

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
 Data File : BF100793.D
 Acq On : 21 Nov 2017 21:00
 Operator : SJ/JU
 Sample : I6499-05
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PG1-1-E(7-8)

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	5.098	509	512	521	rBV	93081	122379	6.01%	0.723%
2	5.493	574	579	582	rBV	1690631	1601250	78.69%	9.461%
3	6.504	745	751	755	rBV	1608187	1792933	88.10%	10.593%
4	6.640	770	774	778	rBV	1695061	1738198	85.42%	10.270%
5	6.875	810	814	817	rBV	469032	416461	20.46%	2.461%
6	7.028	836	840	843	rBV	1495437	1287539	63.27%	7.607%
7	7.434	904	909	912	rBV	1108820	1078852	53.01%	6.374%
8	7.510	916	922	928	rVB	28202	29036	1.43%	0.172%
9	8.151	1027	1031	1035	rBV	628215	527062	25.90%	3.114%
10	9.228	1209	1214	1217	rBV	2267647	2034997	100.00%	12.023%
11	9.616	1277	1280	1283	rBV	171755	146003	7.17%	0.863%
12	9.833	1313	1317	1320	rBV	59281	51888	2.55%	0.307%
13	9.910	1326	1330	1334	rBV	618630	531640	26.12%	3.141%
14	10.304	1395	1397	1399	rBV	29002	23133	1.14%	0.137%
15	10.333	1399	1402	1404	rVB	59186	51018	2.51%	0.301%
16	10.698	1460	1464	1467	rBV	1145379	978116	48.06%	5.779%
17	10.804	1479	1482	1491	rVB	65588	70922	3.49%	0.419%
18	11.251	1555	1558	1560	rBV	48228	33967	1.67%	0.201%
19	11.392	1579	1582	1585	rBV	514627	458492	22.53%	2.709%
20	11.416	1585	1586	1589	rVB	113529	72020	3.54%	0.426%
21	11.674	1627	1630	1637	rVB2	28797	24709	1.21%	0.146%
22	11.910	1664	1670	1678	rBV3	68032	99584	4.89%	0.588%
23	12.004	1683	1686	1689	rBV2	19846	24597	1.21%	0.145%
24	12.604	1785	1788	1792	rBV	192798	161555	7.94%	0.954%
25	12.698	1801	1804	1807	rBV2	28258	28087	1.38%	0.166%
26	12.833	1821	1827	1833	rBV	164663	175043	8.60%	1.034%
27	12.974	1847	1851	1855	rVB	1362081	1301970	63.98%	7.692%
28	13.051	1860	1864	1868	rBV2	13996	23526	1.16%	0.139%
29	13.263	1897	1900	1903	rVB2	23653	22567	1.11%	0.133%
