

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\
 Data File : BF103628.D
 Acq On : 14 Mar 2018 4:09
 Operator : SJ/JU
 Sample : J1894-01
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

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-BF022218.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

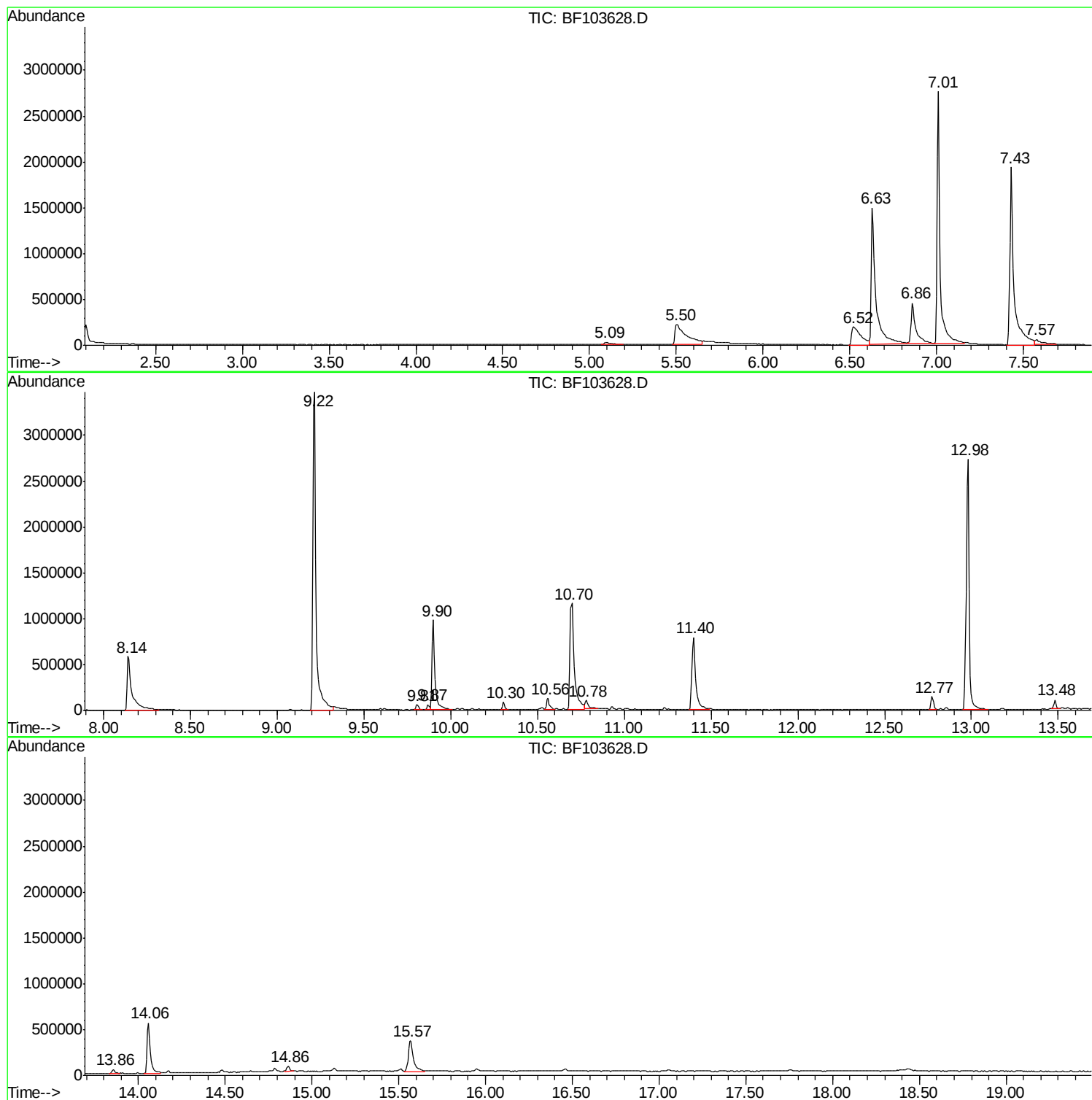
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.092	507	511	528	rBV2	28076	79676	1.72%	0.286%
2	5.498	576	580	606	rBV	220881	1029087	22.15%	3.695%
3	6.522	749	754	769	rBV	197776	729046	15.69%	2.618%
4	6.628	769	772	808	rVV	1489617	2917978	62.81%	10.478%
5	6.857	808	811	833	rVB	441519	859157	18.49%	3.085%
6	7.010	833	837	863	rBV	2745584	3447743	74.21%	12.380%
7	7.428	904	908	931	rBV	1940831	3177798	68.40%	11.411%
8	7.575	931	933	952	rVB	51252	139339	3.00%	0.500%
9	8.139	1026	1029	1059	rBV	584271	1189484	25.60%	4.271%
