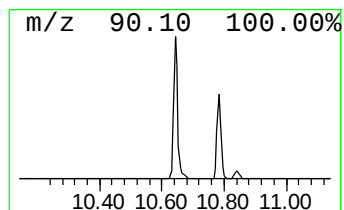
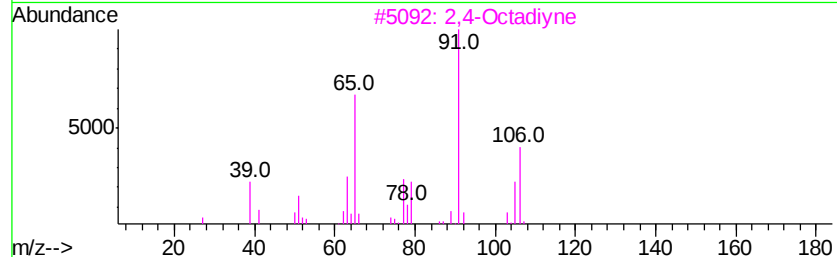
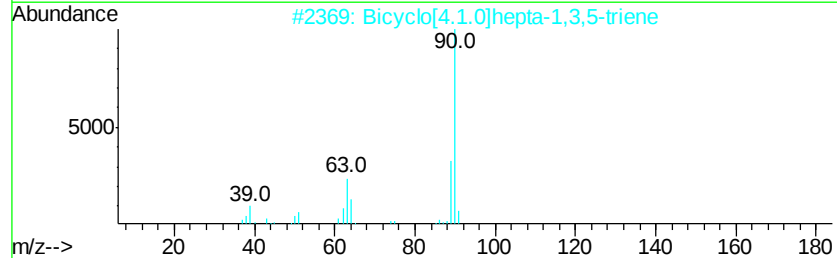
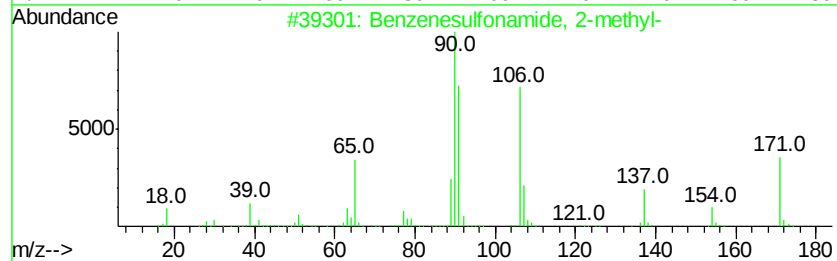
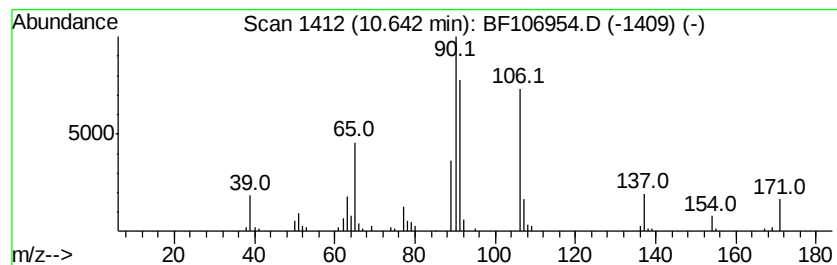
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Peak Number 4 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	4.39 ng	86662	Acenaphthene-d10	9.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	95
2		Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	43
3		2,4-Octadiyne	106	C8H10	002809-71-4	38
4		Gluconic acid	196	C6H12O7	000526-95-4	38
5		Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	35



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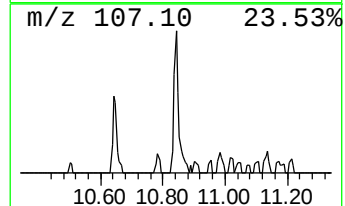
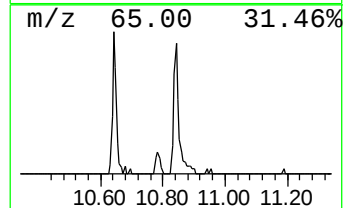
