

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071817\
 Data File : BF096851.D
 Acq On : 18 Jul 2017 16:46
 Operator : SJ/JU
 Sample : I4248-05
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-COMP-(0-8)

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-BF071317.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	4.787	472	476	492	rVB	243651	399841	11.58%	1.292%
2	5.216	543	549	552	rBV	3066881	3313131	95.95%	10.705%
3	6.257	720	726	730	rBV	2822239	3453002	100.00%	11.157%
4	6.375	740	746	749	rBV	3104480	3258539	94.37%	10.529%
5	6.598	780	784	787	rBV	836845	708060	20.51%	2.288%
6	6.757	806	811	814	rBV	2583950	2399618	69.49%	7.754%
7	7.163	874	880	883	rBV	1915223	2198159	63.66%	7.103%
8	7.881	997	1002	1004	rBV	1084366	987860	28.61%	3.192%
9	7.898	1004	1005	1009	rVB	64595	39950	1.16%	0.129%
10	8.957	1180	1185	1189	rBV	2921762	3152979	91.31%	10.188%
11	9.051	1198	1201	1205	rVB2	50805	43979	1.27%	0.142%
12	9.351	1248	1252	1255	rBV	444916	346363	10.03%	1.119%
13	9.580	1287	1291	1294	rVB	52632	42494	1.23%	0.137%
14	9.628	1294	1299	1302	rBV	1138153	1019772	29.53%	3.295%
15	9.828	1331	1333	1338	rVB2	40849	39398	1.14%	0.127%
16	10.075	1372	1375	1378	rVB	83482	69977	2.03%	0.226%
17	10.298	1408	1413	1415	rBV2	32333	41343	1.20%	0.134%
18	10.416	1428	1433	1436	rBV	1841789	1807478	52.35%	5.840%
19	10.545	1451	1455	1465	rBV	104321	132896	3.85%	0.429%
20	10.910	1514	1517	1522	rVB	51223	46040	1.33%	0.149%
21	10.992	1528	1531	1534	rBV2	82616	66463	1.92%	0.215%
22	11.104	1545	1550	1552	rBV	919605	901619	26.11%	2.913%
23	11.122	1552	1553	1557	rVV	297651	227361	6.58%	0.735%
24	11.174	1557	1562	1566	rVB	81321	72329	2.09%	0.234%
25	11.627	1637	1639	1641	rBV	66448	49932	1.45%	0.161%
26	11.710	1650	1653	1655	rBV	64210	58538	1.70%	0.189%
27	11.821	1669	1672	1677	rVB2	43335	46756	1.35%	0.151%