10	9.216	1207	1212	1230	rBV	3467158	4645693	100.00%	16.682%
11	9.810	1309	1313	1317	rBV	55115	54650	1.18%	0.196%
12	9.869	1320	1323	1325	rVV	54519	46587	1.00%	0.167%
13	9.898	1325	1328	1346	rVB	973080	1218250	26.22%	4.375%
14	10.304	1394	1397	1401	rBV	77586	63545	1.37%	0.228%
15	10.563	1437	1441	1447	rBV	117439	127435	2.74%	0.458%
16	10.698	1460	1464	1476	rBV	1159196	1855806	39.95%	6.664%
17	10.780	1476	1478	1489	rVB	90081	126891	2.73%	0.456%
18	11.398	1579	1583	1599	rBV	789873	1187181	25.55%	4.263%
19	12.774	1814	1817	1821	rBV	138769	121318	2.61%	0.436%
20	12.980	1847	1852	1871	rBV	2728017	3153570	67.88%	11.324%
21	13.480	1934	1937	1942	rBV	100520	84672	1.82%	0.304%
22	13.857	1997	2001	2007	rBV	44597	54683	1.18%	0.196%
23	14.057	2031	2035	2047	rBV	548746	781264	16.82%	2.805%
24	14.862	2169	2172	2177	rVB	54661	53784	1.16%	0.193%
