

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101917\
 Data File : BF099664.D
 Acq On : 19 Oct 2017 18:36
 Operator : SJ/JU
 Sample : I5879-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1(6-8)

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-BF092317.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	5.045	500	503	520	rBV	253434	376817	14.76%	1.651%
2	5.451	568	572	587	rBV	2109735	2105891	82.51%	9.226%
3	6.469	740	745	762	rBV	1949947	2162646	84.73%	9.475%
4	6.598	762	767	770	rBV	2174270	2171094	85.06%	9.512%
5	6.816	801	804	813	rBB	607616	524974	20.57%	2.300%
6	6.975	827	831	834	rBV	1946655	1754109	68.72%	7.685%
7	7.386	896	901	904	rBV	1380544	1323053	51.84%	5.796%
8	8.098	1018	1022	1026	rBV	847471	732362	28.69%	3.209%
9	9.175	1199	1205	1208	rBV	2725961	2552362	100.00%	11.182%
10	9.569	1269	1272	1278	rVB	74341	66624	2.61%	0.292%
11	9.851	1315	1320	1324	rBV2	939798	811703	31.80%	3.556%
12	10.645	1451	1455	1458	rBV	1449343	1308124	51.25%	5.731%
13	11.339	1569	1573	1575	rBV	934492	762433	29.87%	3.340%
14	11.363	1575	1577	1581	rVB	295718	228502	8.95%	1.001%
15	11.416	1584	1586	1589	rBV	44100	34281	1.34%	0.150%