28	11.898	1680	1685	1687	rBV	52340	59475	1.72%	0.192%
29	12.151	1725	1728	1731	rBV3	34102	38360	1.11%	0.124%
30	12.210	1735	1738	1740	rVV2	48360	43334	1.25%	0.140%
31	12.233	1740	1742	1746	rVB2	39526	36737	1.06%	0.119%
32	12.304	1751	1754	1759	rBV	500163	455719	13.20%	1.472%
33	12.533	1788	1793	1795	rBV	429293	443297	12.84%	1.432%
34	12.580	1799	1801	1807	rVB3	43323	48619	1.41%	0.157%

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TP-1-COMP-(0-8)

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.686	1815	1819	1822	rBV	2053989	1958208	56.71%	6.327%
36	12.863	1847	1849	1853	rVB	48363	43718	1.27%	0.141%
37	12.927	1858	1860	1863	rVB3	35547	37295	1.08%	0.121%
38	12.963	1863	1866	1871	rBV4	50665	71831	2.08%	0.232%
39	13.368	1932	1935	1939	rBV	50515	50541	1.46%	0.163%
40	13.474	1950	1953	1956	rBV	50800	47994	1.39%	0.155%
41	13.592	1967	1973	1978	rBV2	104353	162142	4.70%	0.524%