30	13.668	1966	1969	1973	rVB	37797	35722	1.76%	0.211%
31	13.780	1983	1988	1991	rBV3	24069	32729	1.61%	0.193%
32	13.863	1999	2002	2010	rVB2	93297	128239	6.30%	0.758%
33	14.033	2023	2031	2033	rBV2	517726	590475	29.02%	3.489%
34	14.057	2033	2035	2041	rVB	117991	106873	5.25%	0.631%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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35	14.415	2092	2096	2099	rBV	33943	35956	1.77%	0.212%
36	14.498	2106	2110	2111	rBV3	27710	35904	1.76%	0.212%
37	15.074	2203	2208	2211	rBV2	110752	175185	8.61%	1.035%
38	15.133	2215	2218	2223	rVV7	15906	26158	1.29%	0.155%
39	15.180	2223	2226	2229	rVB	28433	30673	1.51%	0.181%
40	15.374	2256	2259	2266	rVB	63343	86367	4.24%	0.510%
41	15.439	2266	2270	2276	rBV	92506	115455	5.67%	0.682%
42	15.504	2276	2281	2285	rBV2	353880	468766	23.04%	2.770%
43	15.951	2354	2357	2362	rVB5	16305	23908	1.17%	0.141%
44	16.980	2528	2532	2539	rVB3	36858	72640	3.57%	0.429%
