

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112717\
 Data File : BF100899.D
 Acq On : 27 Nov 2017 18:28
 Operator : SJ/JU
 Sample : I6548-09
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAU-4-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-BF110817.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	5.081	505	509	518	rBV	79644	93579	6.07%	0.698%
2	5.481	572	577	580	rBV	1248619	1176419	76.31%	8.780%
3	6.492	744	749	757	rBV	1245395	1253185	81.29%	9.353%
4	6.628	768	772	776	rBV	1304511	1268959	82.31%	9.470%
5	6.857	808	811	815	rBV	497512	416104	26.99%	3.105%
6	7.016	834	838	841	rBV	1187245	981645	63.67%	7.326%
7	7.422	902	907	910	rBV	855201	759895	49.29%	5.671%
8	8.139	1025	1029	1033	rBV	660552	537938	34.89%	4.015%
9	9.216	1207	1212	1215	rBV	1872347	1541713	100.00%	11.506%
10	9.604	1275	1278	1281	rBV	108274	87282	5.66%	0.651%
11	9.816	1308	1314	1318	rBV2	45386	39946	2.59%	0.298%
12	9.898	1324	1328	1331	rBV	642944	567722	36.82%	4.237%
13	10.316	1396	1399	1402	rVB	54355	41141	2.67%	0.307%
14	10.686	1458	1462	1465	rBV	883946	801321	51.98%	5.980%
15	10.792	1476	1480	1487	rBV	37100	42168	2.74%	0.315%
16	11.380	1576	1580	1583	rBV	581358	521997	33.86%	3.896%
17	11.404	1583	1584	1587	rVB	115578	69293	4.49%	0.517%
18	11.898	1662	1668	1675	rBV2	144393	214381	13.91%	1.600%
19	11.992	1681	1684	1686	rBV2	27552	29869	1.94%	0.223%
20	12.015	1686	1688	1694	rVB	82658	69379	4.50%	0.518%
21	12.327	1737	1741	1744	rBV	40914	35470	2.30%	0.265%
22	12.486	1766	1768	1771	rVB	61011	50542	3.28%	0.377%
23	12.557	1777	1780	1783	rBV	23540	21449	1.39%	0.160%
24	12.592	1783	1786	1791	rVB	150251	138230	8.97%	1.032%
25	12.686	1799	1802	1805	rBV2	61749	66548	4.32%	0.497%
26	12.821	1819	1825	1828	rBV	140835	146401	9.50%	1.093%
27	12.880	1832	1835	1838	rVB2	57547	47547	3.08%	0.355%
28	12.963	1845	1849	1853	rBV	1139318	1091910	70.82%	8.149%
