

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
 Data File : BF103630.D
 Acq On : 14 Mar 2018 5:02
 Operator : SJ/JU
 Sample : J1894-03
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

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-BF022218.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

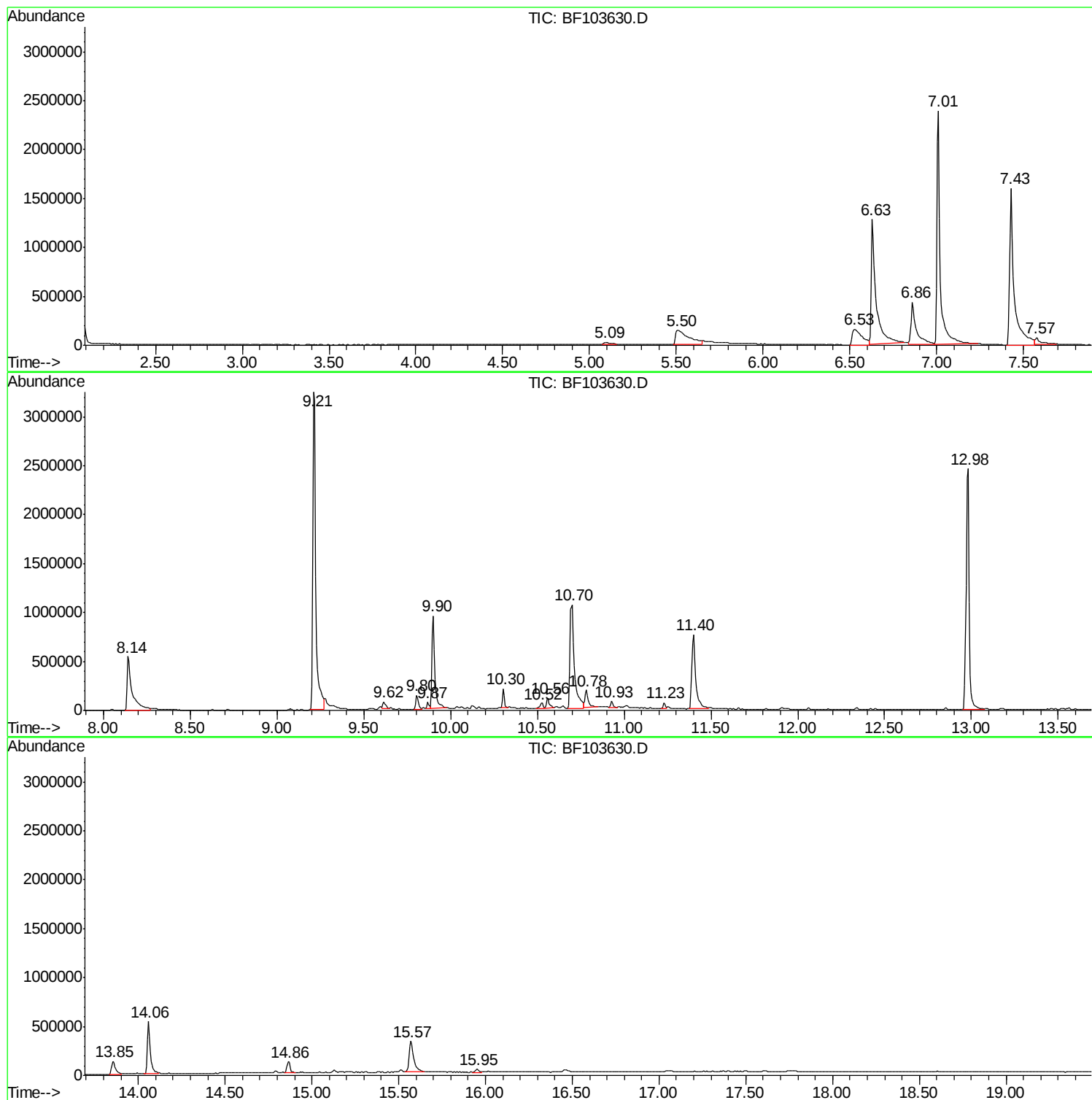
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.093	508	511	521	rBV	25345	65150	1.57%	0.250%
2	5.504	577	581	606	rBV2	148414	797552	19.20%	3.065%
3	6.528	750	755	769	rBV	160298	609241	14.67%	2.341%
4	6.628	769	772	803	rVB	1267868	2487768	59.90%	9.560%
5	6.857	808	811	833	rVV	430420	903205	21.75%	3.471%
6	7.010	833	837	875	rVB	2382250	3284597	79.09%	12.622%
7	7.428	904	908	931	rBV	1600842	2867430	69.05%	11.019%
8	7.575	931	933	952	rVB	68377	150348	3.62%	0.578%
9	8.140	1026	1029	1051	rBV	546181	1126055	27.11%	4.327%
10	9.210	1207	1211	1221	rBV	3244902	4152977	100.00%	15.959%
11	9.616	1278	1280	1285	rVB	70880	77466	1.87%	0.298%