45	17.427	2603	2608	2617	rVB2	25511	53038	2.61%	0.313%

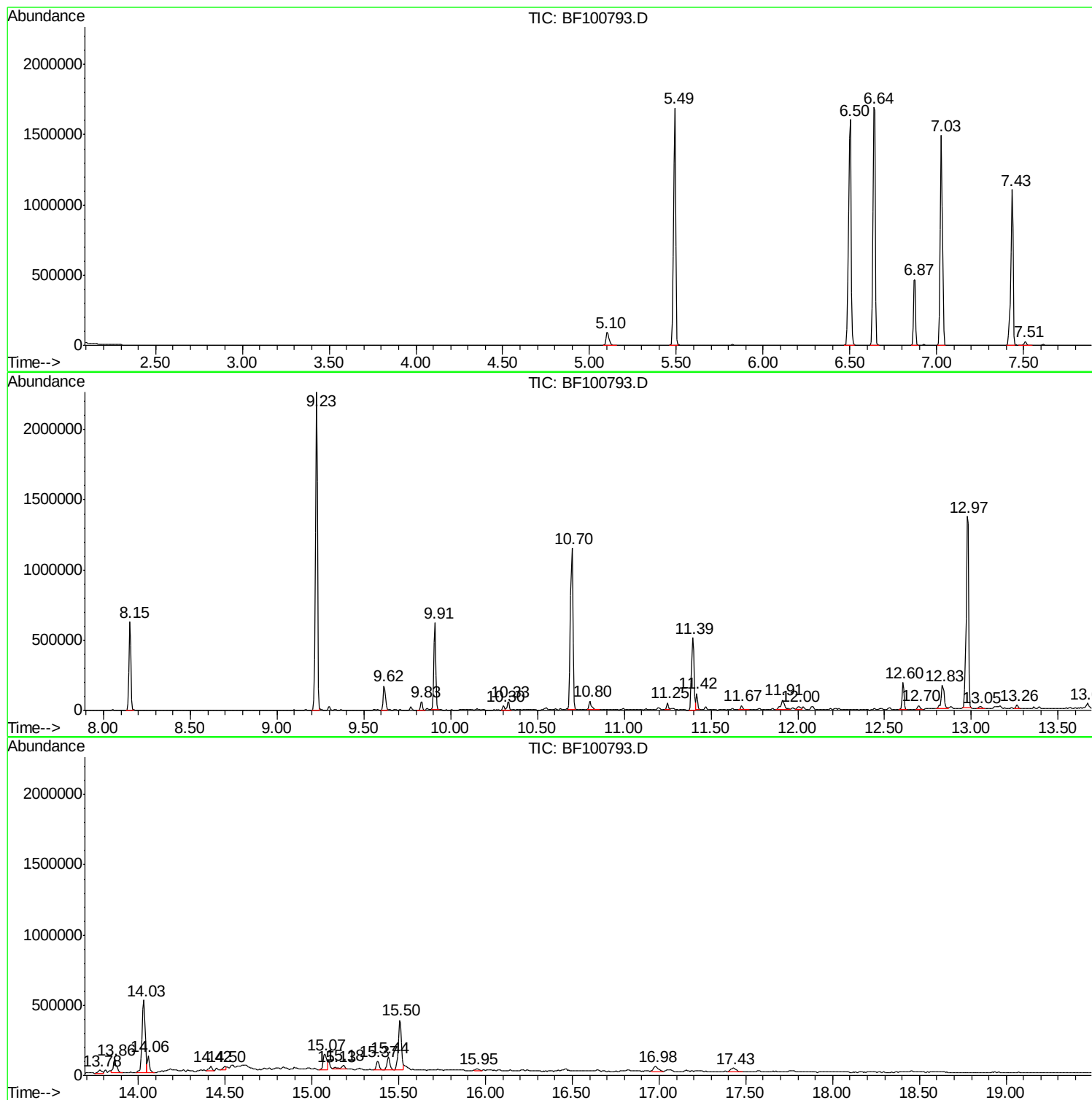
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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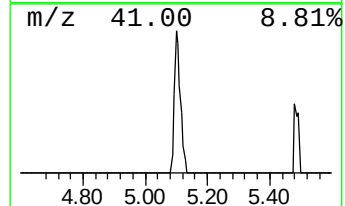
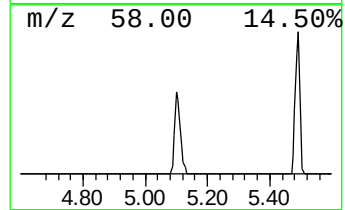
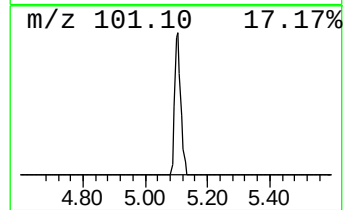
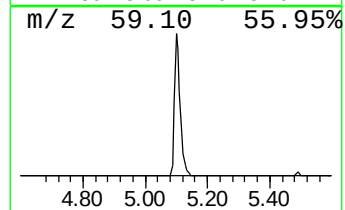
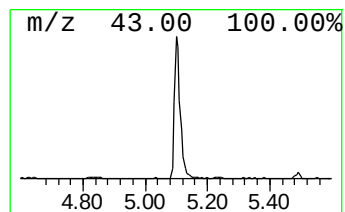
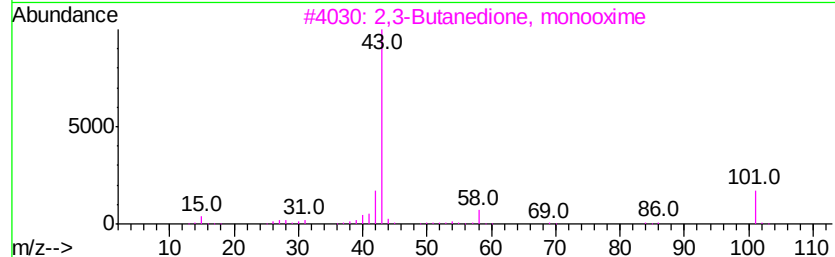
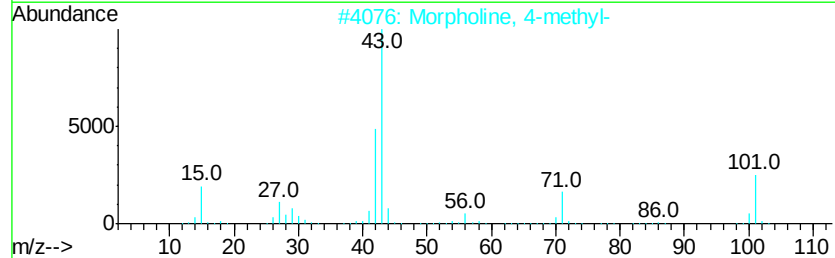
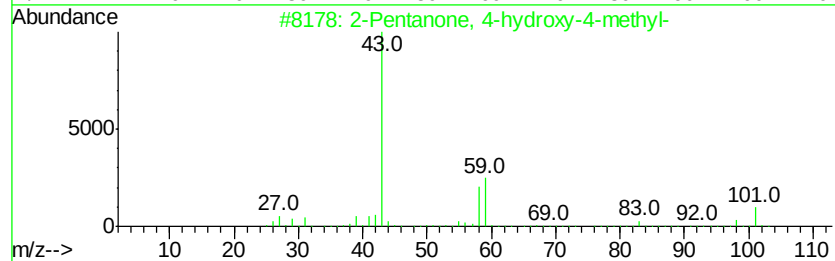
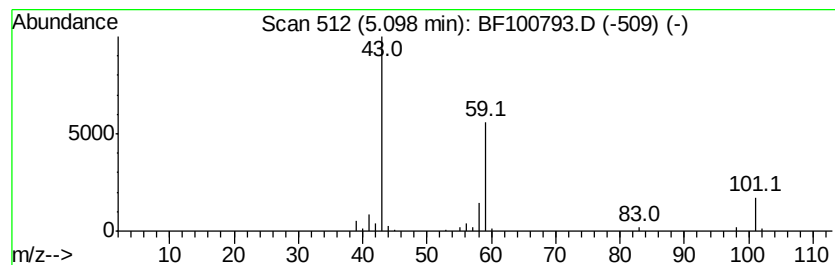
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	5.88 ng	122379	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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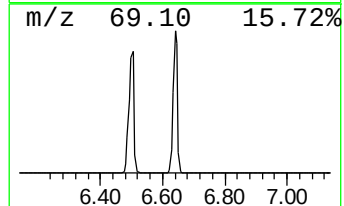
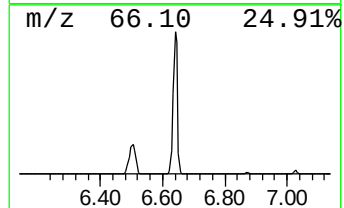
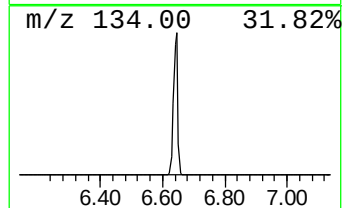
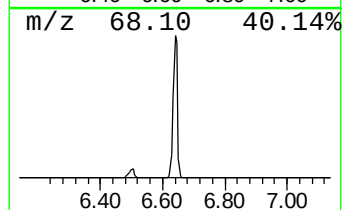
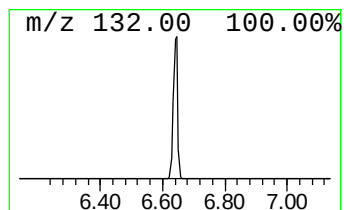