25	15.568	2286	2292	2306	rBV	336207	704128	15.16%	2.528%

Sum of corrected areas: 27848765

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



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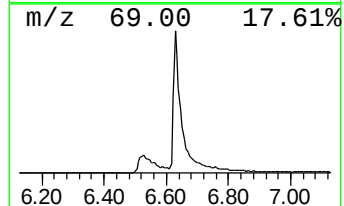
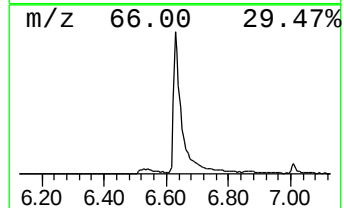
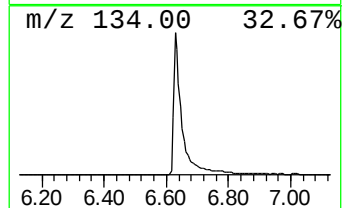
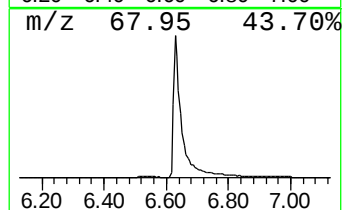
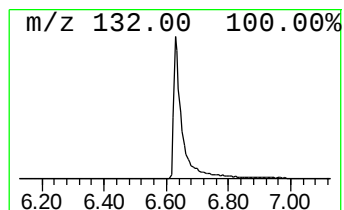
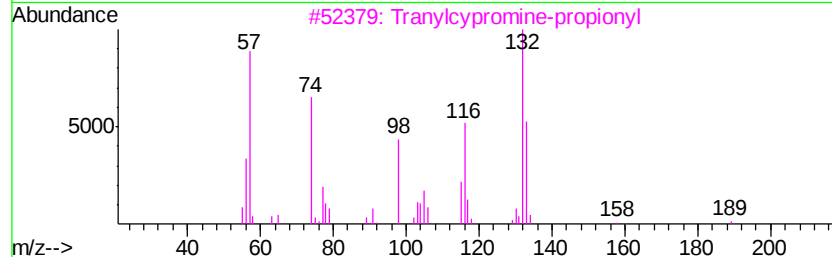
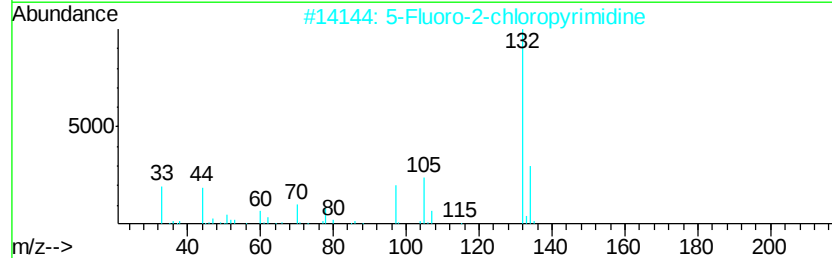
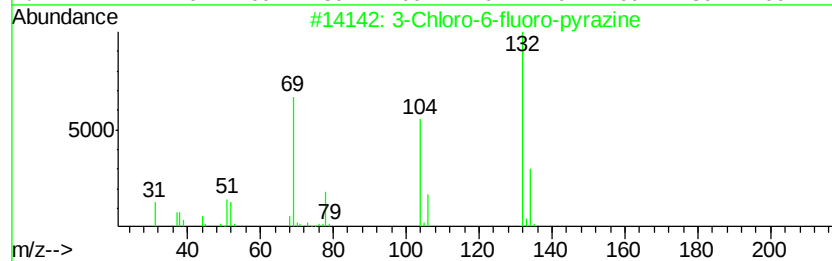
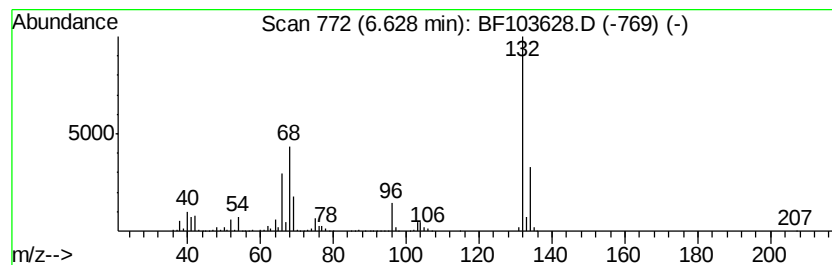
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Peak Number 1 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	67.93 ng	2917980	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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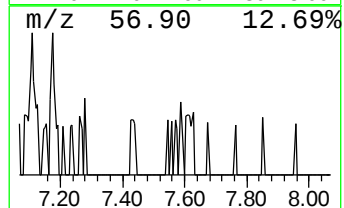
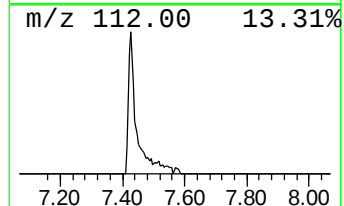