12	9.804	1309	1312	1317	rBV	141045	131088	3.16%	0.504%
13	9.869	1321	1323	1325	rVV	62602	48266	1.16%	0.185%
14	9.898	1325	1328	1341	rVB	940432	1150553	27.70%	4.421%
15	10.304	1395	1397	1401	rBV	195651	146661	3.53%	0.564%
16	10.522	1429	1434	1437	rBV	57328	74172	1.79%	0.285%
17	10.563	1437	1441	1446	rVV	101903	120991	2.91%	0.465%
18	10.698	1460	1464	1475	rBV	1057312	1691853	40.74%	6.502%
19	10.781	1475	1478	1489	rVB	174171	245062	5.90%	0.942%
20	10.928	1500	1503	1508	rVB	64014	57815	1.39%	0.222%
21	11.228	1551	1554	1557	rBV	57385	49422	1.19%	0.190%
22	11.398	1579	1583	1598	rBV	761784	1166085	28.08%	4.481%
23	12.980	1847	1852	1868	rBV	2457842	2948727	71.00%	11.332%
24	13.851	1997	2000	2009	rBV	130510	188694	4.54%	0.725%
25	14.057	2031	2035	2045	rBV	532548	686702	16.54%	2.639%
26	14.863	2169	2172	2179	rVB	111911	127412	3.07%	0.490%
27	15.568	2287	2292	2305	rBV	316273	619677	14.92%	2.381%
28	15.951	2353	2357	2362	rBV	29973	47203	1.14%	0.181%

Sum of corrected areas: 26022172