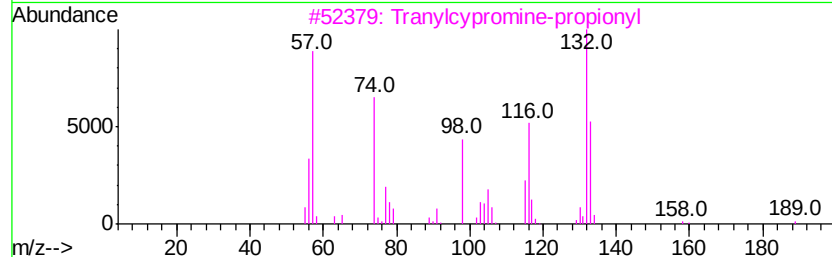
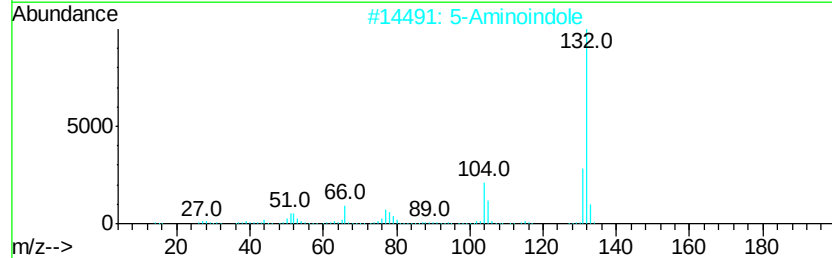
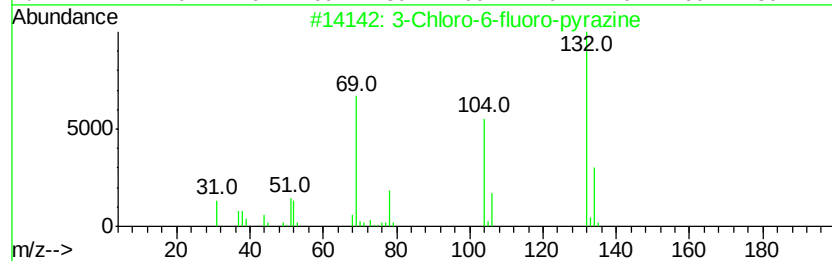
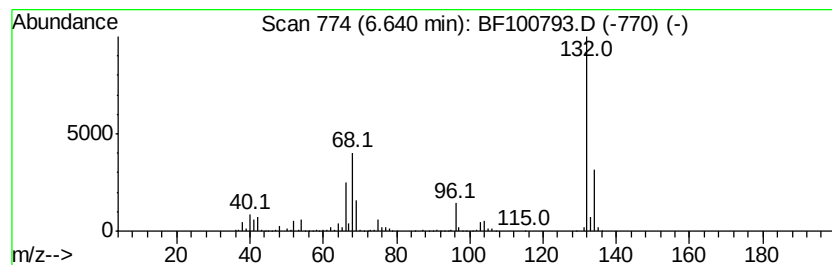
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Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	83.47 ng	1738200	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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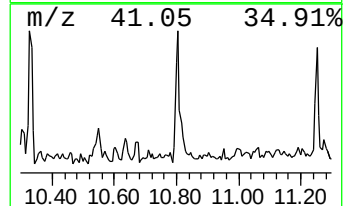
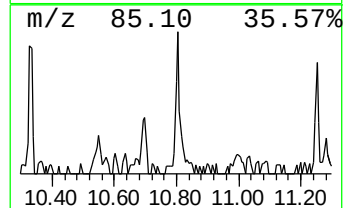
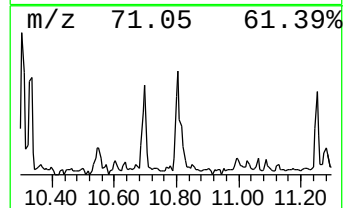
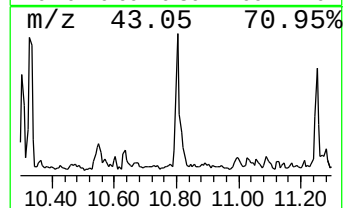
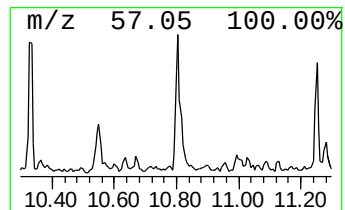
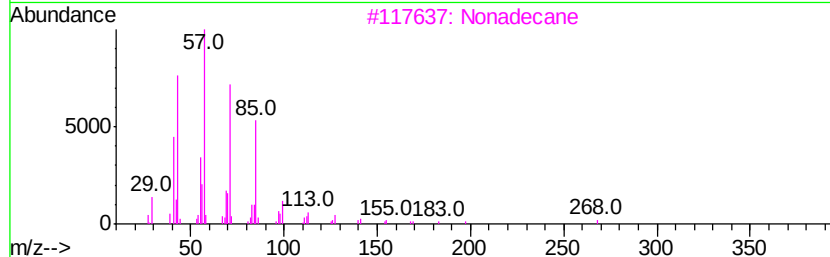
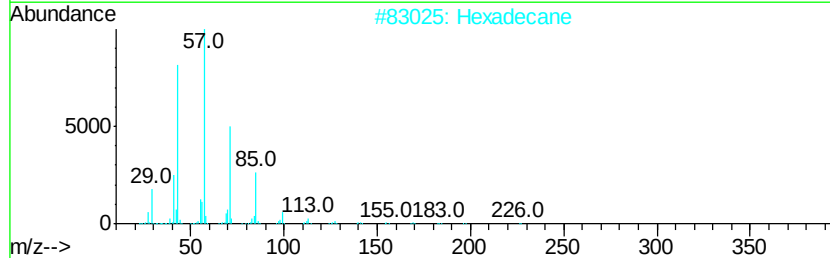
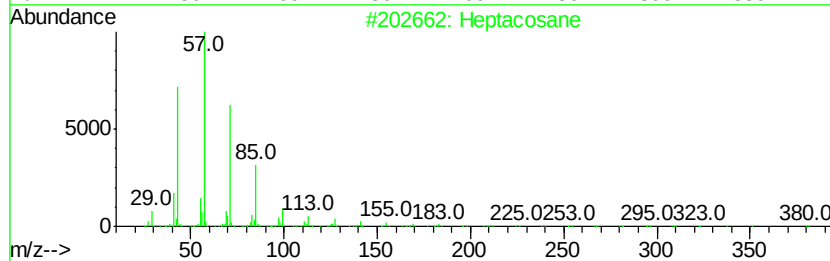
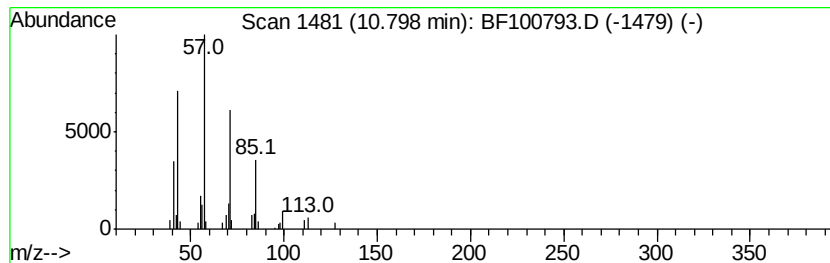
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	3.09 ng	70922	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	90
2		Hexadecane	226	C16H34	000544-76-3	90