29	13.039	1858	1862	1866	rBV5	17080	29883	1.94%	0.223%
30	13.098	1870	1872	1875	rBV	46056	39469	2.56%	0.295%
31	13.257	1896	1899	1901	rVB2	19635	20158	1.31%	0.150%
32	13.657	1965	1967	1971	rVB	19406	18657	1.21%	0.139%
33	13.851	1997	2000	2006	rVB2	79738	99276	6.44%	0.741%
34	14.021	2024	2029	2032	rBV	510493	507899	32.94%	3.791%

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SAU-4-E(4-5)

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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

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35	14.045	2032	2033	2039	rVB	77935	60908	3.95%	0.455%
36	15.062	2203	2206	2209	rBV	37363	48011	3.11%	0.358%
37	15.427	2265	2268	2273	rBV	43500	59128	3.84%	0.441%
38	15.492	2275	2279	2284	rBV2	316887	403804	26.19%	3.014%

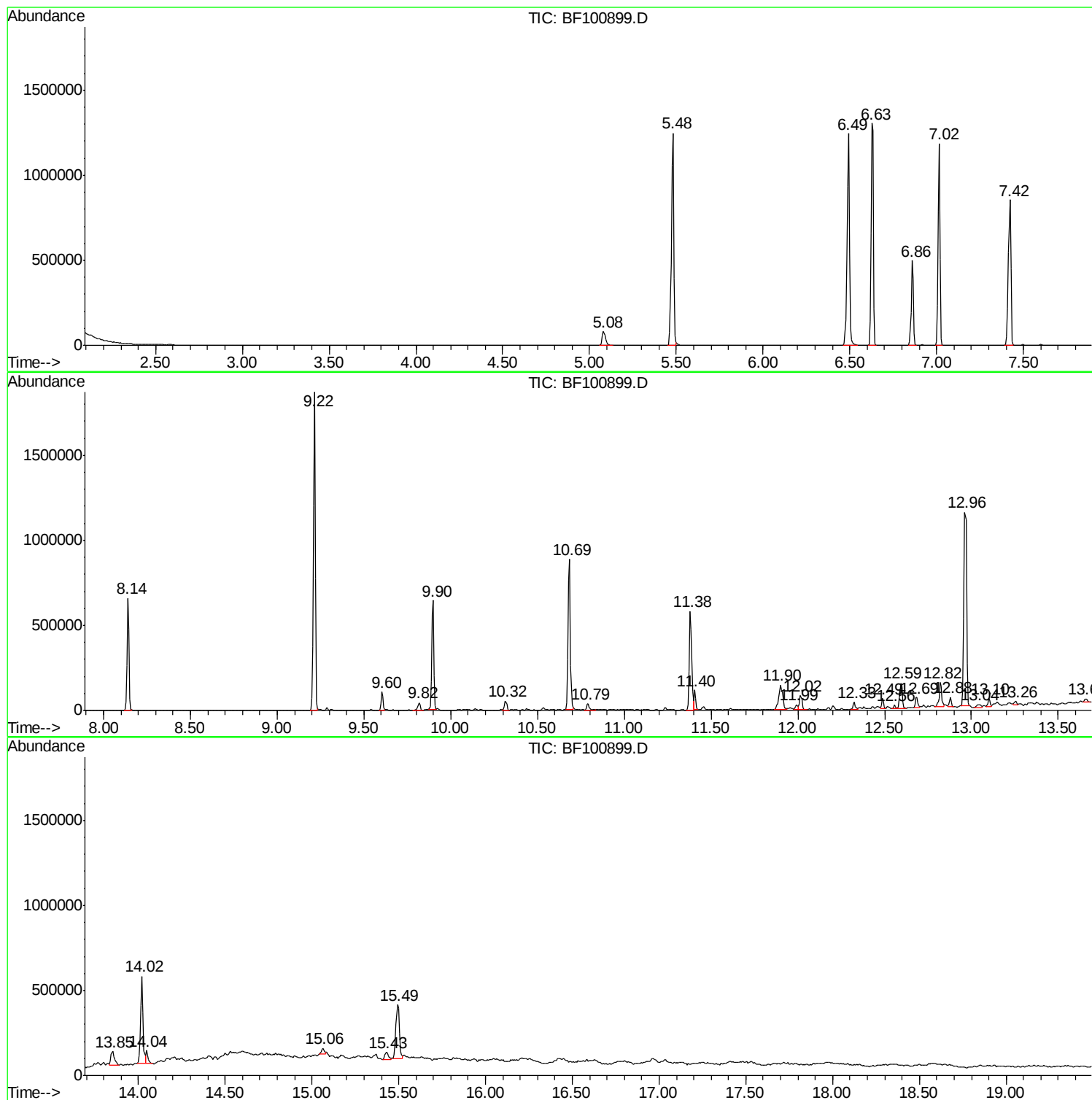
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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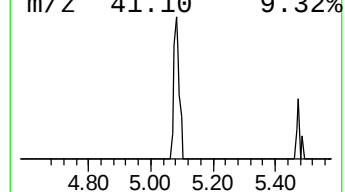
