

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120517\
 Data File : BF101146.D
 Acq On : 6 Dec 2017 1:59
 Operator : SJ/JU
 Sample : I6702-05
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-3-E(4-5)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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	5.087	506	510	522	rBV	51194	75045	5.73%	0.683%
2	5.475	571	576	579	rBV	1169988	1160690	88.55%	10.562%
3	6.481	742	747	760	rBV	1110547	1216054	92.78%	11.066%
4	6.616	766	770	774	rBV	1274675	1235598	94.27%	11.244%
5	6.845	806	809	813	rBV	392121	302804	23.10%	2.756%
6	7.004	832	836	839	rBV	1107799	956876	73.00%	8.708%
7	7.416	900	906	909	rBV	708797	741942	56.61%	6.752%
8	8.128	1023	1027	1036	rBV	478416	392508	29.95%	3.572%
9	9.204	1205	1210	1213	rBV	1571078	1310735	100.00%	11.928%
10	9.598	1273	1277	1284	rVB	121900	120321	9.18%	1.095%
11	9.804	1309	1312	1316	rBV	40261	31658	2.42%	0.288%
12	9.886	1321	1326	1334	rVB	453124	427153	32.59%	3.887%
13	10.304	1393	1397	1400	rVB	41795	31795	2.43%	0.289%
14	10.675	1456	1460	1470	rVV	849061	788527	60.16%	7.176%
15	10.775	1474	1477	1486	rVB	27128	27182	2.07%	0.247%
16	11.375	1575	1579	1582	rBV	470862	403602	30.79%	3.673%
17	11.886	1664	1666	1672	rBV2	23383	22395	1.71%	0.204%
18	12.957	1844	1848	1851	rBV	1167623	980862	74.83%	8.926%
19	13.839	1995	1998	2009	rBV	118601	129954	9.91%	1.183%
20	14.016	2025	2028	2035	rVB	314864	268029	20.45%	2.439%
21	14.474	2100	2106	2111	rBV2	12260	17695	1.35%	0.161%
22	15.492	2274	2279	2291	rVB	216979	281778	21.50%	2.564%
23	15.839	2331	2338	2342	rBV4	19435	34343	2.62%	0.313%