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.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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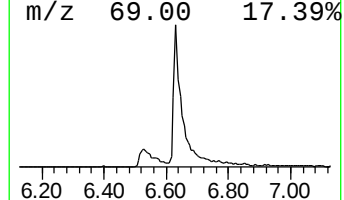
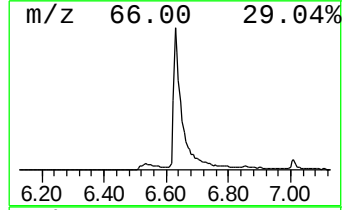
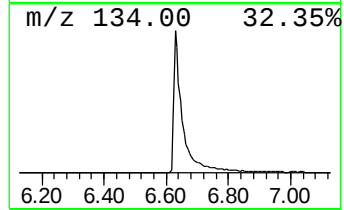
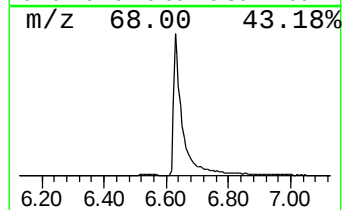
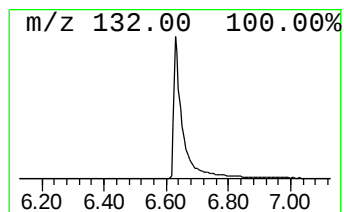
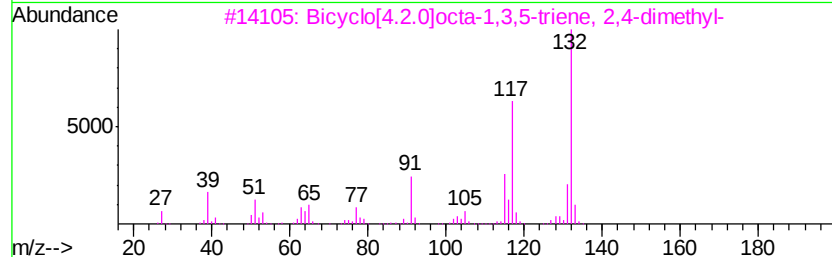
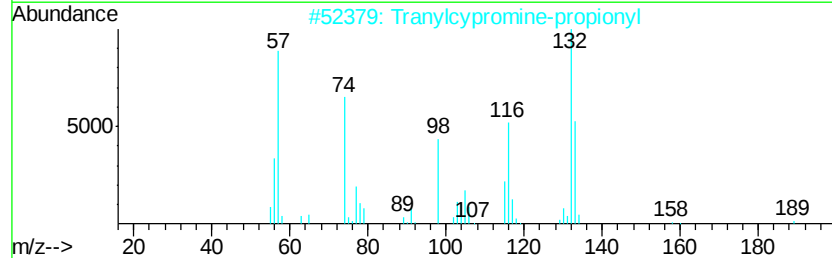
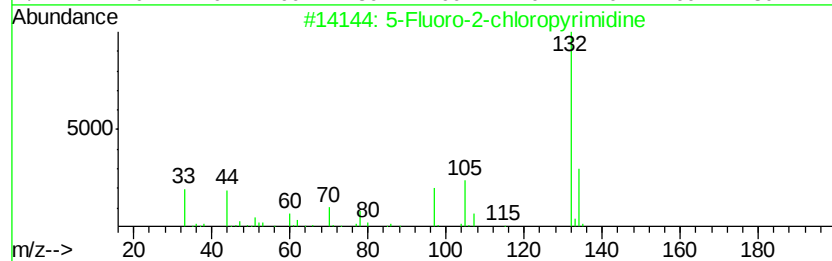
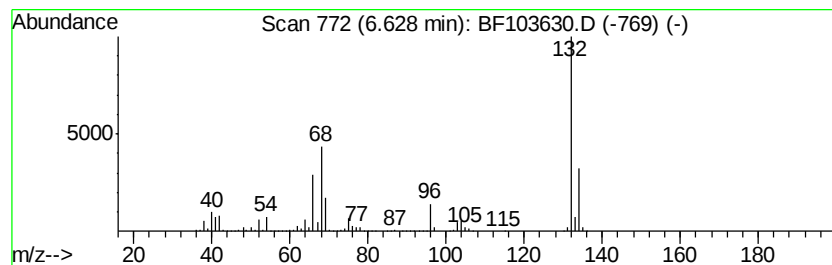
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	55.09 ng	2487770	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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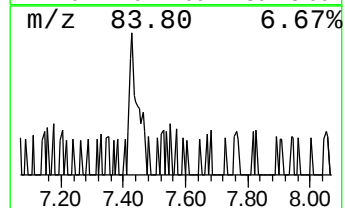
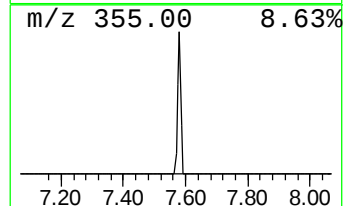
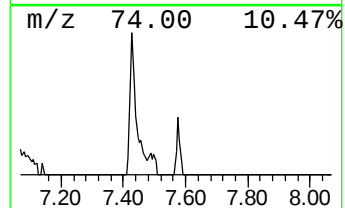
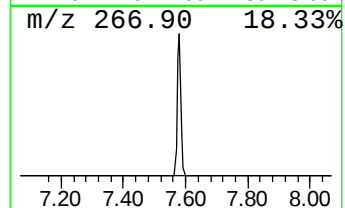
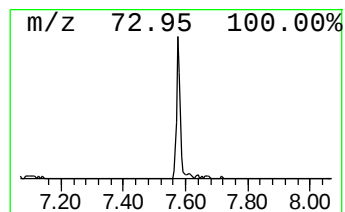
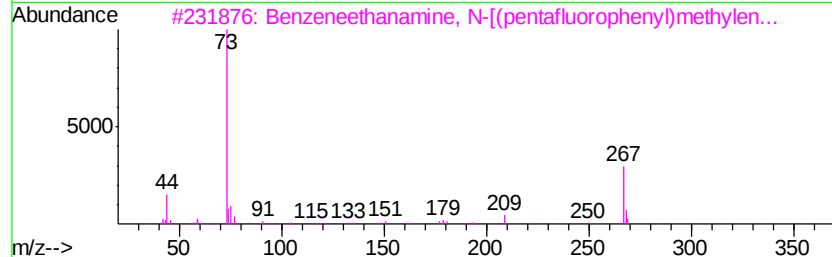
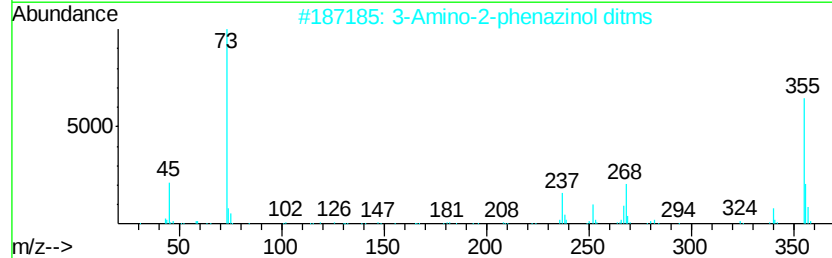