42	13.727	1991	1996	1998	rBV2	709382	797134	23.09%	2.576%
43	13.751	1998	2000	2003	rVB	193227	141416	4.10%	0.457%
44	14.721	2161	2165	2173	rVB	217153	361473	10.47%	1.168%
45	14.815	2179	2181	2184	rVB	55021	47711	1.38%	0.154%
46	14.986	2207	2210	2215	rVB	122822	140786	4.08%	0.455%
47	15.039	2216	2219	2224	rVB	158165	173284	5.02%	0.560%
48	15.098	2225	2229	2232	rBV	482539	561782	16.27%	1.815%
49	16.374	2442	2446	2454	rVB2	99630	180064	5.21%	0.582%
50	16.756	2506	2511	2517	rBV	69303	124039	3.59%	0.401%

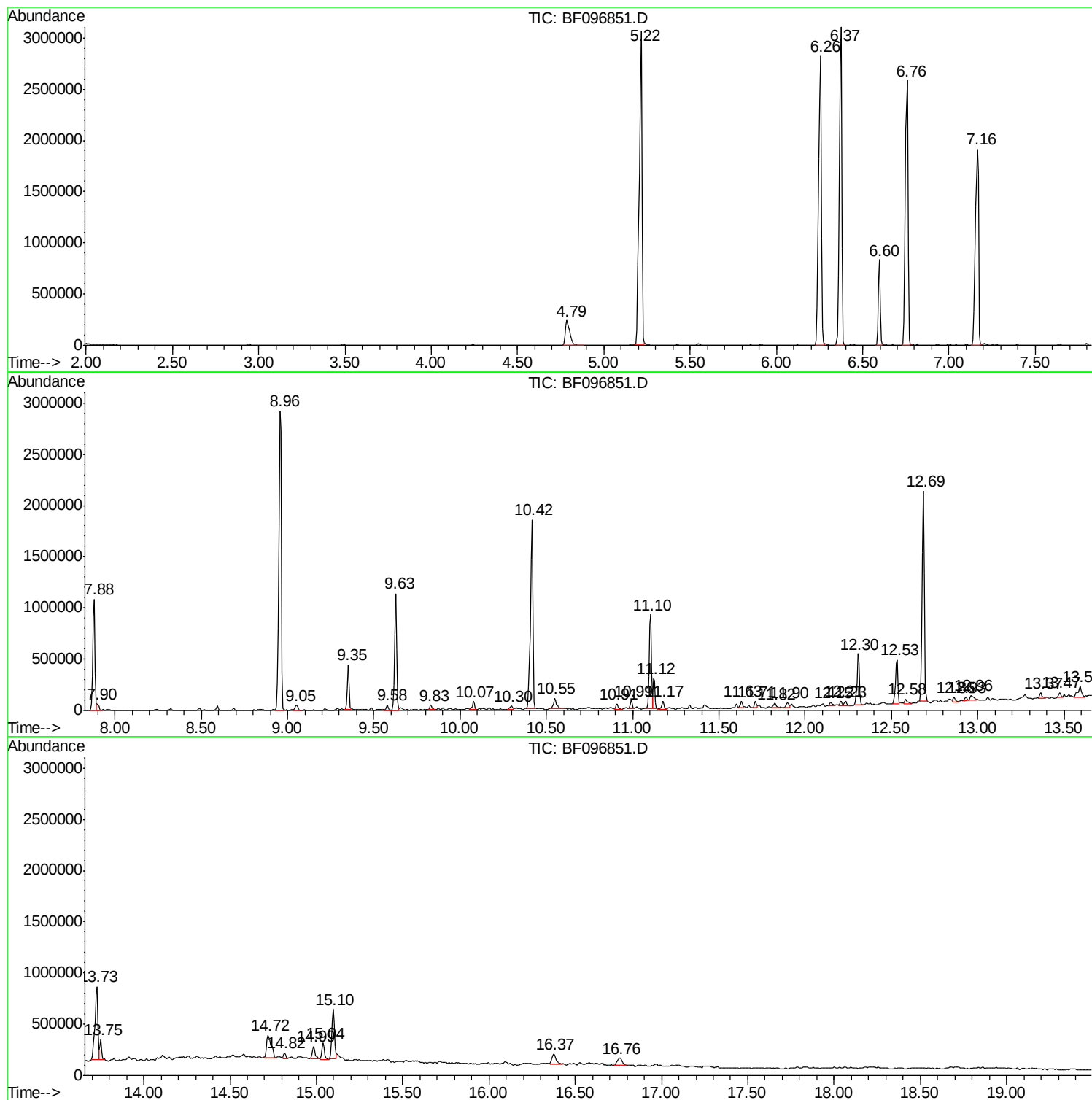
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ClientSampled :
TP-1-COMP-(0-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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Instrument :
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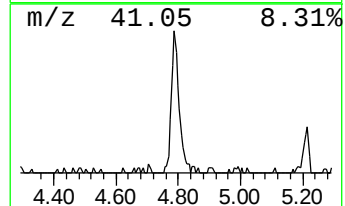
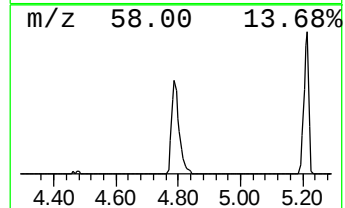