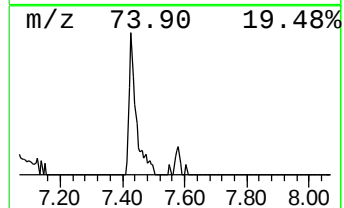
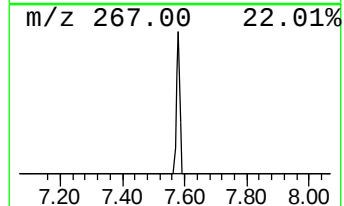
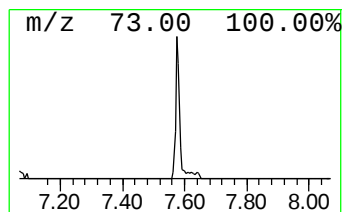
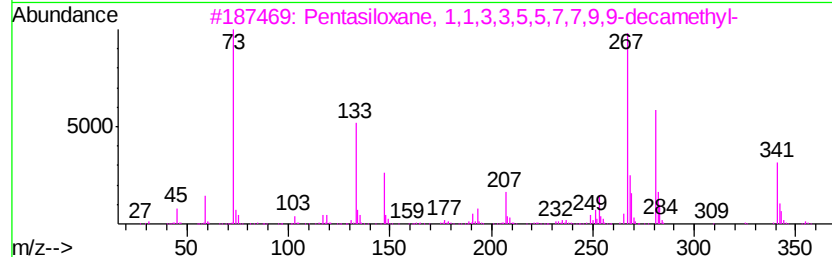
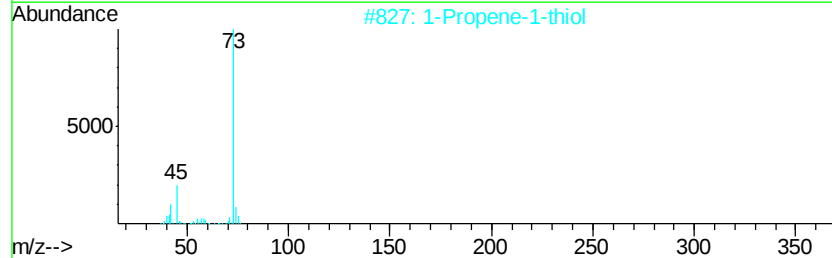
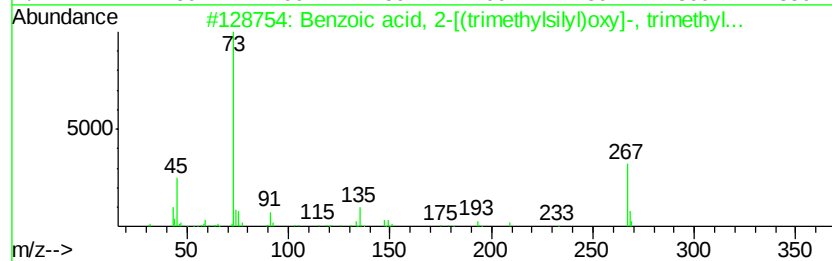
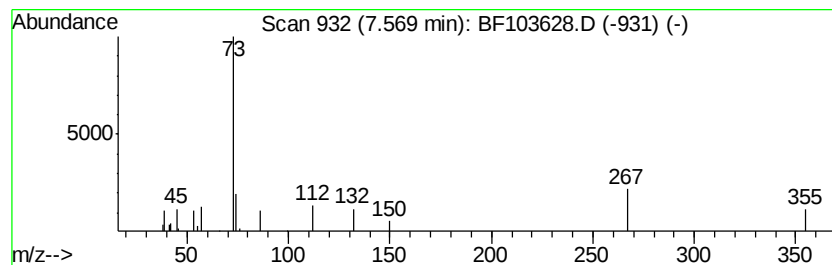
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Peak Number 3 unknown7.57 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	2.34 ng	139339	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	28
2		1-Propene-1-thiol	74	C3H6S	000925-89-3	11
3		Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-	356	C10H32O4Si5	000995-83-5	9
4		Benzeneethanamine, N-[(pentafluoroethyl)oxy]-, trimethyl...	475	C21H26F5NO2Si2	055429-85-1	9
5		Trimethylsilyloxyethane, 2-(3-trimethylsilyloxypropyl)-	282	C14H26O2Si2	1000365-49-0	9



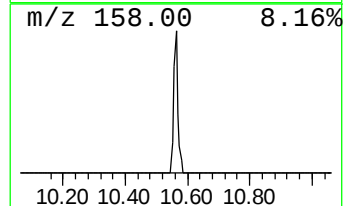