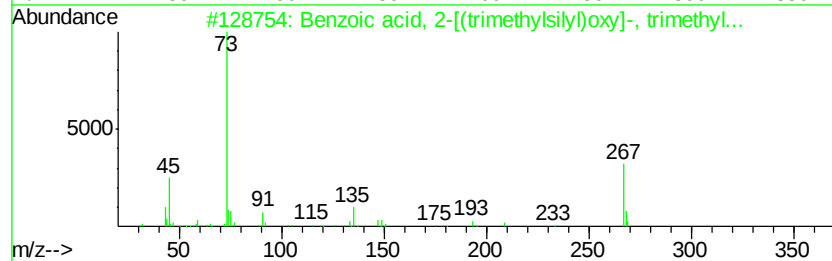
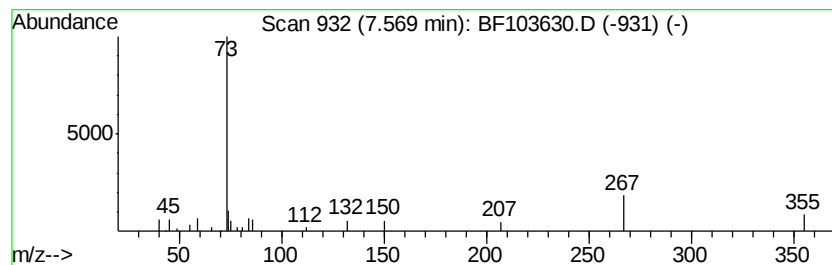
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown7.57 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	2.67 ng	150348	Napthalene-d8	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 2-[(trimethylsilyl)oxy]-, trimethyl...	282	C13H22O3Si2	003789-85-3	45
2		3-Amino-2-phenazolin ditms	355	C18H25N3O2Si2	1000332-15-5	38
3		Benzeneethanamine, N-[(pentafluorophenyl)methyl]-	475	C21H26F5N2Si2	055429-85-1	36
4		Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	36
5		Tetrasiloxane, 1,1,3,3,5,5,7,7-octamethyl-	282	C8H26O3Si4	001000-05-1	33



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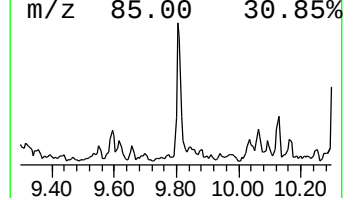
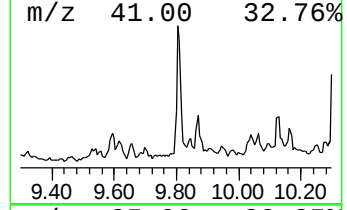
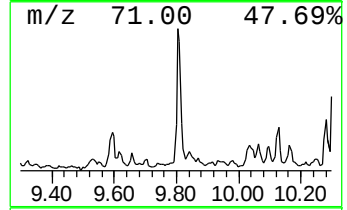
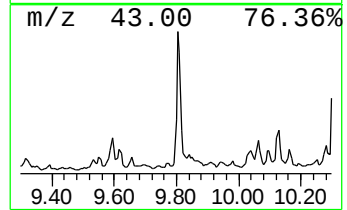
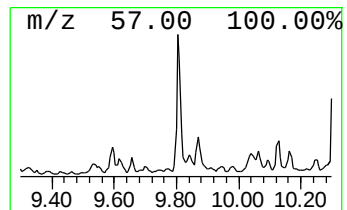
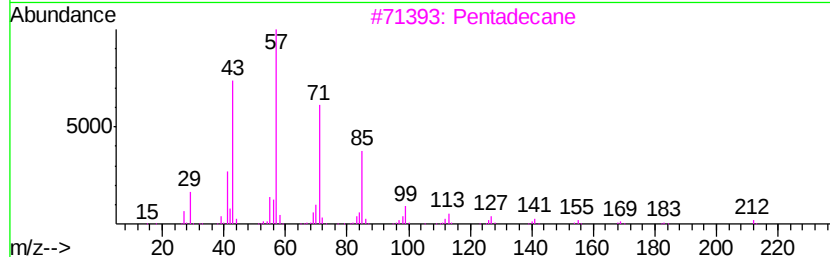
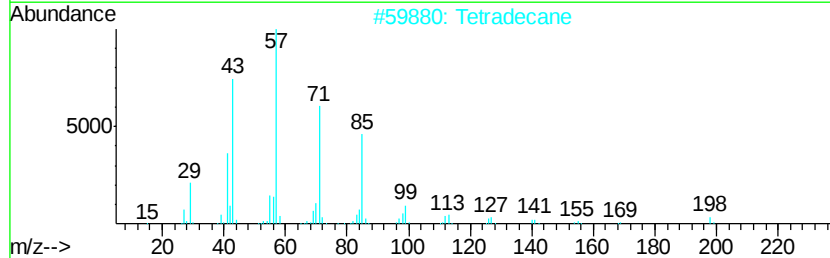