16	11.839	1655	1658	1659	rBV	55704	44403	1.74%	0.195%
17	11.869	1662	1663	1668	rVB2	79384	57711	2.26%	0.253%
18	11.951	1674	1677	1680	rBV2	77852	83698	3.28%	0.367%
19	11.974	1680	1681	1684	rVB	42088	27644	1.08%	0.121%
20	12.133	1706	1708	1712	rBV	35667	28826	1.13%	0.126%
21	12.174	1712	1715	1718	rVB2	34413	33092	1.30%	0.145%
22	12.386	1746	1751	1754	rBV	52626	56948	2.23%	0.249%
23	12.486	1764	1768	1771	rBV2	36527	41287	1.62%	0.181%
24	12.557	1776	1780	1783	rBV	434861	392048	15.36%	1.718%
25	12.704	1801	1805	1808	rBV3	22647	25970	1.02%	0.114%
26	12.786	1812	1819	1824	rBV	406968	431913	16.92%	1.892%
27	12.921	1837	1842	1845	rBV	2014931	1855001	72.68%	8.127%
28	13.004	1851	1856	1860	rBV2	27339	44700	1.75%	0.196%
29	13.092	1867	1871	1872	rBV3	24219	30279	1.19%	0.133%
30	13.116	1872	1875	1877	rVB	41000	39123	1.53%	0.171%
31	13.215	1888	1892	1896	rBV2	42659	51795	2.03%	0.227%
32	13.310	1905	1908	1910	rBV	33611	28785	1.13%	0.126%
33	13.339	1910	1913	1916	rVV2	31264	31294	1.23%	0.137%
34	13.627	1959	1962	1965	rVB	34708	29034	1.14%	0.127%

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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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35	13.733	1975	1980	1982	rBV	43543	48207	1.89%	0.211%