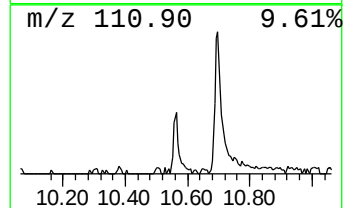
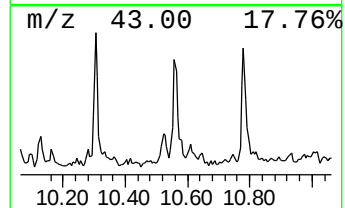
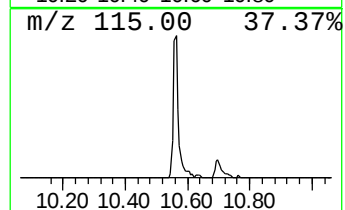
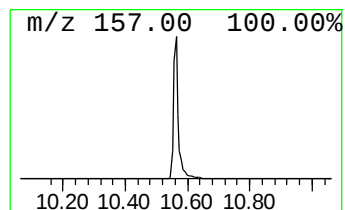
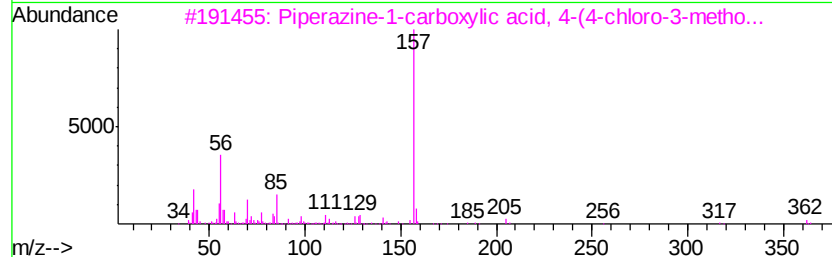
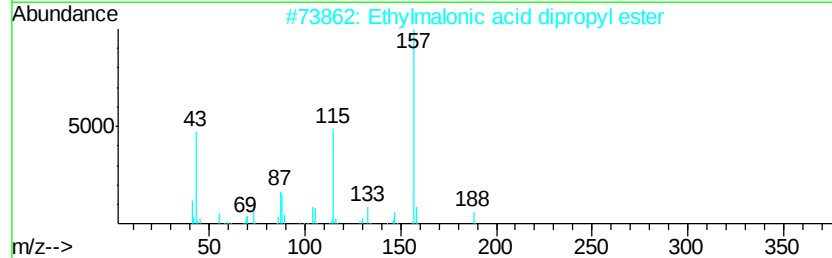
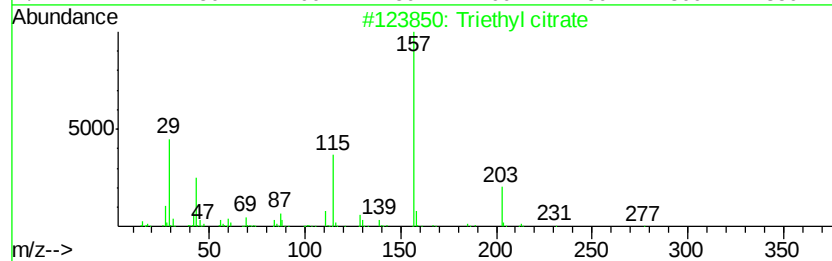
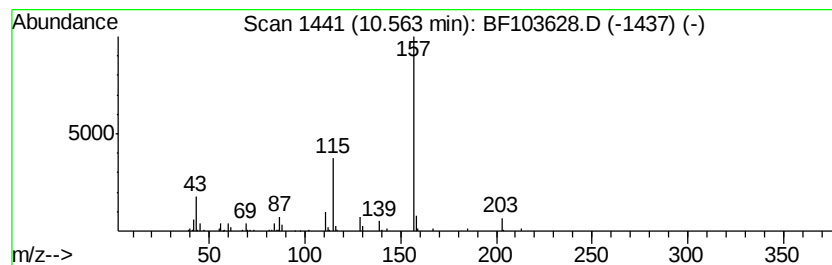
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Peak Number 4 Triethyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.56	2.09 ng	127435	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		Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	42
4		Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	40
5		Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	40



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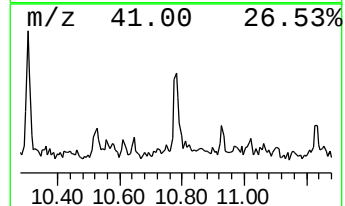
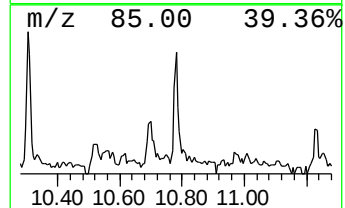
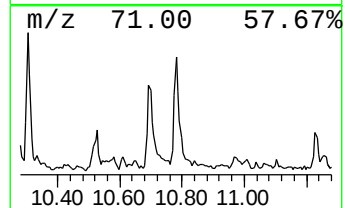