24	15.974	2355	2361	2368	rBV4	15740	31336	2.39%	0.285%

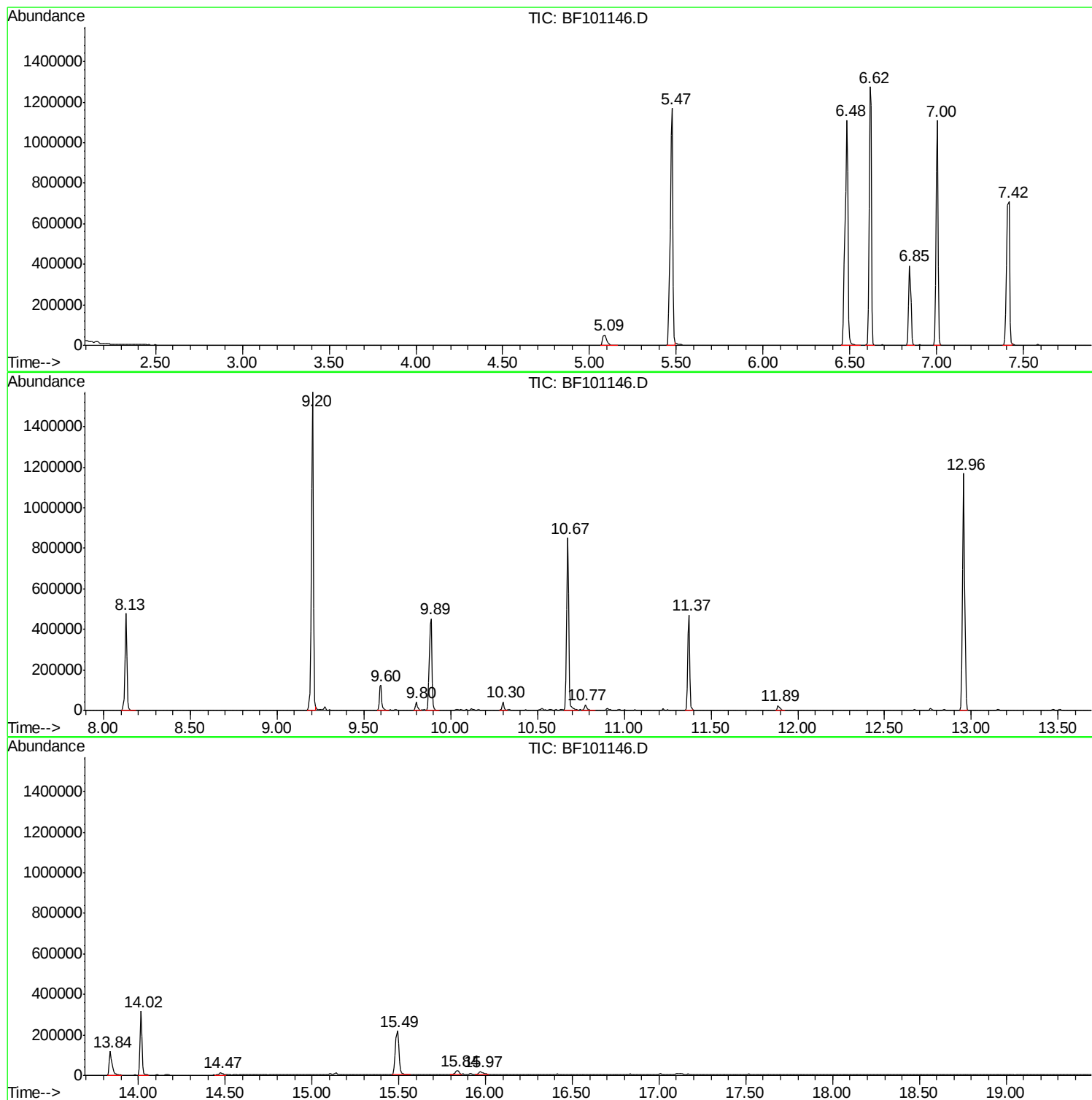
Sum of corrected areas: 10988882

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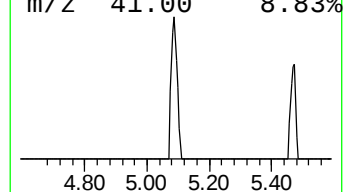
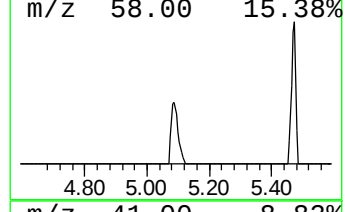
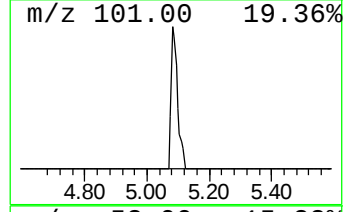
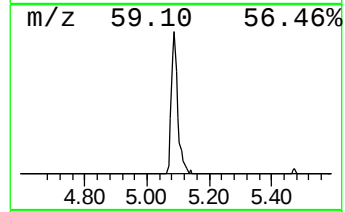
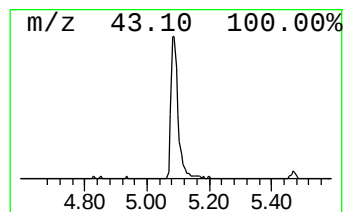
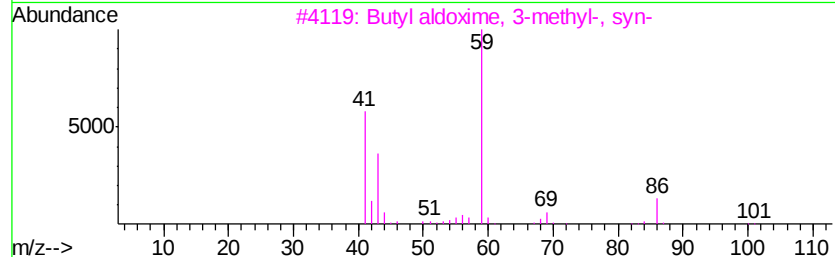
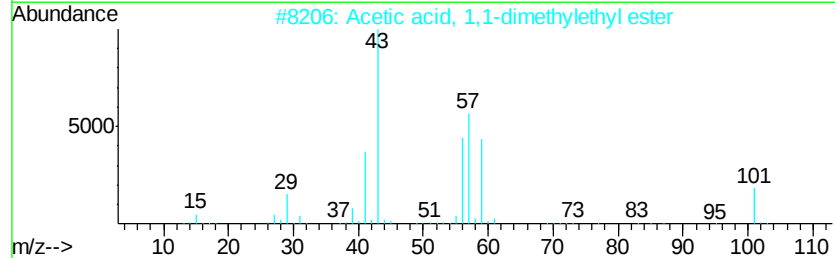
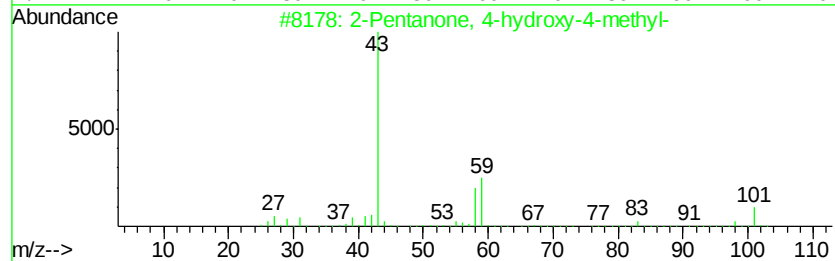
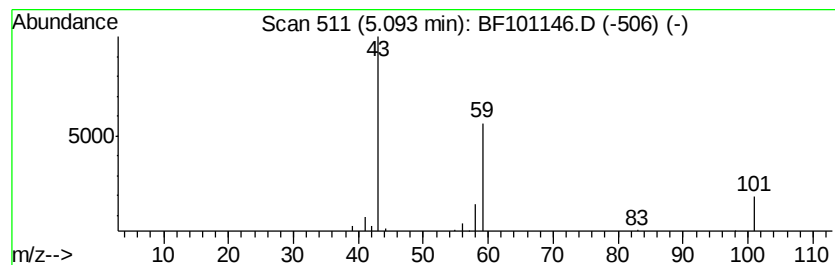
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.96 ng	75045	1,4-Dichlorobenzene-d4	6.85

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	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32	
4	3-Hexanol	102	C6H14O	000623-37-0	28	