36	13.804	1987	1992	1995	rBV3	94919	119575	4.68%	0.524%
37	13.839	1995	1998	2000	rVB	46061	41097	1.61%	0.180%
38	13.980	2017	2022	2025	rBV2	549842	588069	23.04%	2.576%
39	14.010	2025	2027	2031	rVB	118872	97466	3.82%	0.427%
40	14.368	2084	2088	2091	rBV	30481	31428	1.23%	0.138%
41	14.439	2096	2100	2103	rVV5	30719	49120	1.92%	0.215%
42	14.798	2156	2161	2164	rBV2	38081	44751	1.75%	0.196%
43	14.868	2170	2173	2177	rVB3	41085	42102	1.65%	0.184%
44	15.021	2195	2199	2202	rBV	101073	156999	6.15%	0.688%
45	15.086	2207	2210	2215	rVV4	33195	54388	2.13%	0.238%
46	15.127	2215	2217	2221	rVB	28070	29885	1.17%	0.131%
47	15.215	2227	2232	2238	rBV8	13485	32349	1.27%	0.142%
48	15.321	2246	2250	2257	rVB	66530	76967	3.02%	0.337%
49	15.380	2257	2260	2264	rBV	88665	111099	4.35%	0.487%
50	15.445	2264	2271	2275	rBV	369865	494817	19.39%	2.168%
51	15.845	2334	2339	2344	rBV	53658	78597	3.08%	0.344%
52	15.898	2344	2348	2356	rVV8	15894	35814	1.40%	0.157%
53	16.333	2417	2422	2430	rVB4	33152	60238	2.36%	0.264%
54	16.909	2514	2520	2529	rVB	77809	149167	5.84%	0.654%
55	17.080	2546	2549	2556	rBV6	14000	30930	1.21%	0.136%