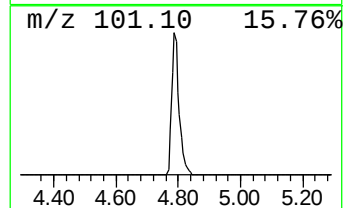
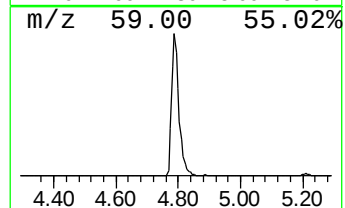
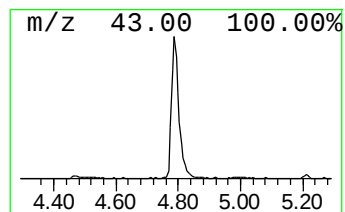
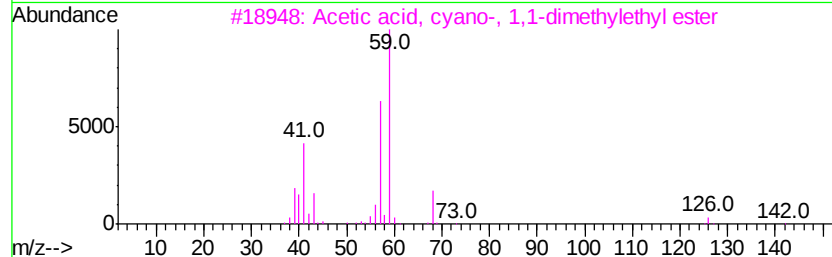
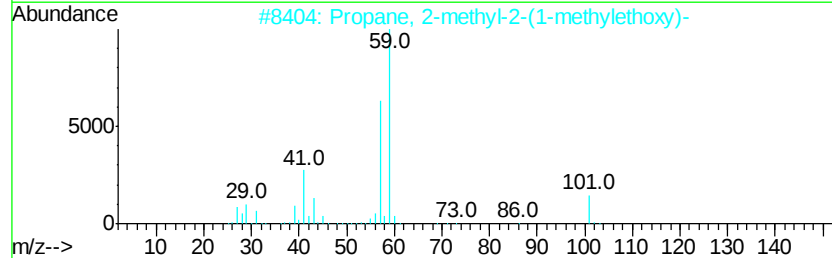
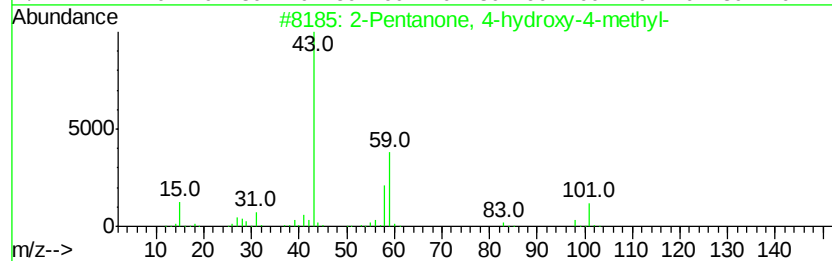
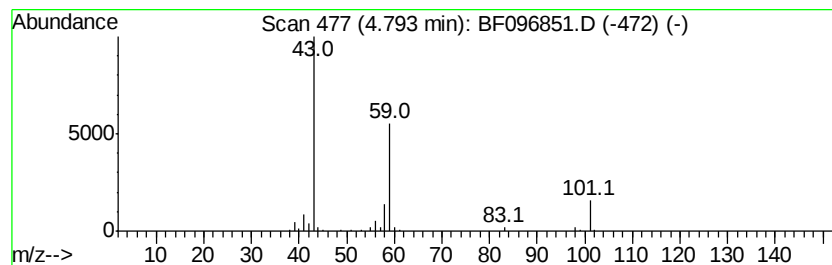
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.79	11.29 ng	399841	1,4-Dichlorobenzene-d4	6.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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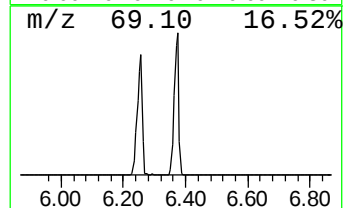
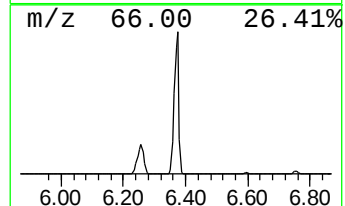
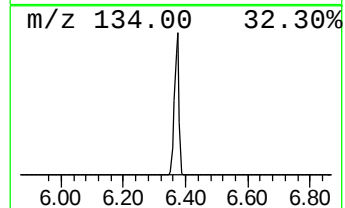
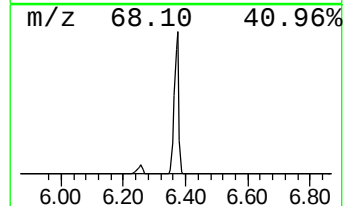
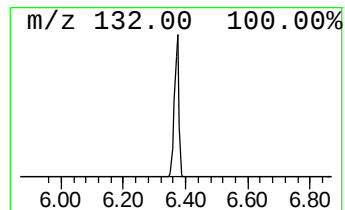
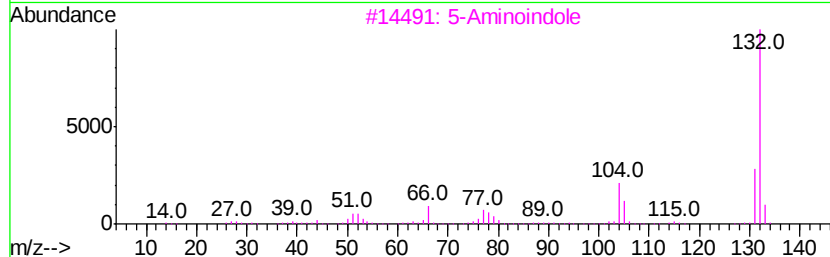
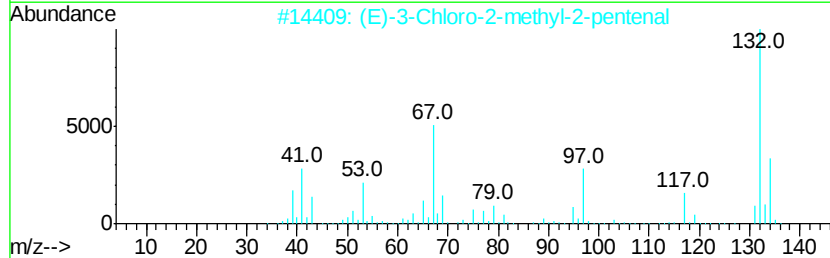
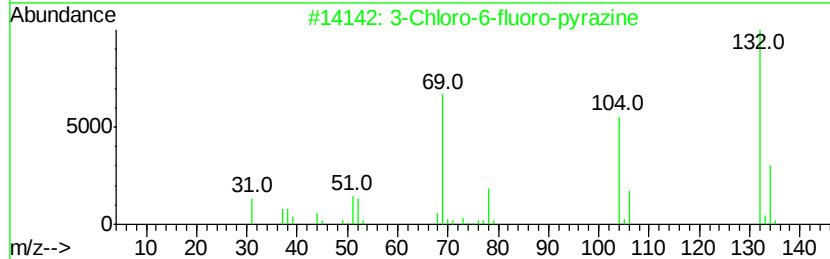
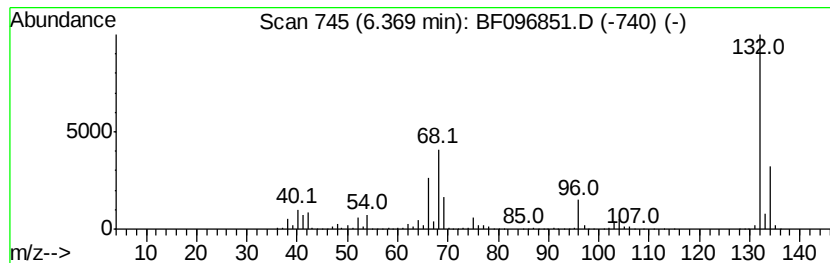