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28	



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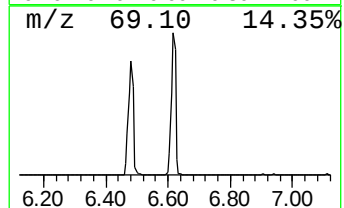
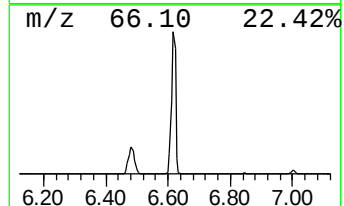
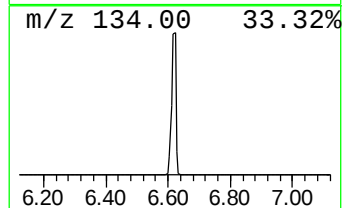
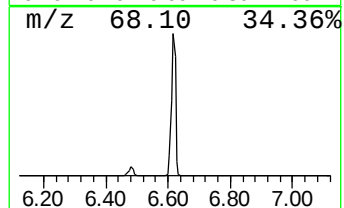
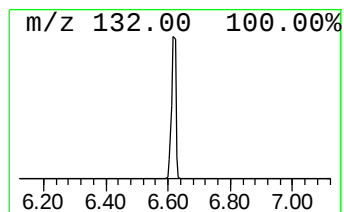
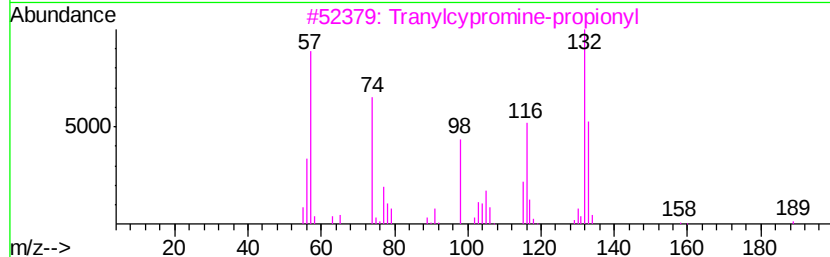
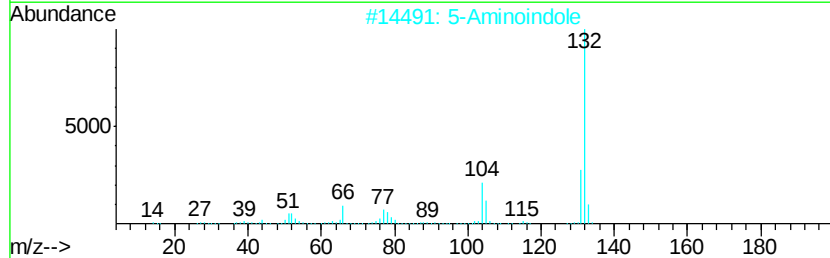
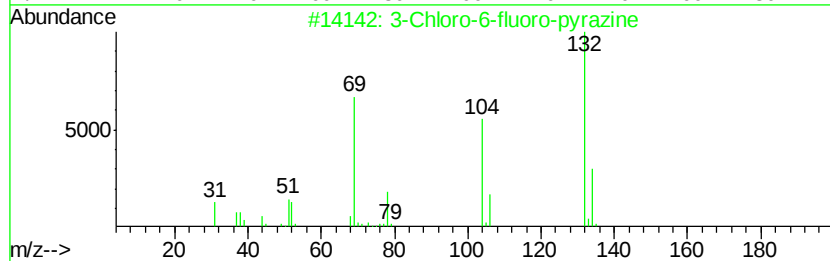
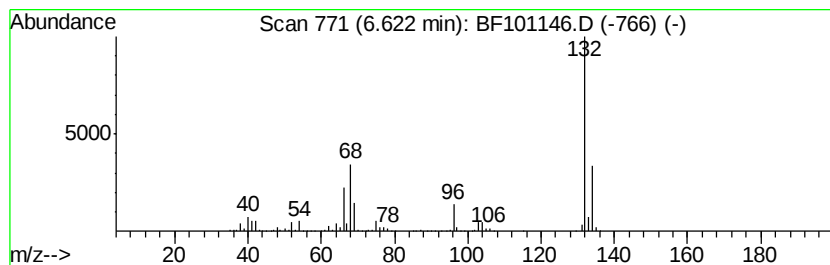
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	81.61 ng	1235600	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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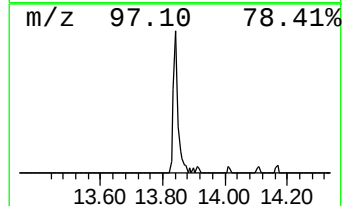
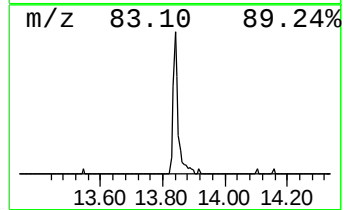
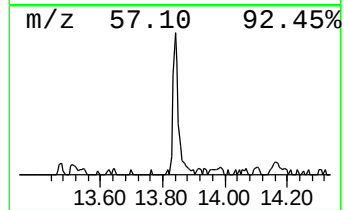
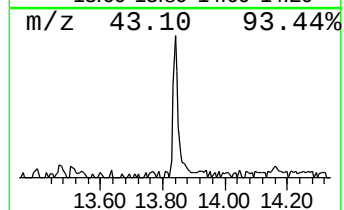