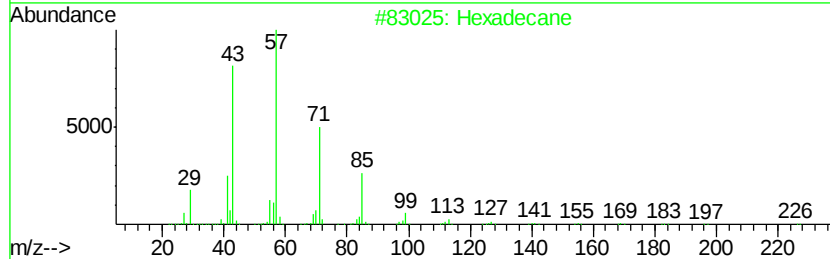
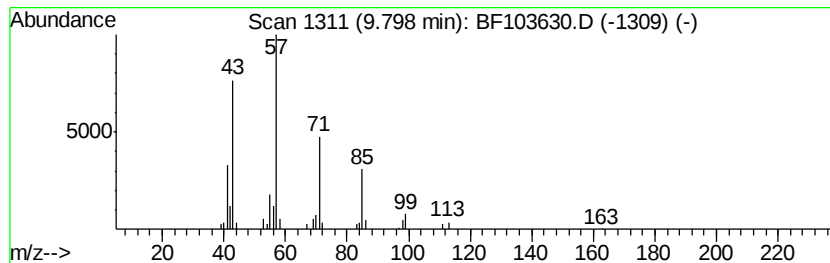
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.80	2.28 ng	131088	Acenaphthene-d10	9.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Tetradecane	198	C14H30	000629-59-4	90
3		Pentadecane	212	C15H32	000629-62-9	86
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	86
5		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72



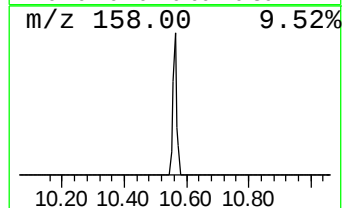
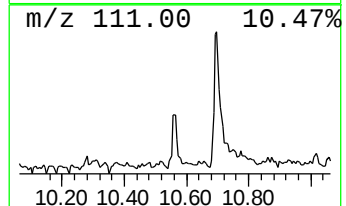
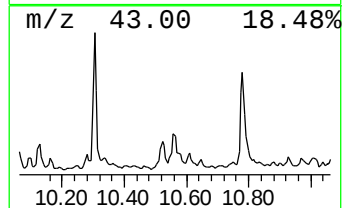
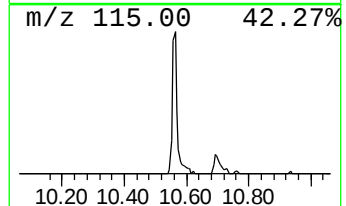
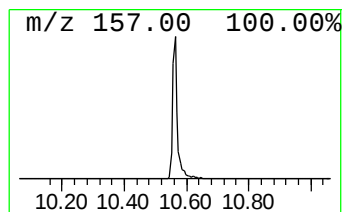
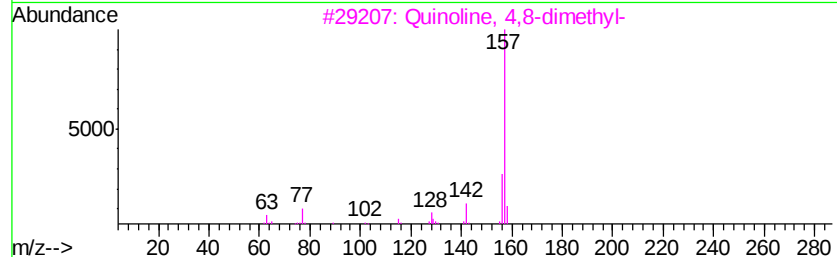
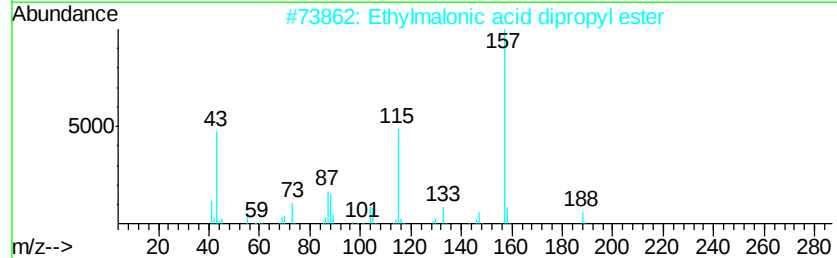
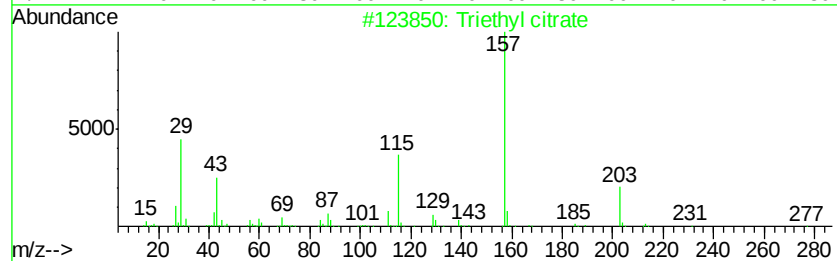
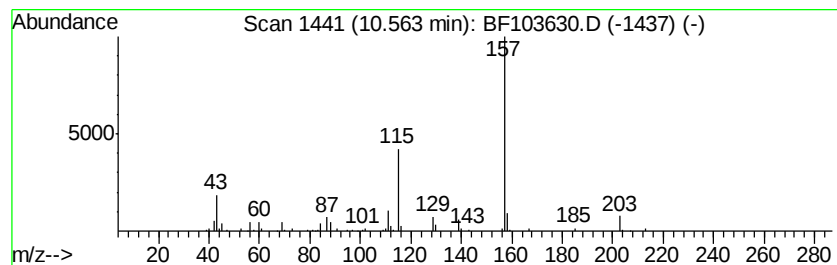
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Triethyl citrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.56	2.10 ng	120991	Acenaphthene-d10	9.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	90