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	92.04 ng	3258540	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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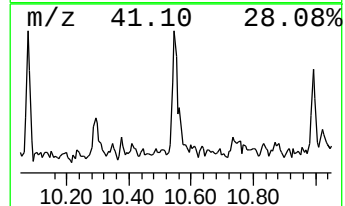
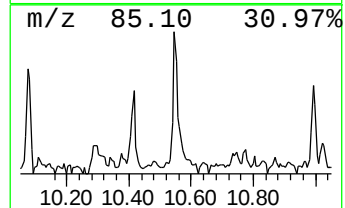
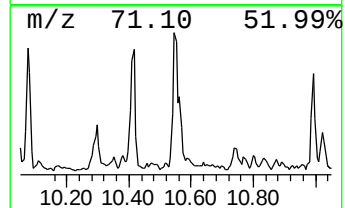
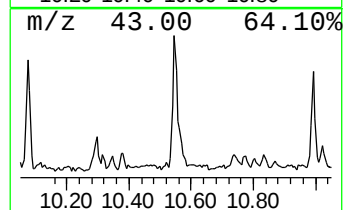
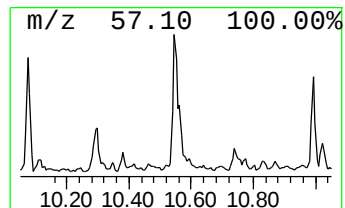
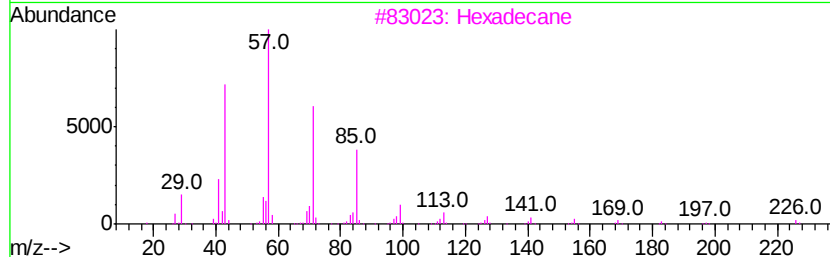
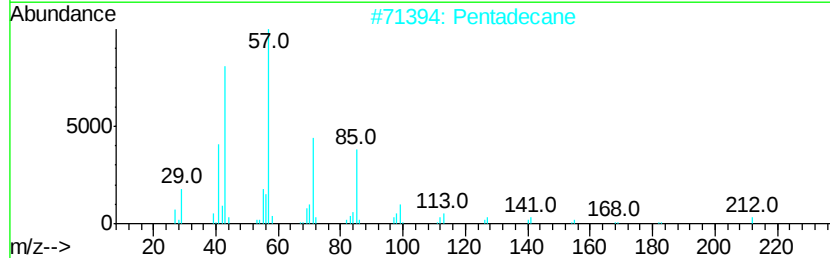
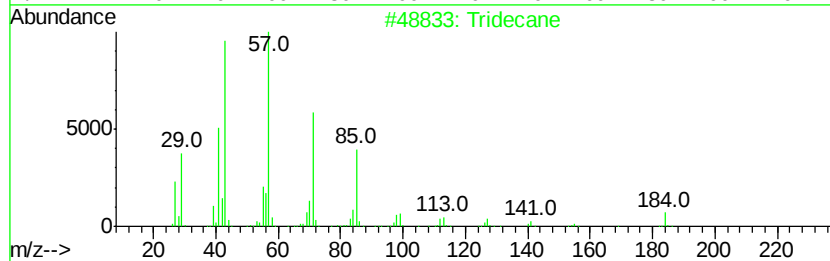
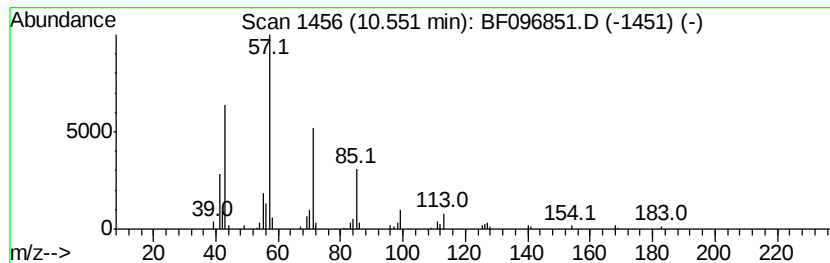
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
10.55	2.95 ng	132896	Phenanthrene-d10		11.10		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	95
2			Pentadecane	212	C15H32	000629-62-9	87
3			Hexadecane	226	C16H34	000544-76-3	86
4			Octacosane	394	C28H58	000630-02-4	86
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86



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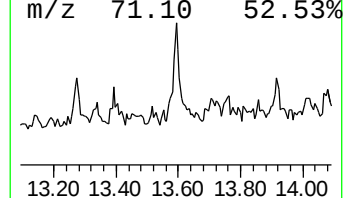