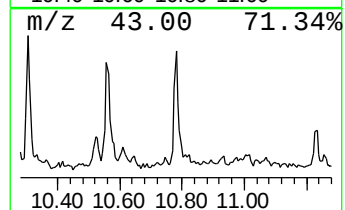
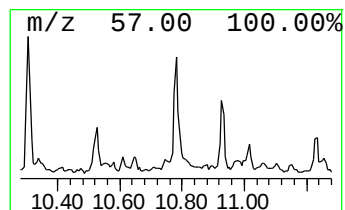
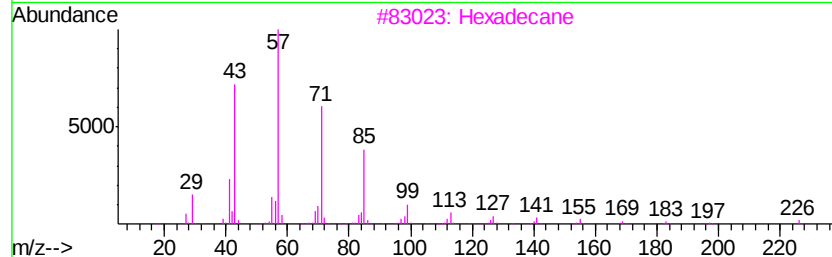
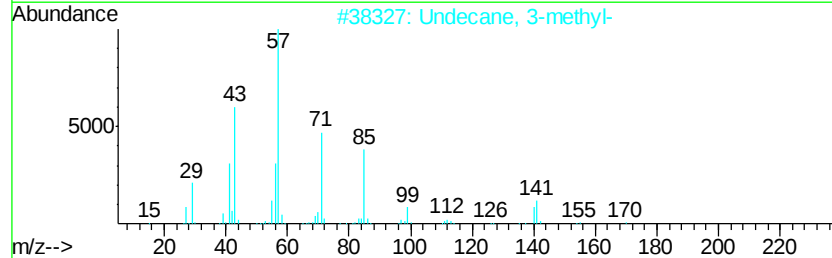
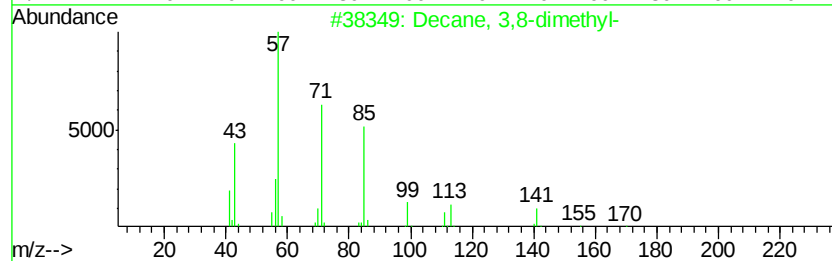
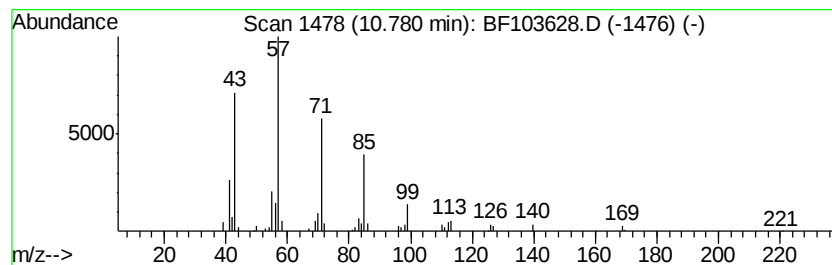
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Peak Number 5 Decane, 3,8-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.78	2.14 ng	126891	Phenanthrene-d10		11.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83
2			Undecane, 3-methyl-	170	C12H26	001002-43-3	80
3			Hexadecane	226	C16H34	000544-76-3	78
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64



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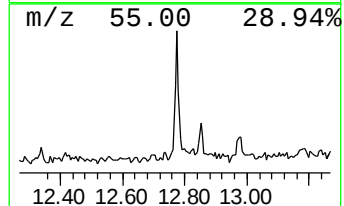
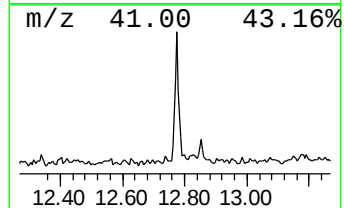
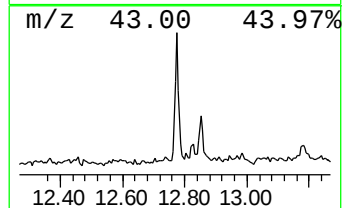
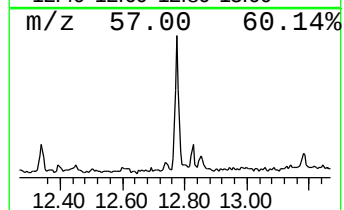
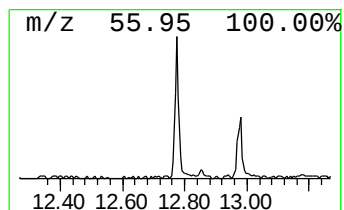