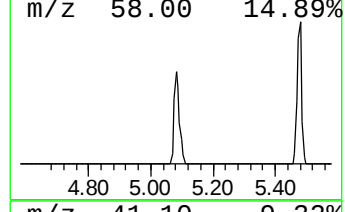
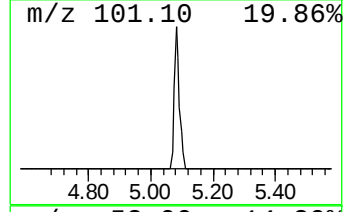
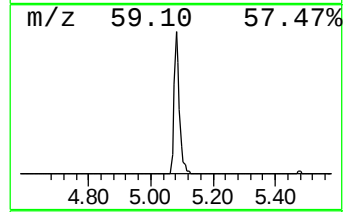
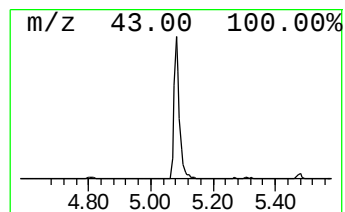
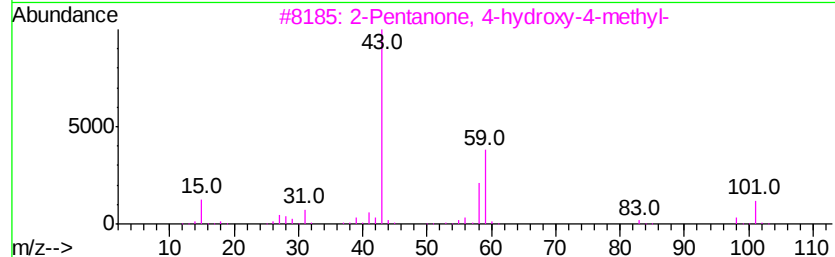
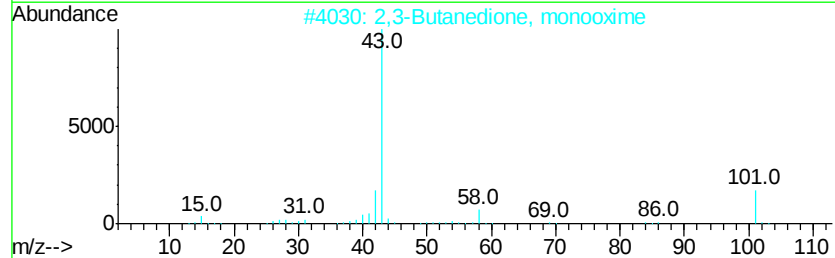
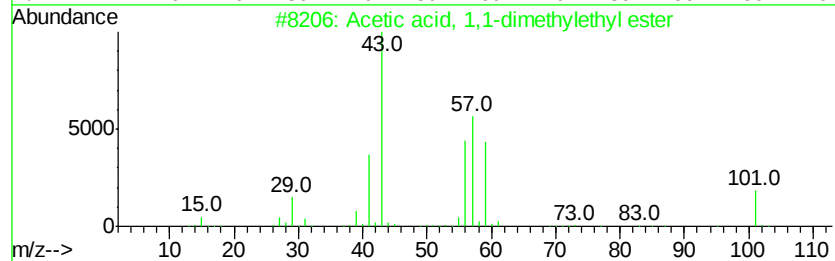
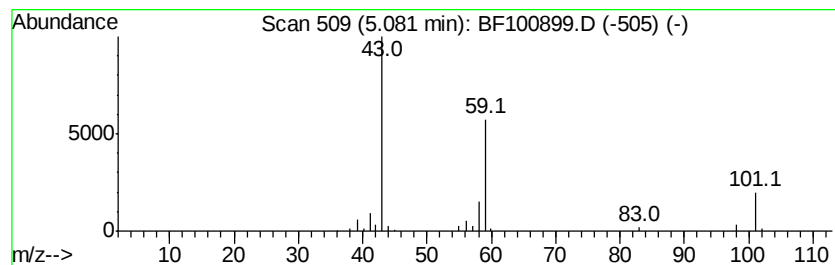
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.08 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	4.50 ng	93579	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			3-Hexanol	102	C6H14O	000623-37-0	9



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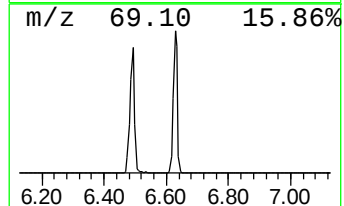
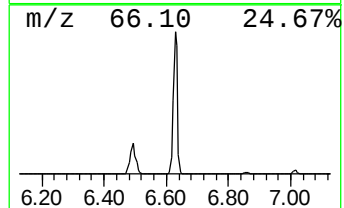
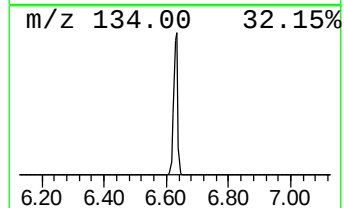
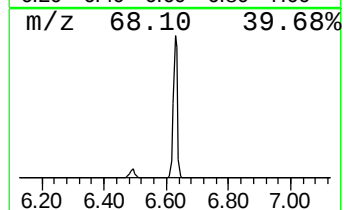
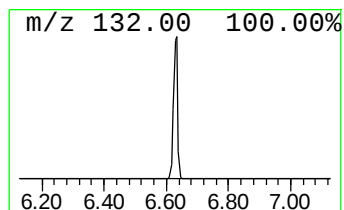
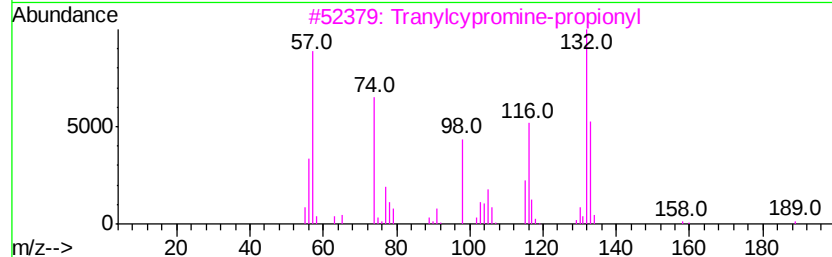
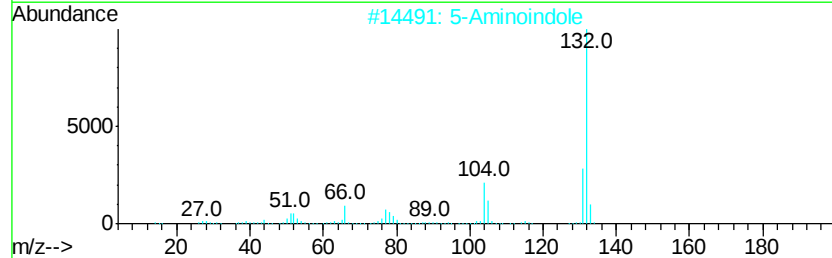
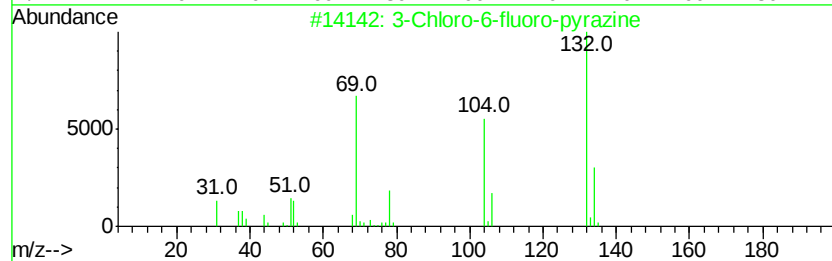