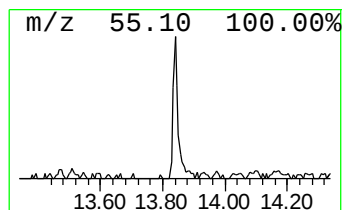
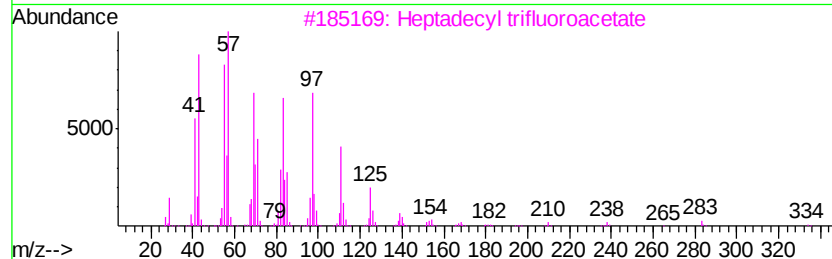
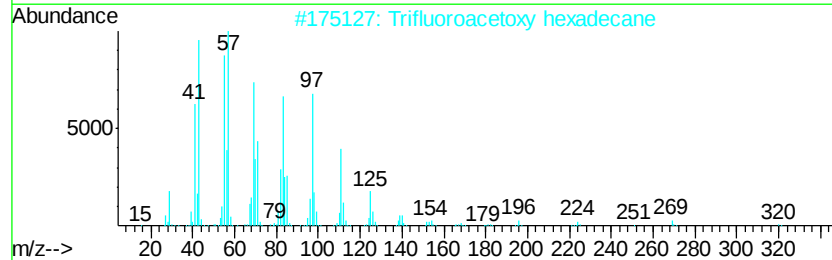
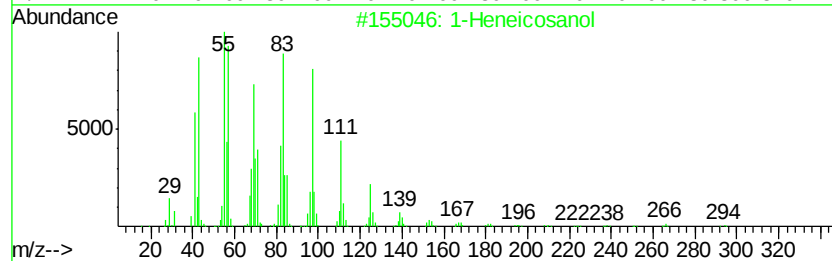
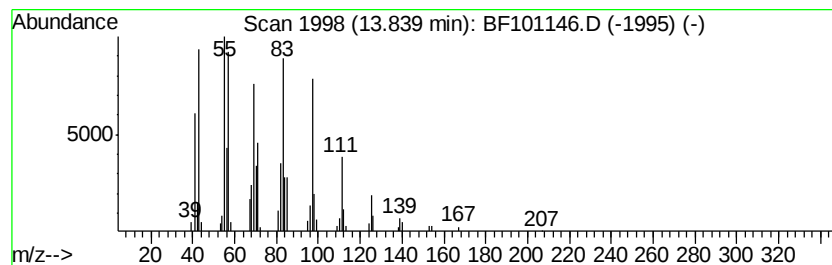
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	9.70 ng	129954	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	92



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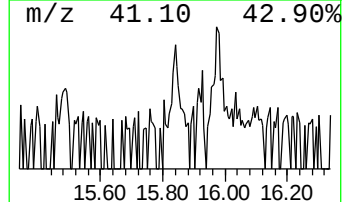
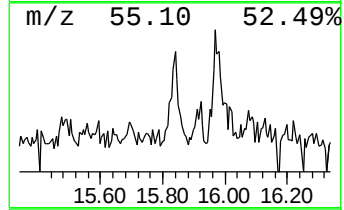
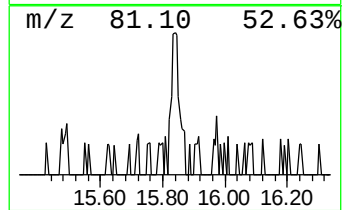
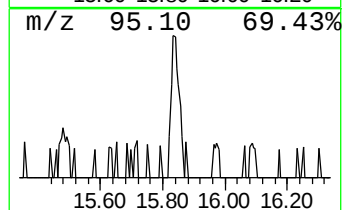
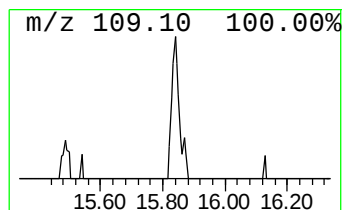
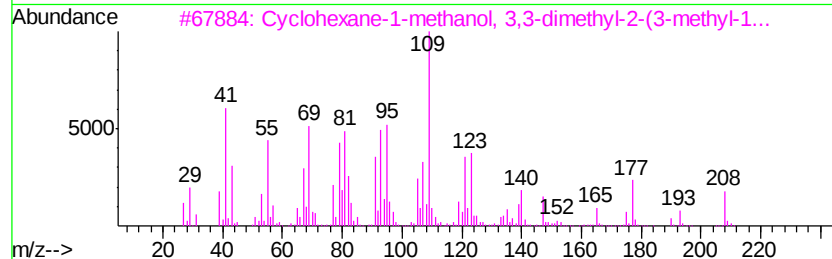
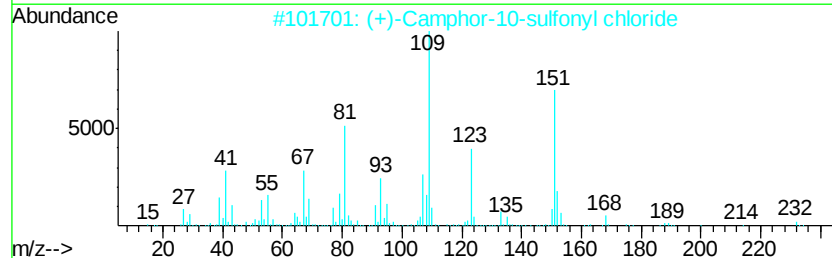
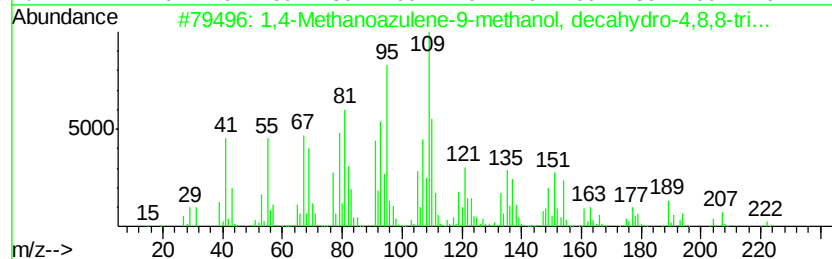
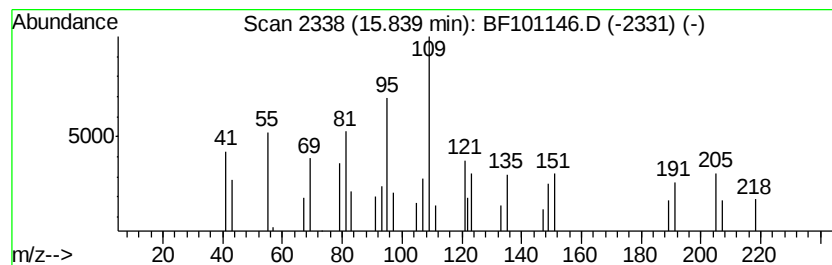