3		Nonadecane	268	C19H40	000629-92-5	87
4		Tridecane	184	C13H28	000629-50-5	86
5		Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86



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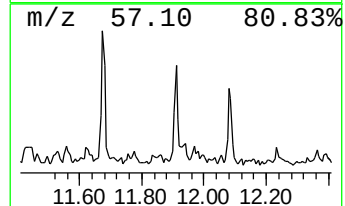
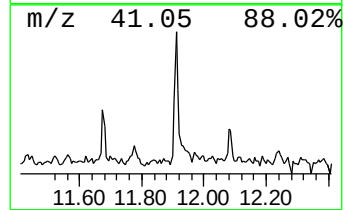
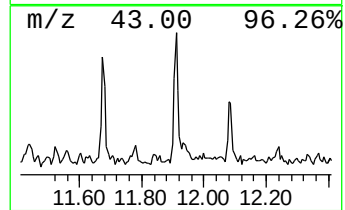
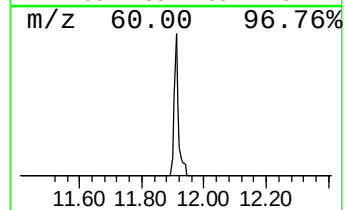
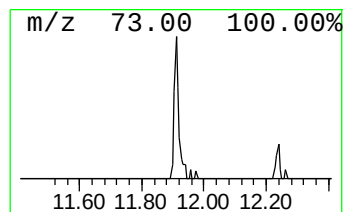
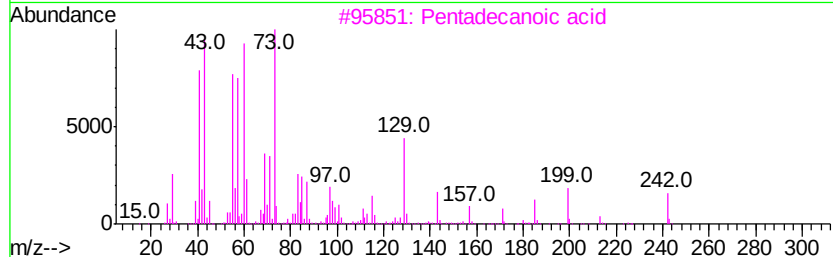
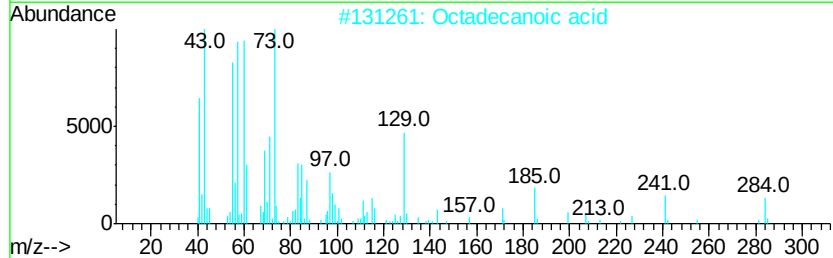
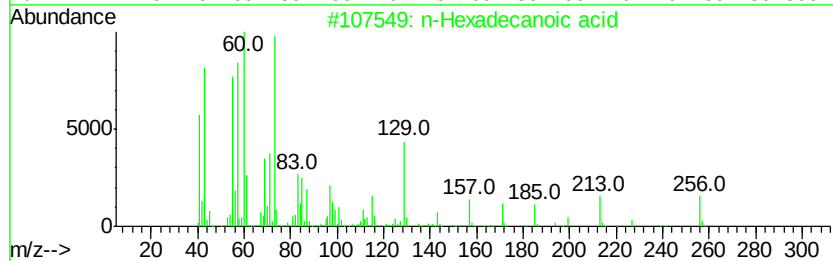
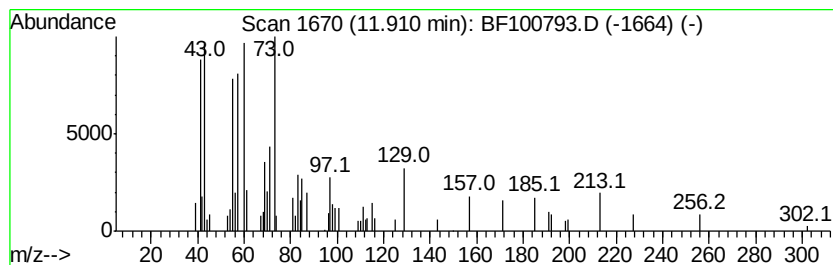
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	4.34 ng	99584	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Octadecanoic acid	284	C18H36O2	000057-11-4	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64



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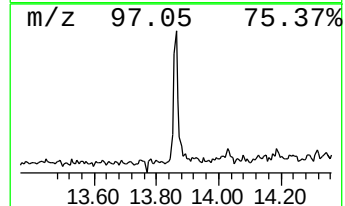
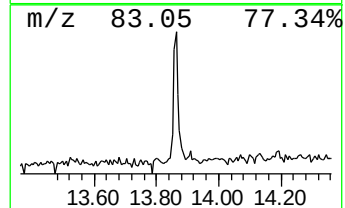