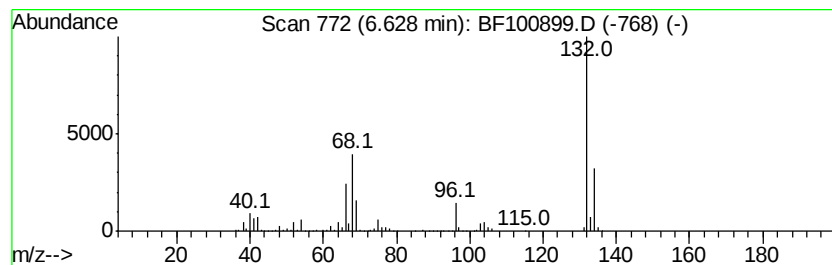
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	60.99 ng	1268960	1,4-Dichlorobenzene-d4	6.86

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	Tranvlcvpromine-propionyl			189	C12H15NO	1000123-86-3	10
4	4-Methylpvrrolo[1,2-apyrazine			132	C8H8N2	064608-60-2	9
5	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	9



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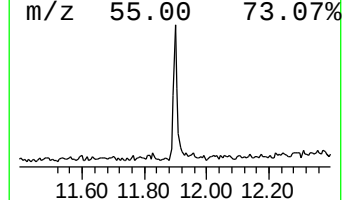
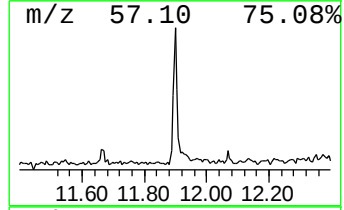
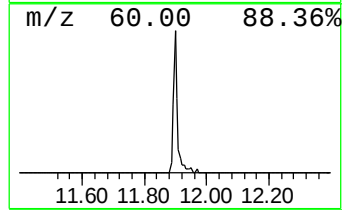
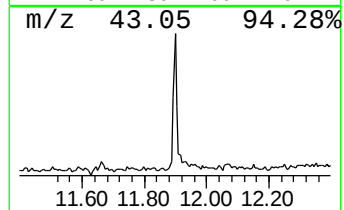
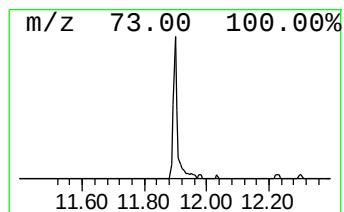
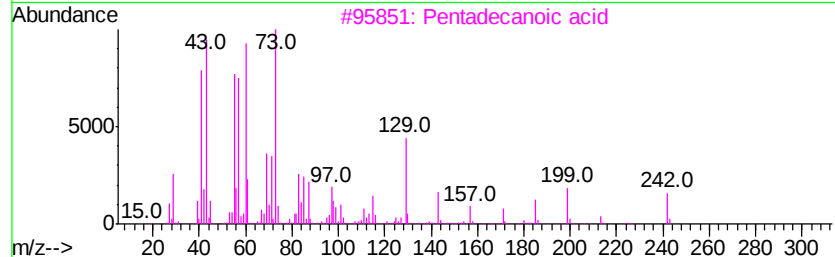
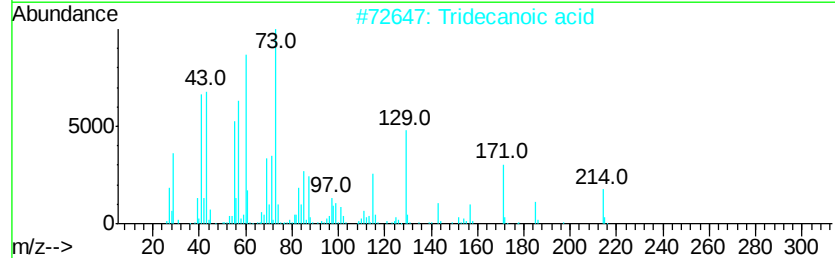
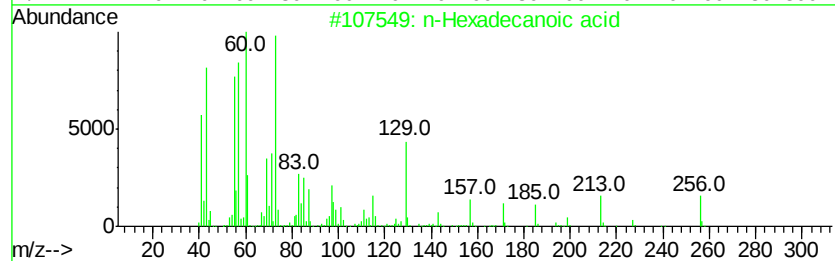
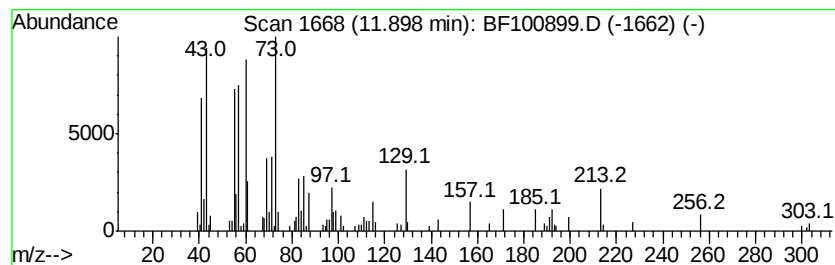
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.90	8.21 ng	214381	Phenanthrene-d10		11.38	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Octadecanoic acid	284	C18H36O2	000057-11-4	58