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	49
4	Hexanedioic acid, 3-ethyl-, bis(...	286	C16H30O4	057983-54-7	40
5	3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClF02	1000338-64-9	40



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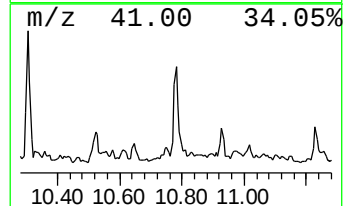
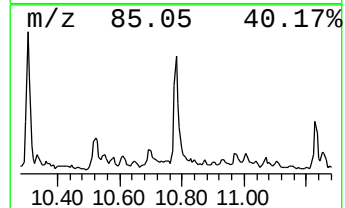
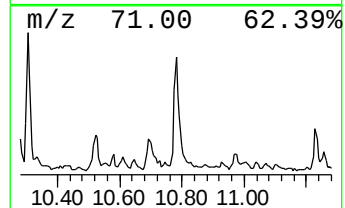
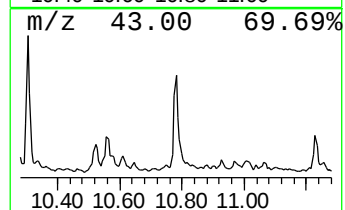
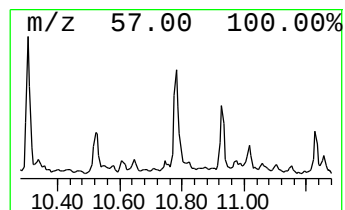
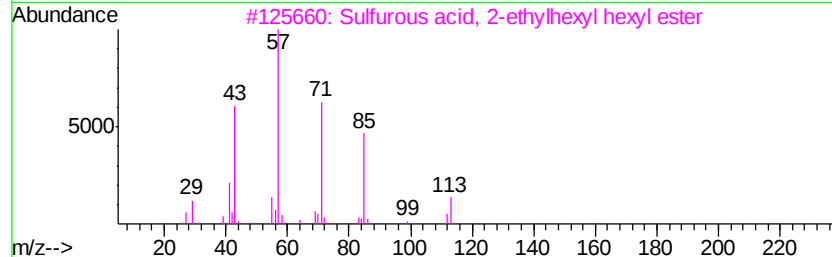
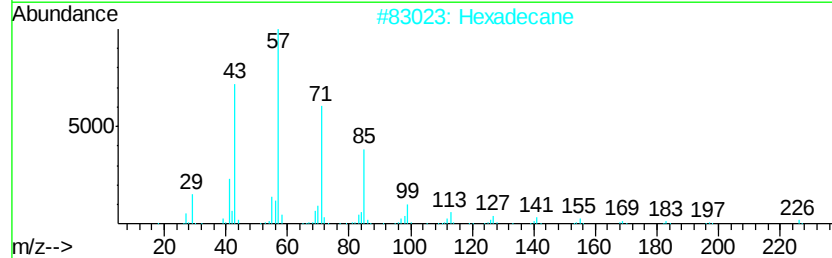
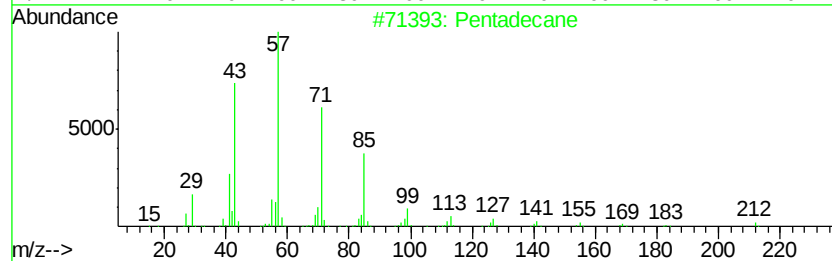
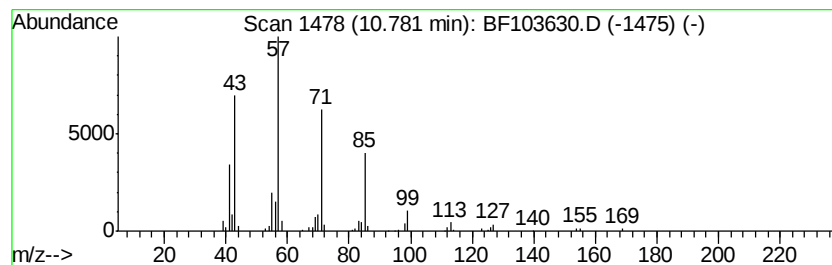
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Pentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	4.20 ng	245062	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane	212	C15H32	000629-62-9	83
2		Hexadecane	226	C16H34	000544-76-3	83
3		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
4		Tridecane	184	C13H28	000629-50-5	53