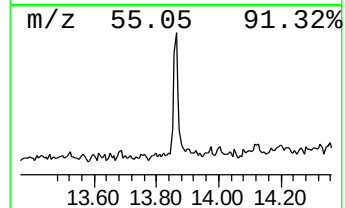
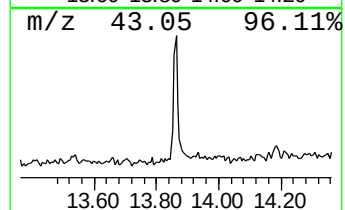
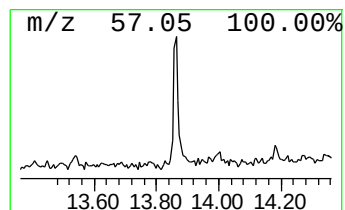
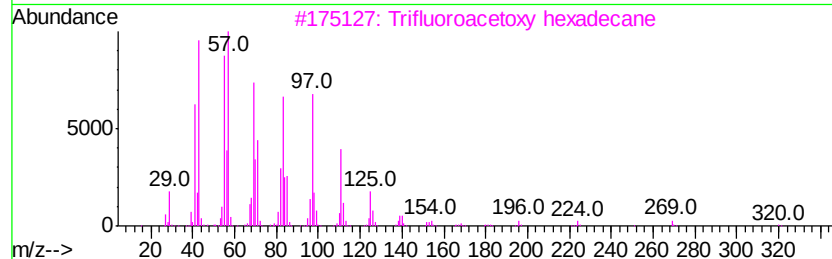
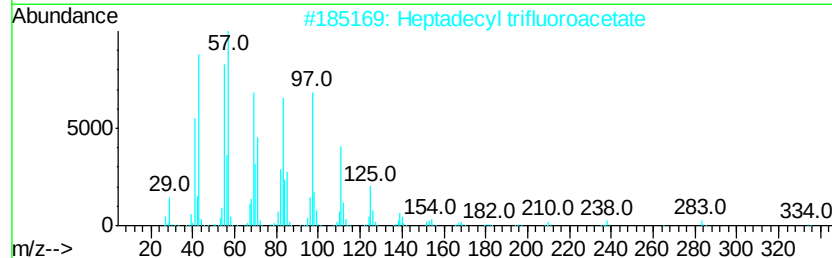
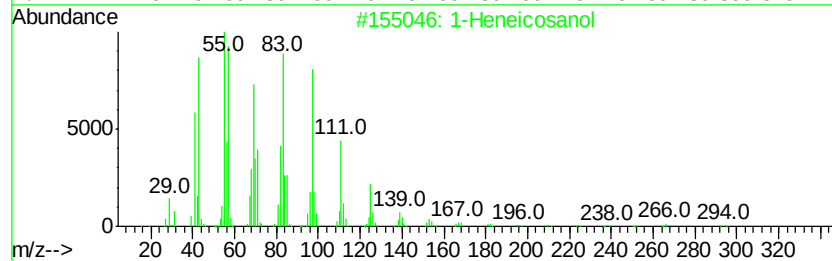
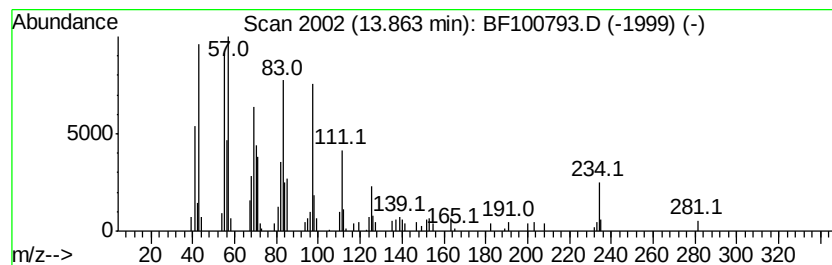
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.34 ng	128239	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4		Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	91
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100793.D
Acq On : 21 Nov 2017 21:00
Operator : SJ/JU
Sample : I6499-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PG1-1-E(7-8)

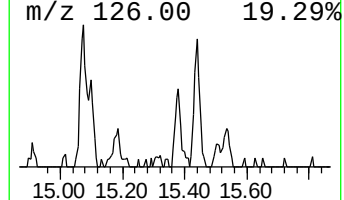
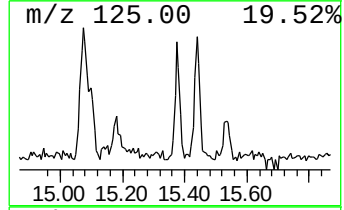
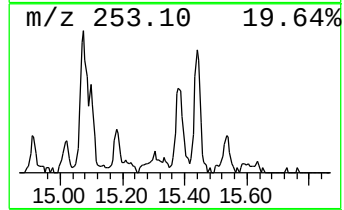
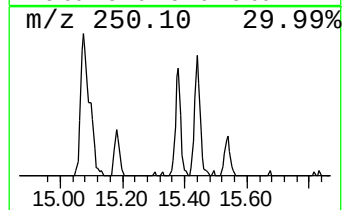
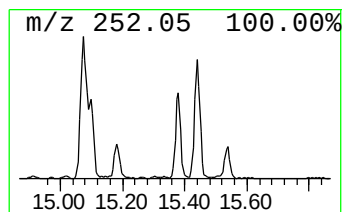
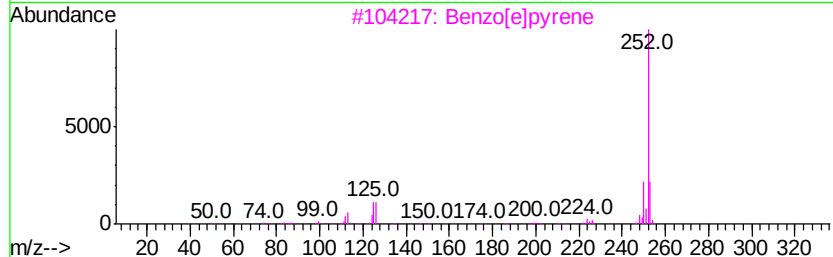
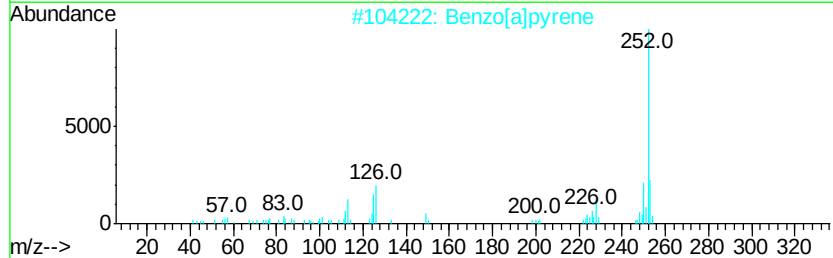