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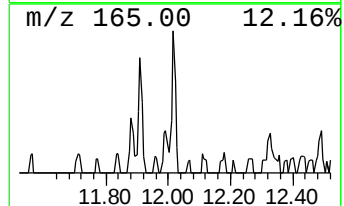
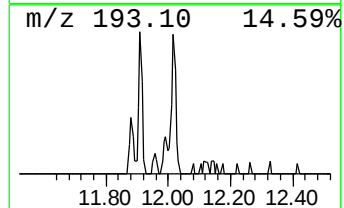
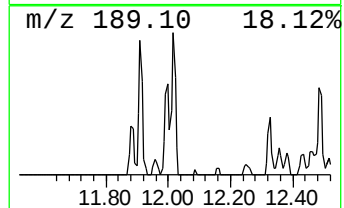
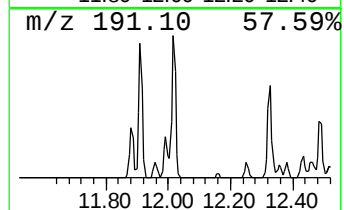
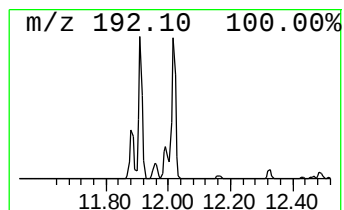
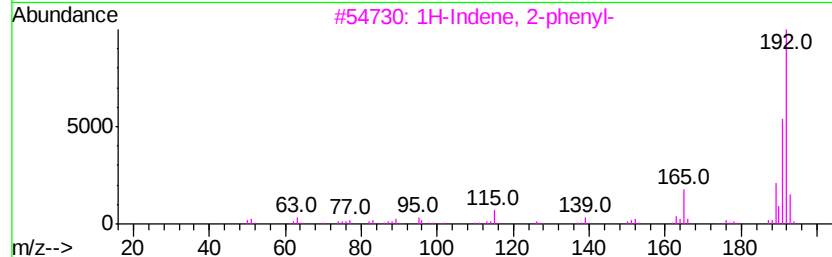
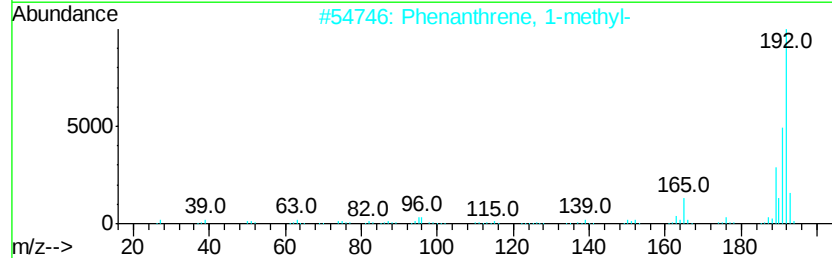
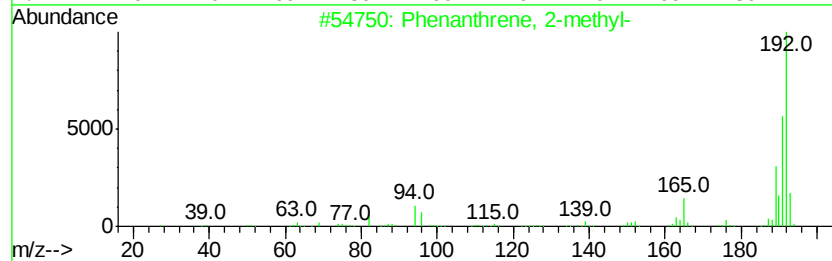
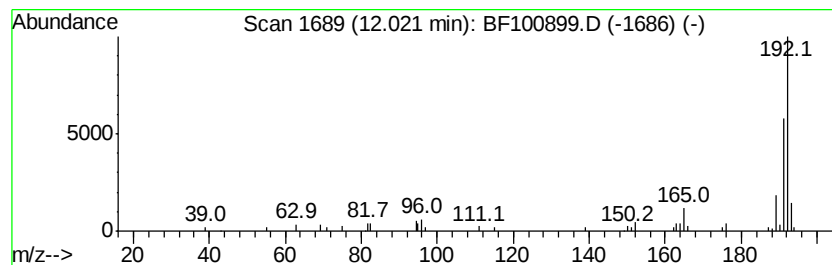
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.66 ng	69379	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91	
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90	
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	90	
4	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	90	
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	90	



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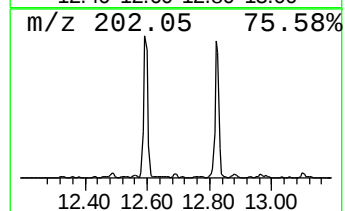