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Peak Number 5 unknown15.84 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.44 ng	34343	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Methanoazulene-9-methanol, d...	222	C15H26O	001139-17-9	38
2		(+)-Camphor-10-sulfonyl chloride	250	C10H15ClO3S	021286-54-4	38
3		Cyclohexane-1-methanol, 3,3-dime...	208	C14H24O	1000196-01-5	37
4		Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	32
5		(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	32



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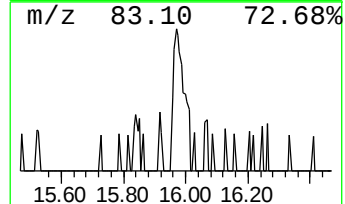
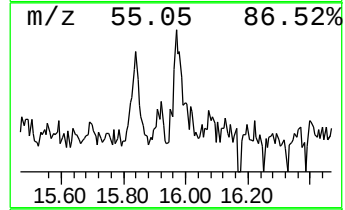
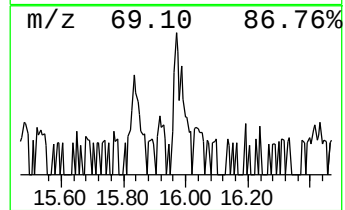
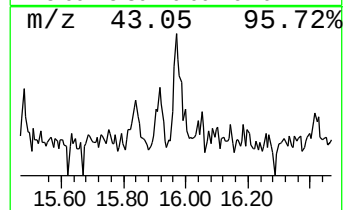
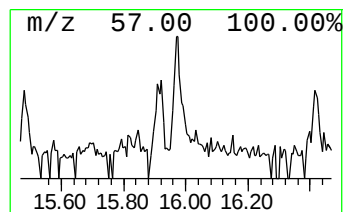
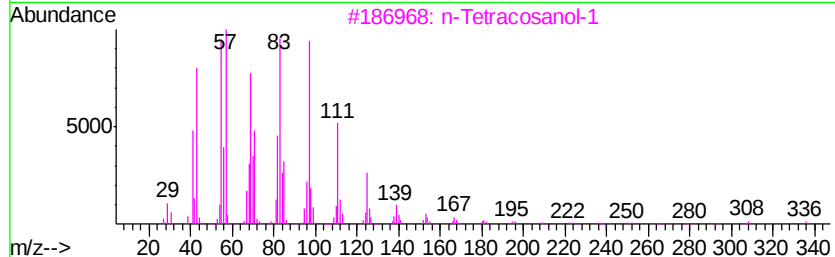
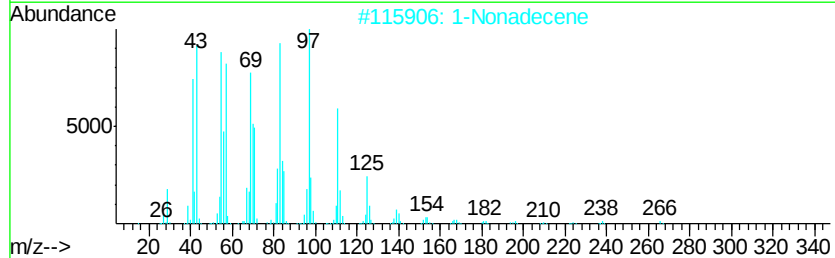