5		2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	50



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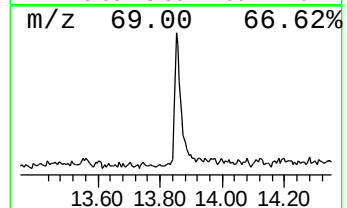
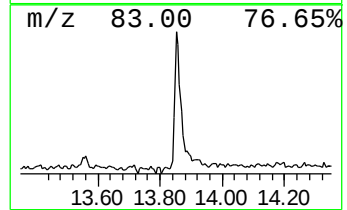
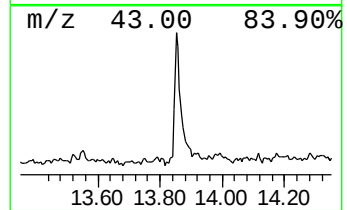
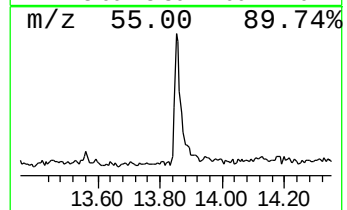
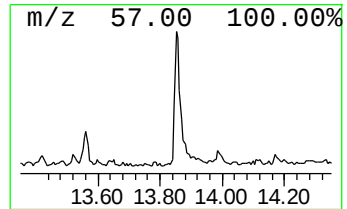
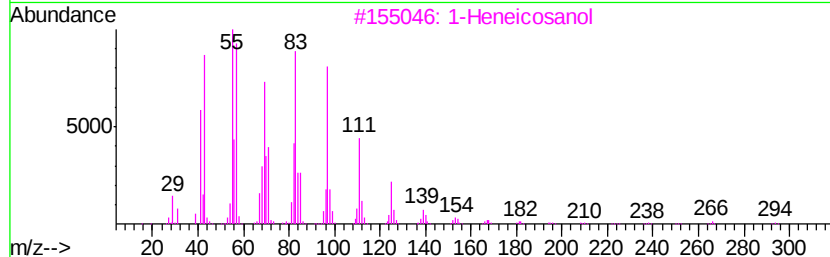
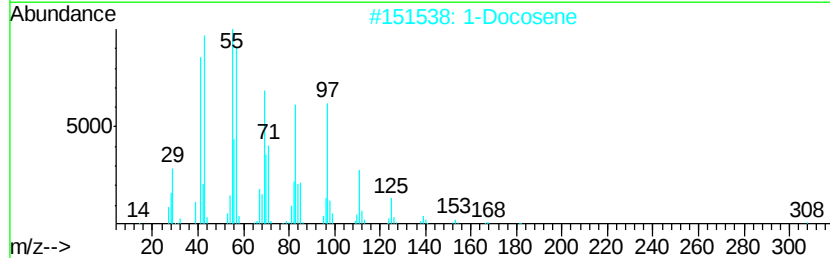
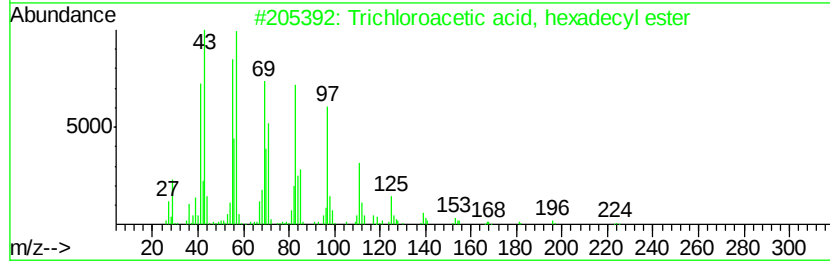
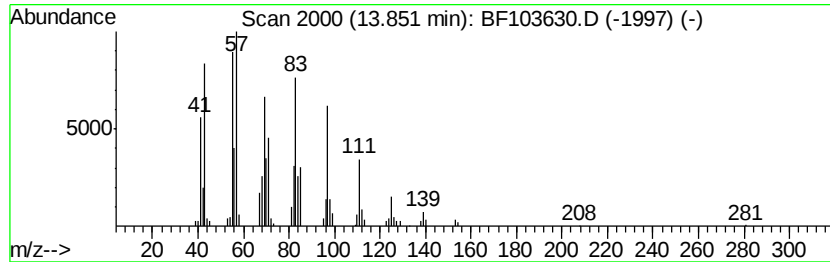
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	5.50 ng	188694	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			1-Docosene	308	C22H44	001599-67-3	95
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
Data File : BF103630.D
Acq On : 14 Mar 2018 5:02
Operator : SJ/JU
Sample : J1894-03
Misc :
ALS Vial : 33 Sample Multiplier: 1

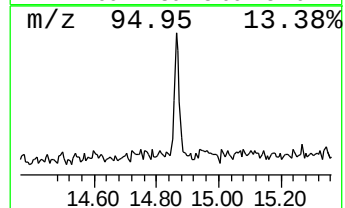
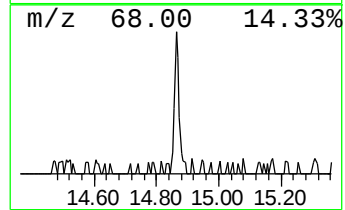
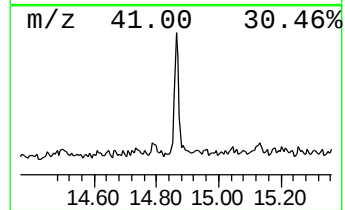