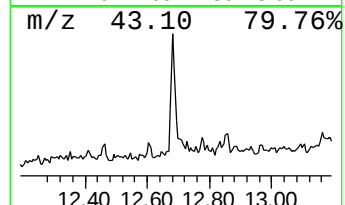
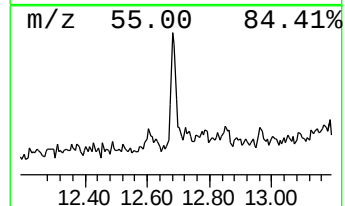
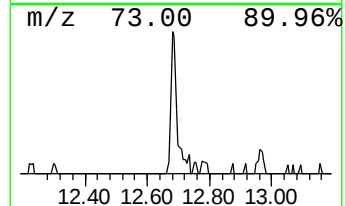
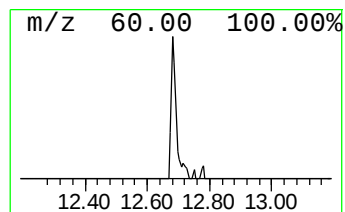
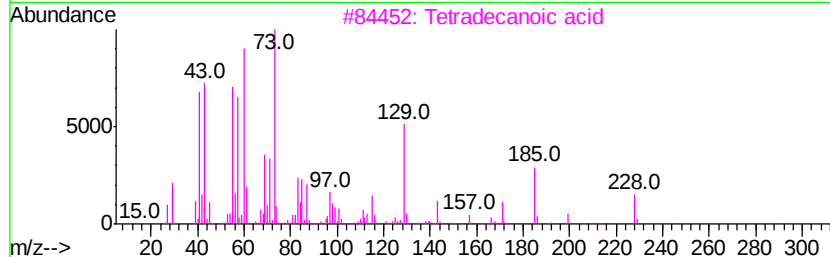
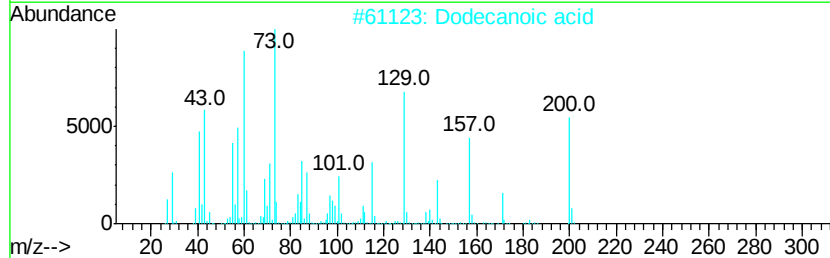
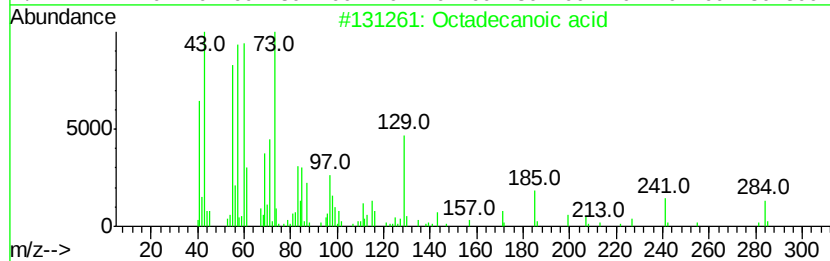
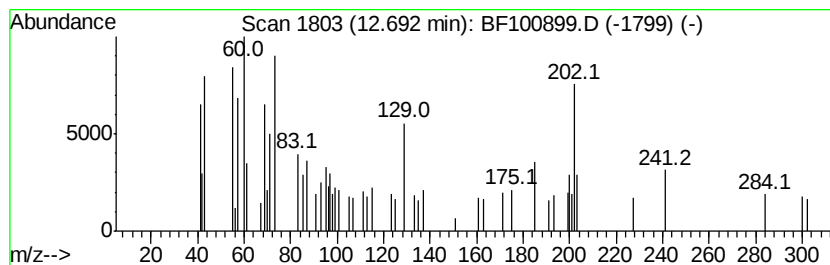
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Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.69	2.55 ng	66548	Phenanthrene-d10	11.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Dodecanoic acid	200	C12H24O2	000143-07-7	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112717\
Data File : BF100899.D
Acq On : 27 Nov 2017 18:28
Operator : SJ/JU
Sample : I6548-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAU-4-E(4-5)

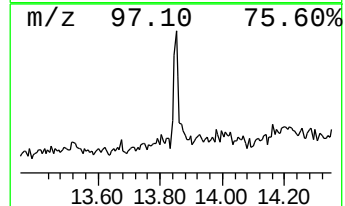
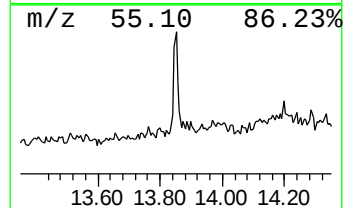
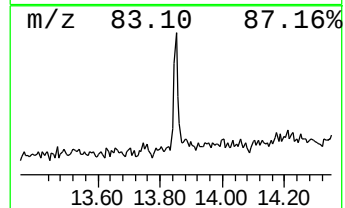
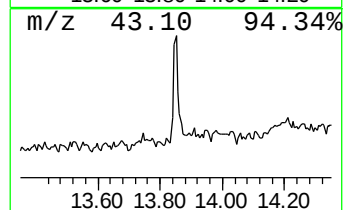