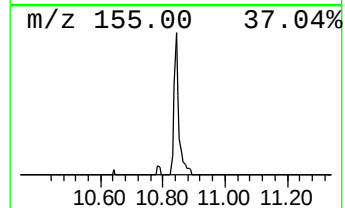
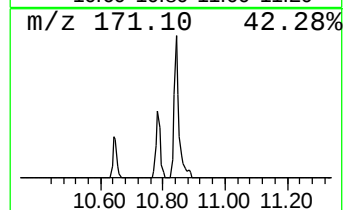
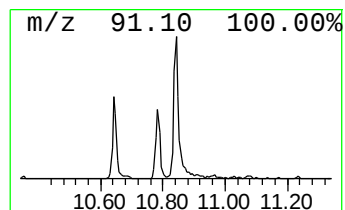
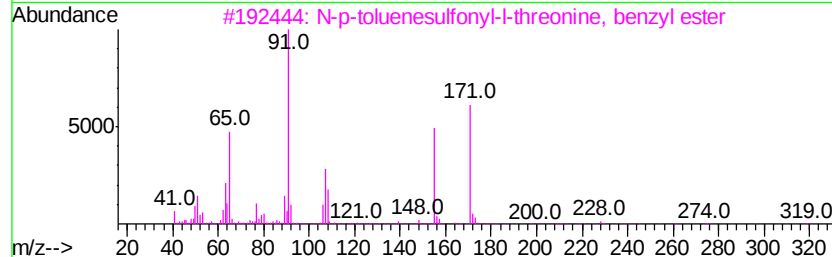
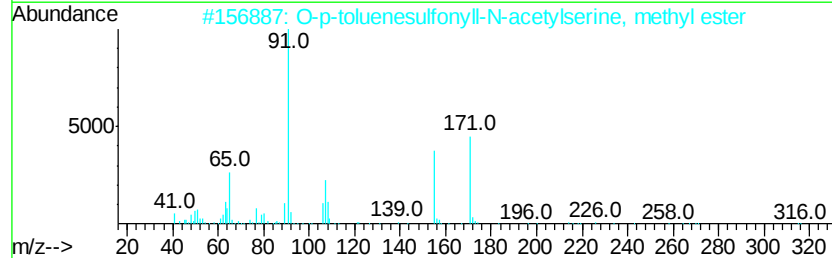
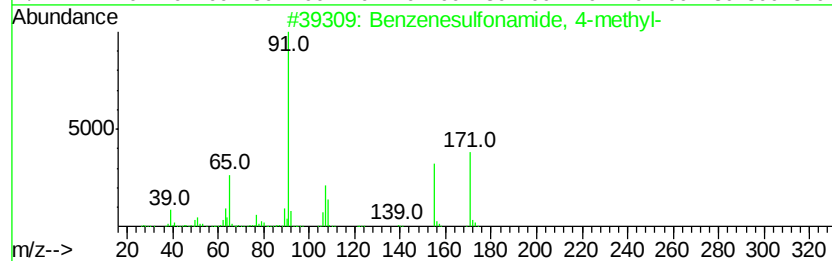
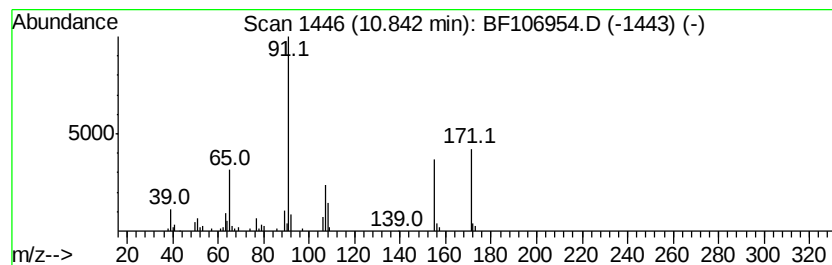
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Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	4.44 ng	85668	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2	O-p-toluenesulfonyl-N-acetylser...	315	C13H17NO6S	1000126-44-8	80
3	N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	64
4	Tolbutamide	270	C12H18N2O3S	000064-77-7	50
5	Thiophene-3-ol, 2,3-dihydro-, 4-...	288	C11H12O5S2	039582-96-2	47



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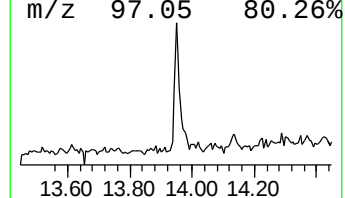