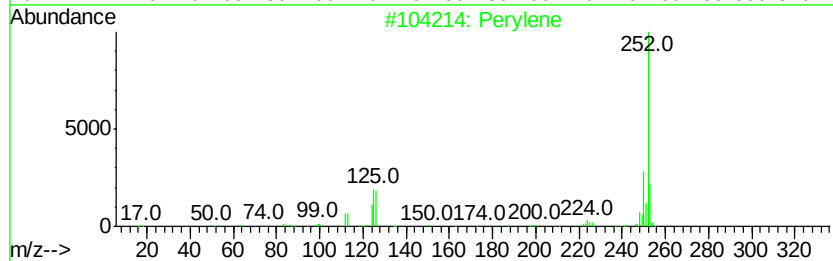
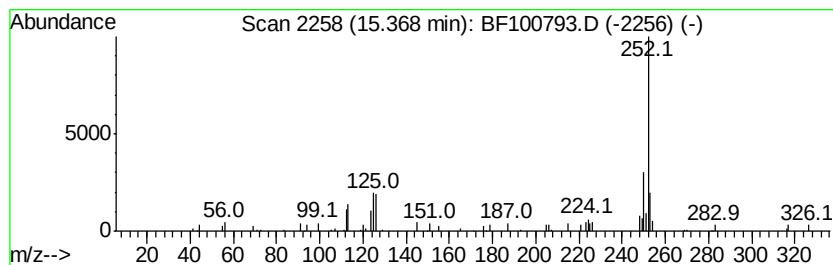
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	3.68 ng	86367	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	93
2		Benzo[a]pyrene	252	C20H12	000050-32-8	93
3		Benzo[e]pyrene	252	C20H12	000192-97-2	93
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	93
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100793.D
Acq On : 21 Nov 2017 21:00
Operator : SJ/JU
Sample : I6499-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PG1-1-E(7-8)

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
2-Pentanone, 4-hy...	5.10	5.9	ng	122379	1	6.87	416461	20.0
unknown6.64	6.64	83.5	ng	1738200	1	6.87	416461	20.0
Heptacosane	10.80	3.1	ng	70922	4	11.39	458492	20.0
n-Hexadecanoic acid	11.91	4.3	ng	99584	4	11.39	458492	20.0
1-Heneicosanol	13.86	4.3	ng	128239	5	14.03	590475	20.0
Perylene	15.37	3.7	ng	86367	6	15.50	468766	20.0