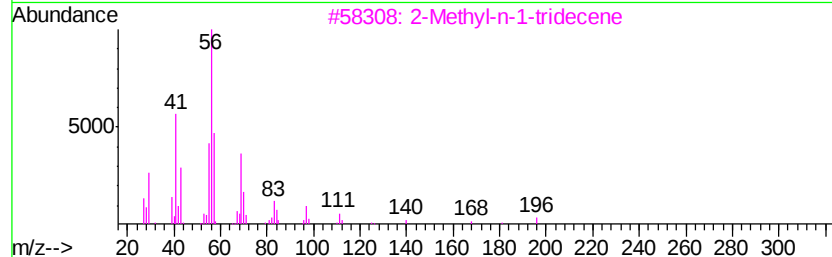
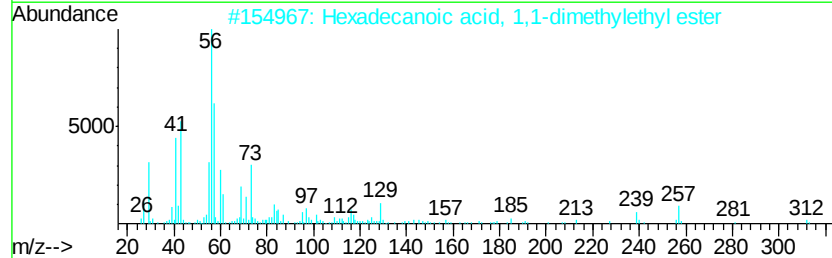
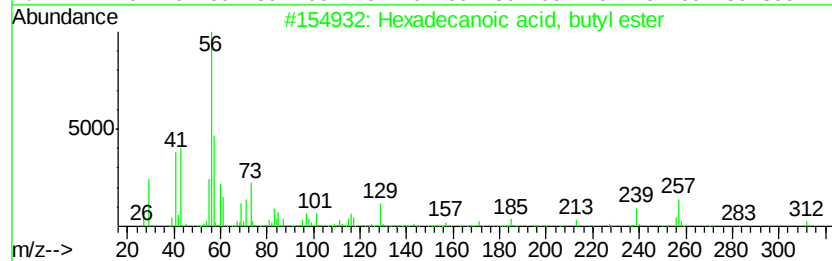
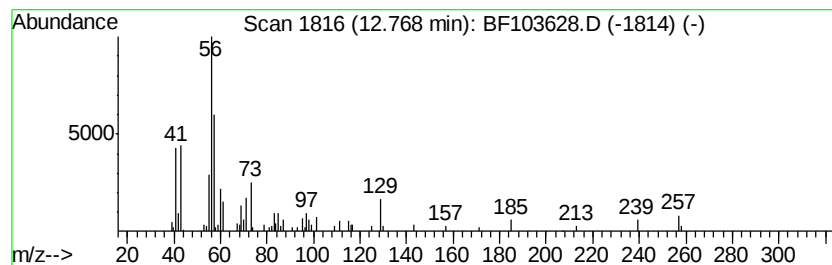
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	3.11 ng	121318	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
3		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35



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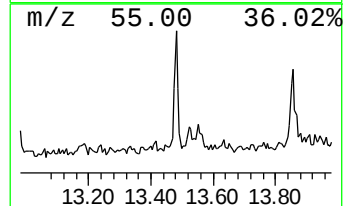
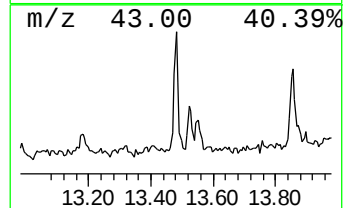
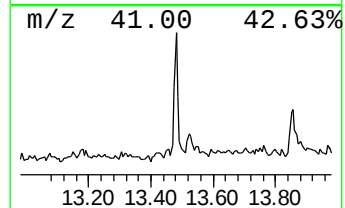
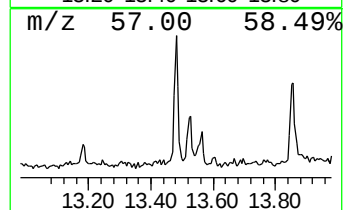
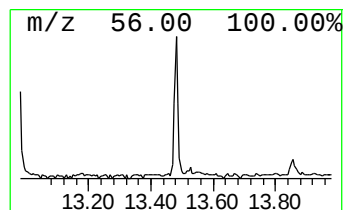
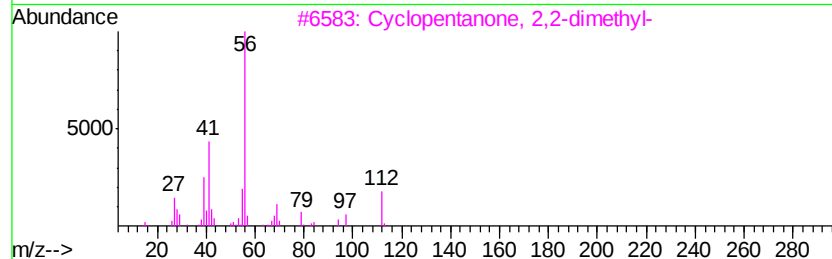
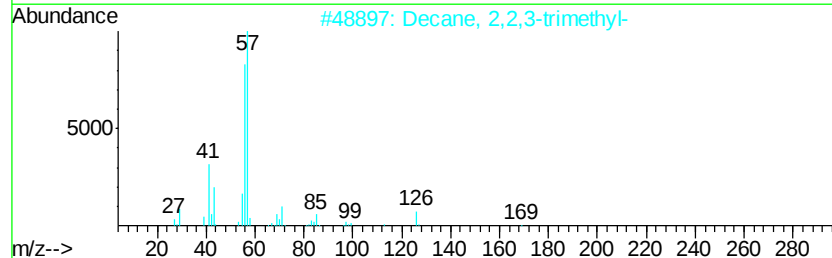
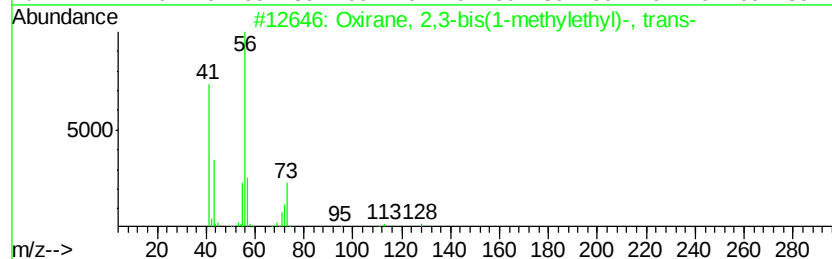
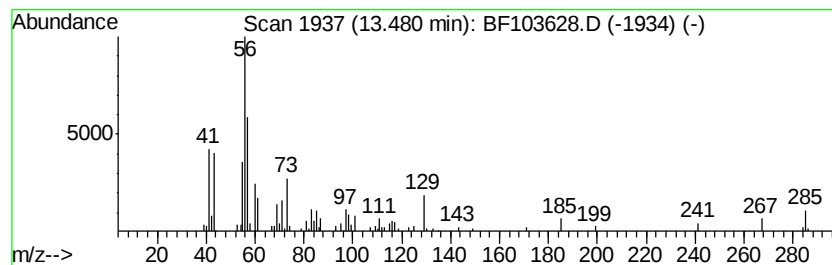
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.48 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.17 ng	84672	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	43
2		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
3		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38
4		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5		5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1000376-27-1	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031318\
Data File : BF103628.D
Acq On : 14 Mar 2018 4:09
Operator : SJ/JU
Sample : J1894-01
Misc :
ALS Vial : 31 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	67.9	ng	2917980	1	6.86	859157	20.0
unknown7.57	7.57	2.3	ng	139339	2	8.14	1189480	20.0
Triethyl citrate	10.56	2.1	ng	127435	3	9.90	1218250	20.0
Decane, 3,8-dimet...	10.78	2.1	ng	126891	4	11.40	1187180	20.0
Hexadecanoic acid...	12.77	3.1	ng	121318	5	14.06	781264	20.0
unknown13.48	13.48	2.2	ng	84672	5	14.06	781264	20.0