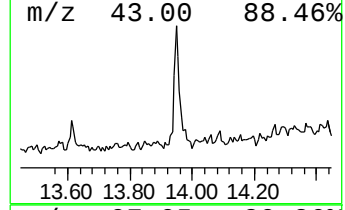
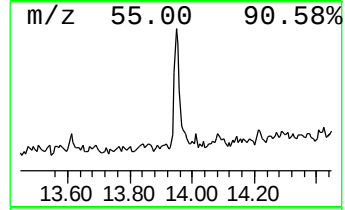
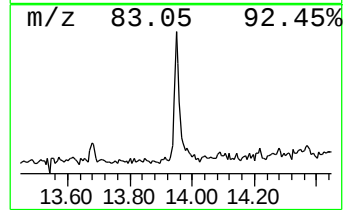
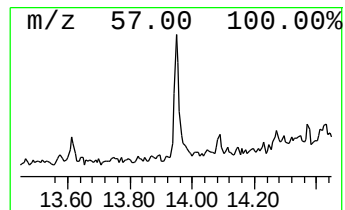
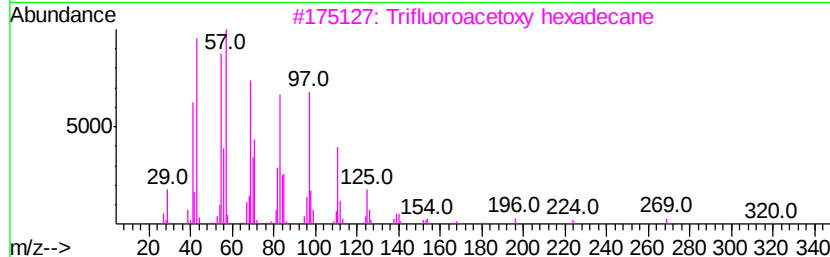
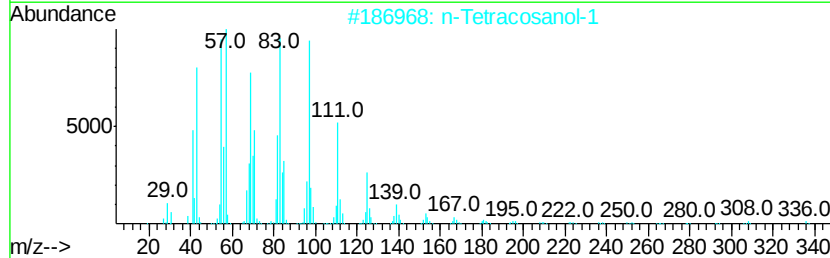
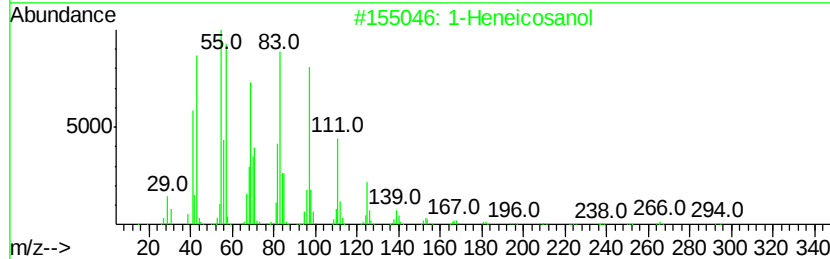
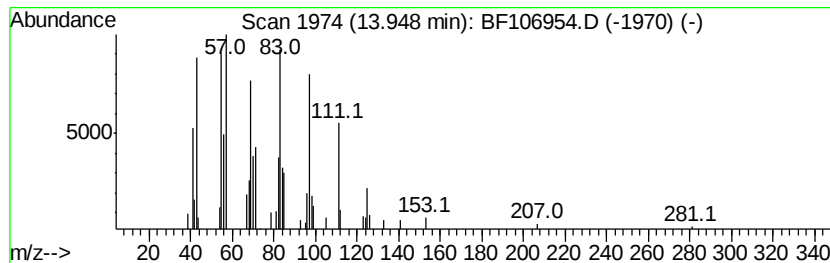
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Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.95	2.55 ng	72846	Chrysene-d12	14.14	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	3.2	ng	62702	1	6.95	390507	20.0
unknown6.73	6.73	69.7	ng	1361360	1	6.95	390507	20.0
Benzenesulfonamid...	10.64	4.4	ng	86662	3	9.99	395005	20.0
Benzenesulfonamid...	10.84	4.4	ng	85668	4	11.48	385738	20.0
1-Heneicosanol	13.95	2.5	ng	72846	5	14.14	572334	20.0