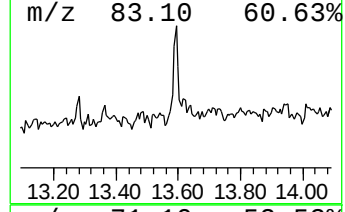
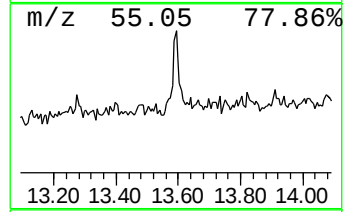
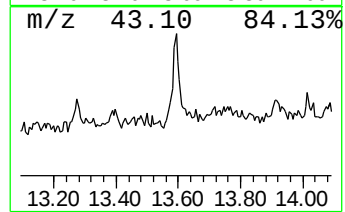
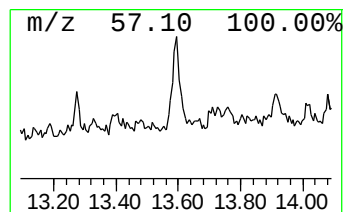
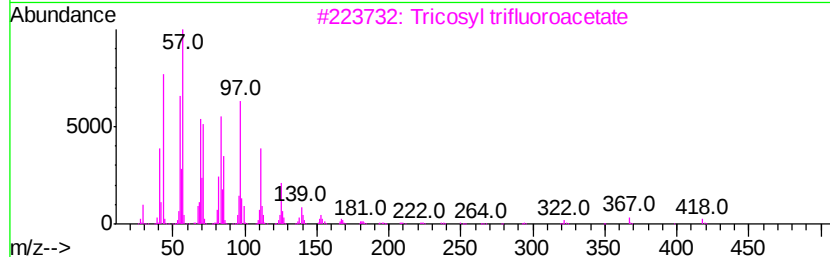
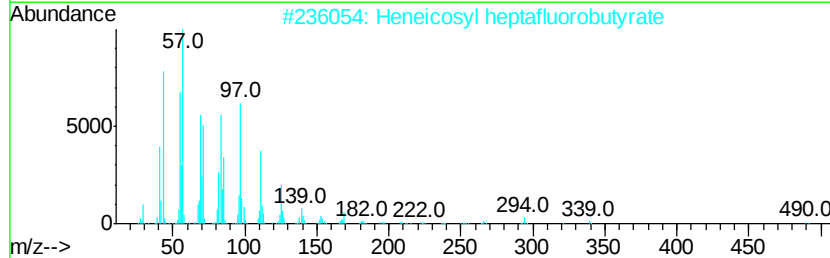
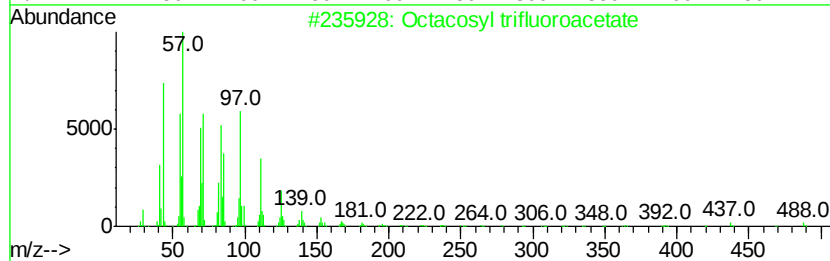
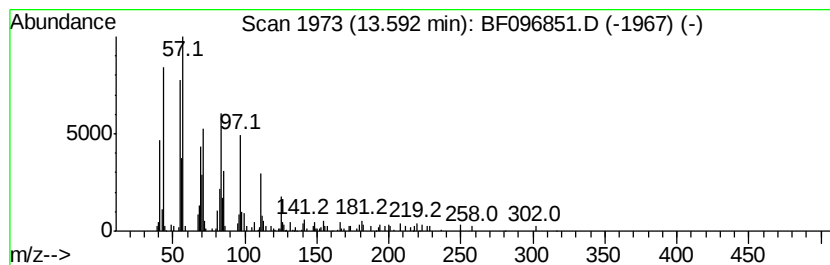
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.59	4.07 ng	162142	Chrysene-d12	13.73	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91



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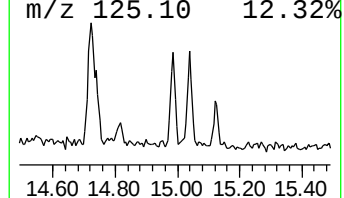
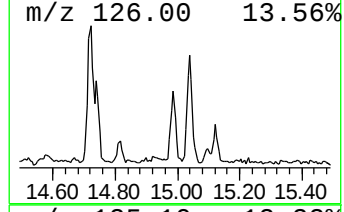
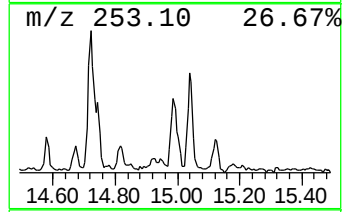
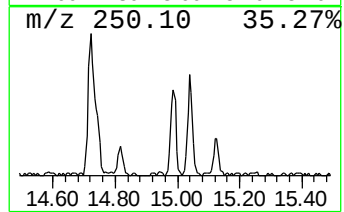
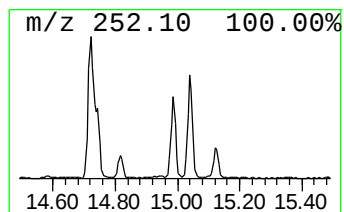
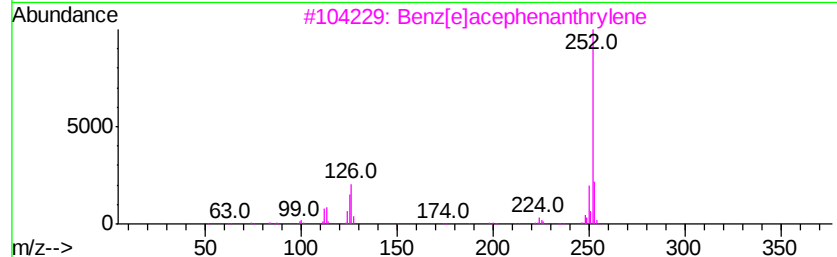
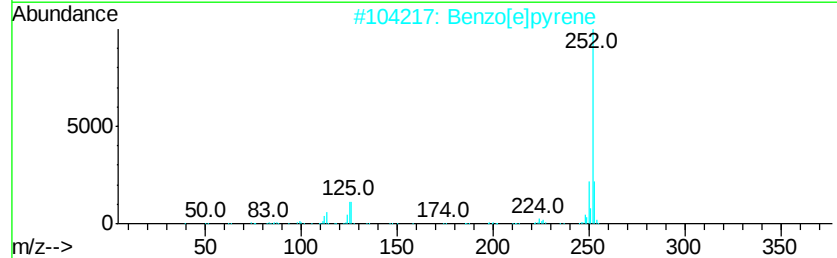
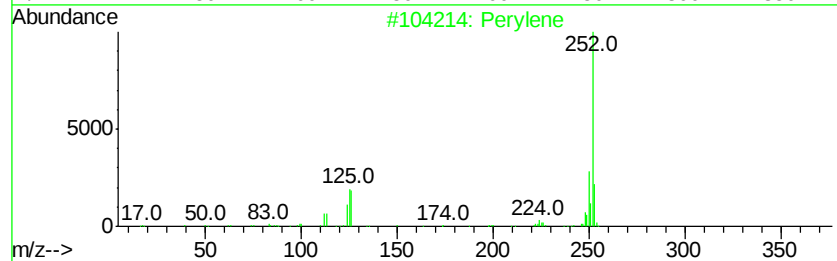