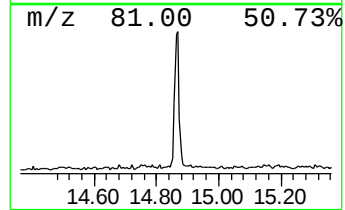
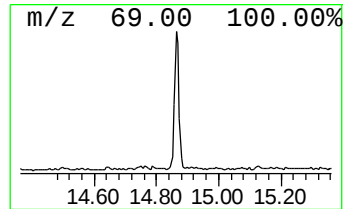
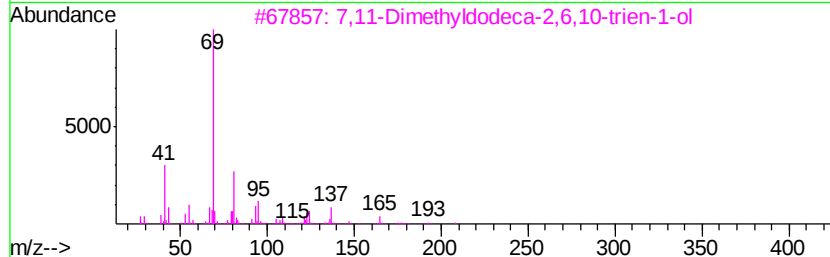
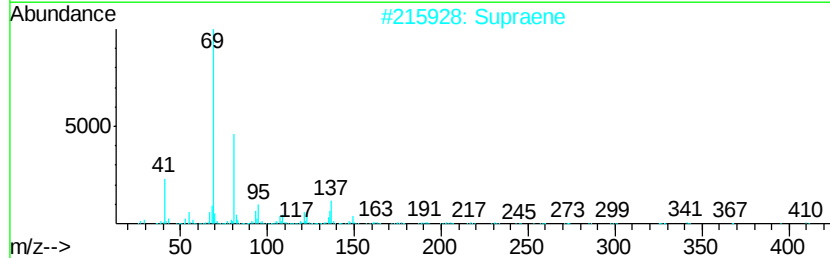
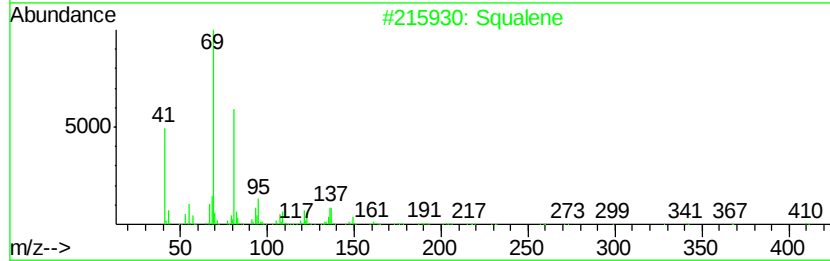
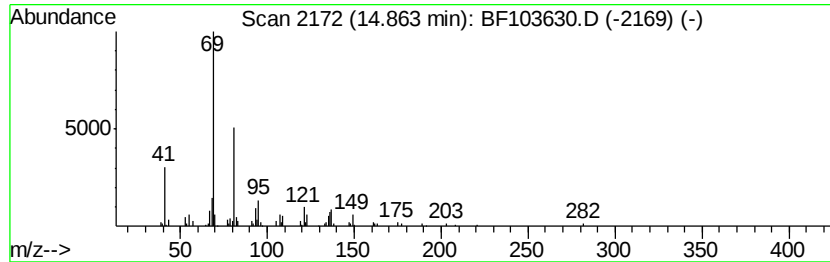
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	4.11 ng	127412	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
4		trans-Farnesol	222	C15H26O	000106-28-5	64
5		6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031318\
Data File : BF103630.D
Acq On : 14 Mar 2018 5:02
Operator : SJ/JU
Sample : J1894-03
Misc :
ALS Vial : 33 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.63	6.63	55.1	ng	2487770	1	6.86	903205	20.0
unknown7.57	7.57	2.7	ng	150348	2	8.14	1126060	20.0
Hexadecane	9.80	2.3	ng	131088	3	9.90	1150550	20.0
Triethyl citrate	10.56	2.1	ng	120991	3	9.90	1150550	20.0
Pentadecane	10.78	4.2	ng	245062	4	11.40	1166090	20.0
Trichloroacetic a...	13.85	5.5	ng	188694	5	14.06	686702	20.0
Squalene	14.86	4.1	ng	127412	6	15.57	619677	20.0