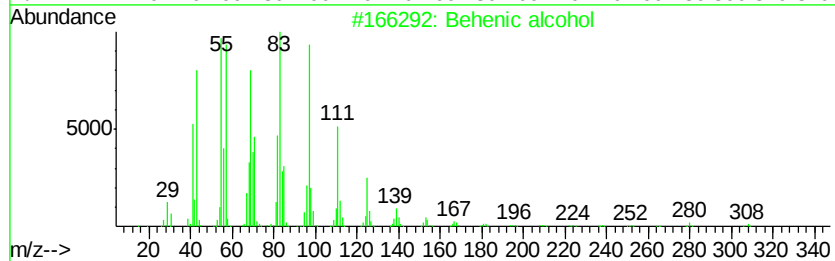
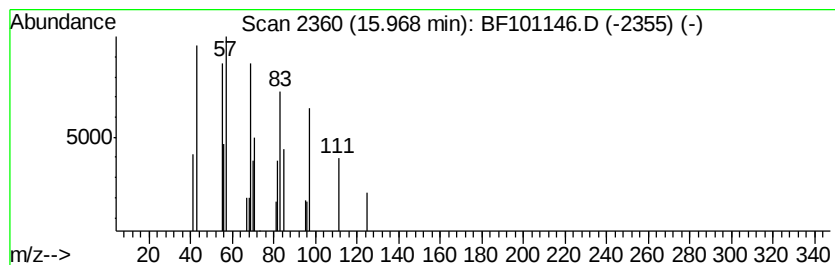
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Peak Number 6 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.97	2.22 ng	31336	Perylene-d12		15.49
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	90
2	1-Nonadecene	266	C19H38	018435-45-5	90
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	1-Heneicosanol	312	C21H44O	015594-90-8	80
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	68



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	5.0	ng	75045	1	6.85	302804	20.0
unknown6.62	6.62	81.6	ng	1235600	1	6.85	302804	20.0
1-Heneicosanol	13.84	9.7	ng	129954	5	14.02	268029	20.0
unknown15.84	15.84	2.4	ng	34343	6	15.49	281778	20.0
Behenic alcohol	15.97	2.2	ng	31336	6	15.49	281778	20.0