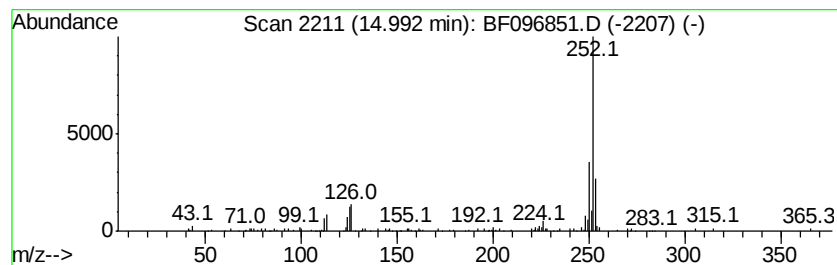
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	5.01 ng	140786	Perylene-d12	15.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Perylene	252	C20H12	000198-55-0	98
2		Benzo[e]pyrene	252	C20H12	000192-97-2	94
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	94
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5		Benzo[a]pyrene	252	C20H12	000050-32-8	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071817\
Data File : BF096851.D
Acq On : 18 Jul 2017 16:46
Operator : SJ/JU
Sample : I4248-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1-COMP-(0-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	4.79	11.3	ng	399841	1	6.60	708060	20.0
unknown6.37	6.37	92.0	ng	3258540	1	6.60	708060	20.0
Tridecane	10.55	3.0	ng	132896	4	11.10	901619	20.0
Octacosyl trifluo...	13.59	4.1	ng	162142	5	13.73	797134	20.0
Perylene	14.99	5.0	ng	140786	6	15.10	561782	20.0