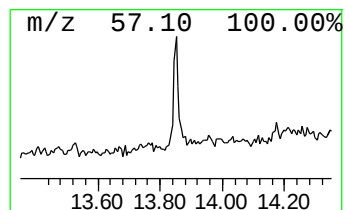
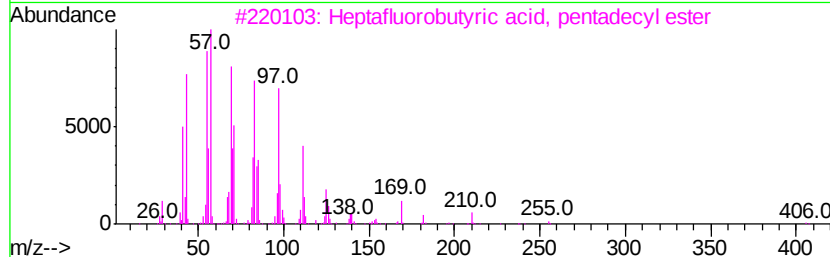
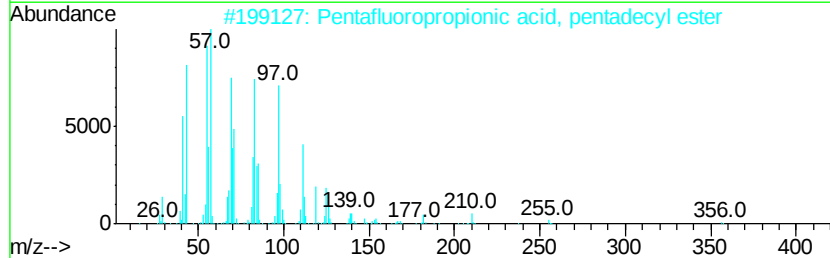
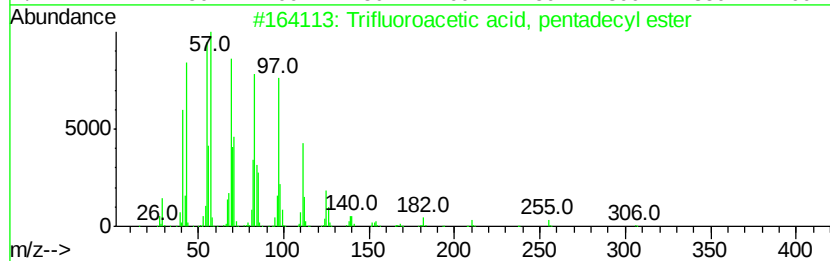
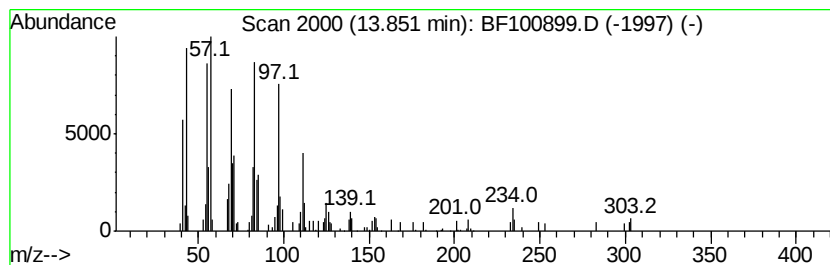
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.91 ng	99276	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	93
5		Trifluoroacetoxyl hexadecane	338	C18H33F3O2	006222-03-3	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112717\
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAU-4-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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
unknown5.08	5.08	4.5	ng	93579	1	6.86	416104	20.0
unknown6.63	6.63	61.0	ng	1268960	1	6.86	416104	20.0
n-Hexadecanoic acid	11.90	8.2	ng	214381	4	11.38	521997	20.0
Phenanthrene, 2-m...	12.02	2.7	ng	69379	4	11.38	521997	20.0
Octadecanoic acid	12.69	2.5	ng	66548	4	11.38	521997	20.0
Trifluoroacetic a...	13.85	3.9	ng	99276	5	14.02	507899	20.0