56	17.356	2590	2596	2602	rBV2	39398	83400	3.27%	0.365%
57	17.592	2631	2636	2647	rVB6	27225	75596	2.96%	0.331%
58	17.909	2685	2690	2697	rVB9	19866	44577	1.75%	0.195%

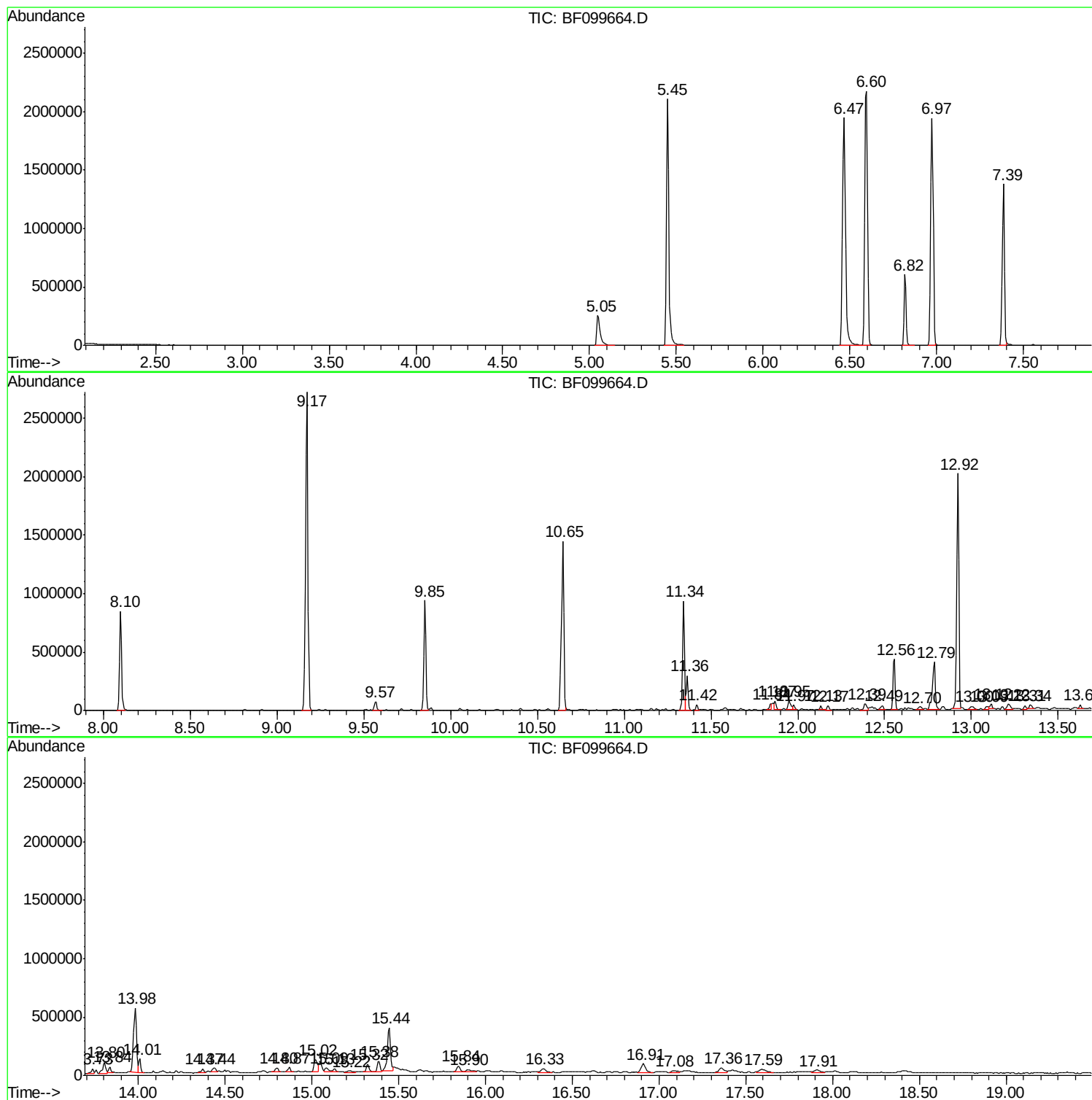
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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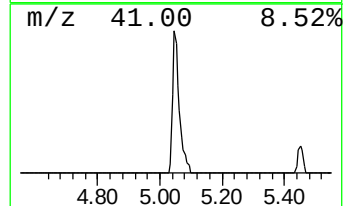
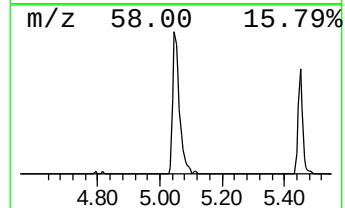
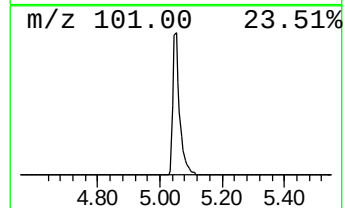
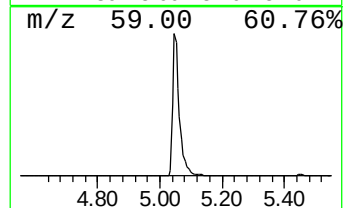
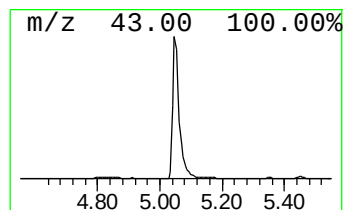
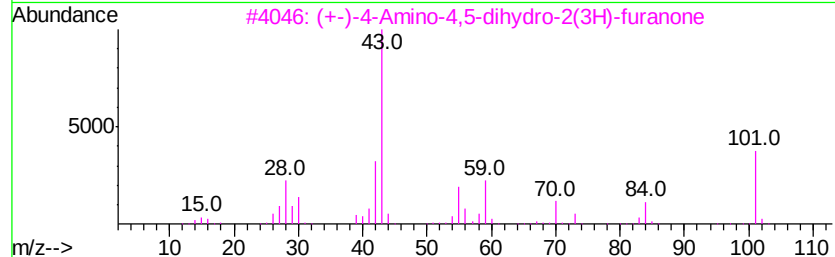
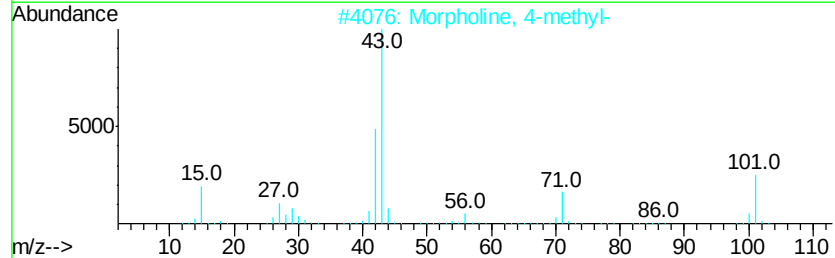
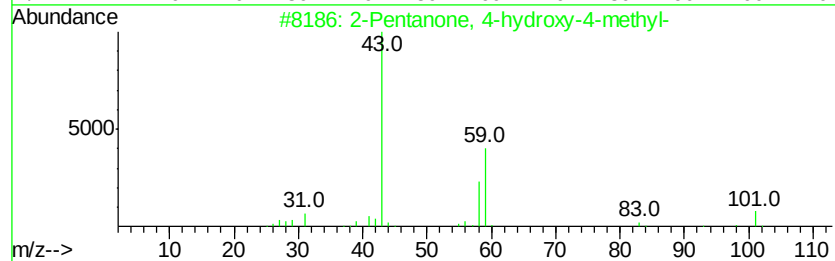
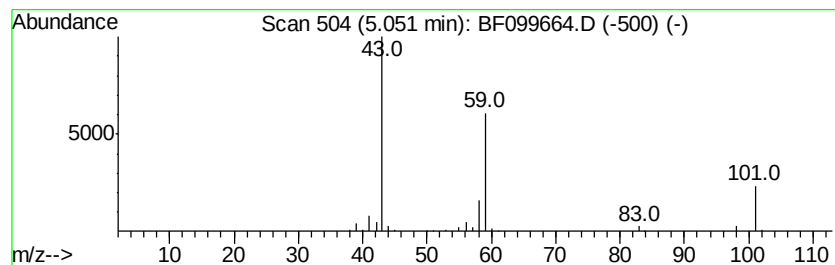
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.05	14.36 ng	376817	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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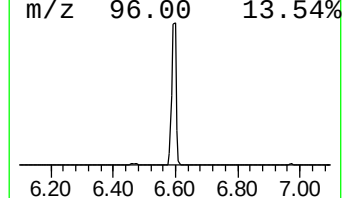
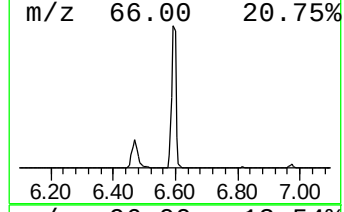
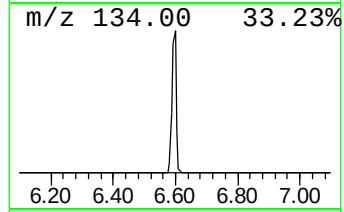
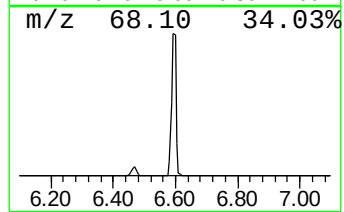
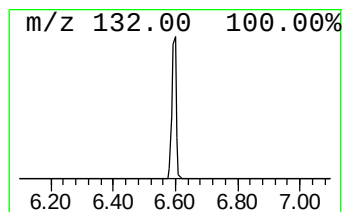
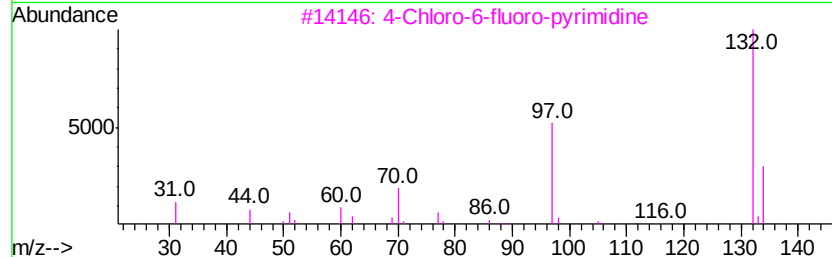
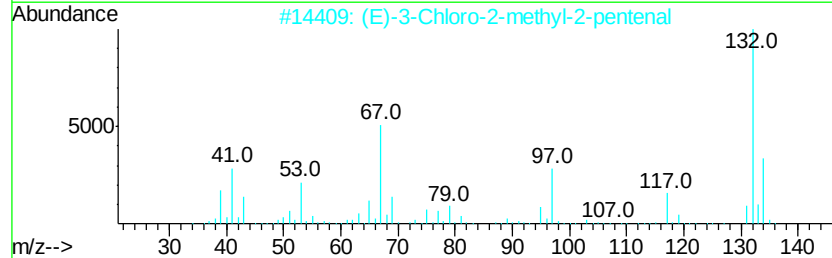
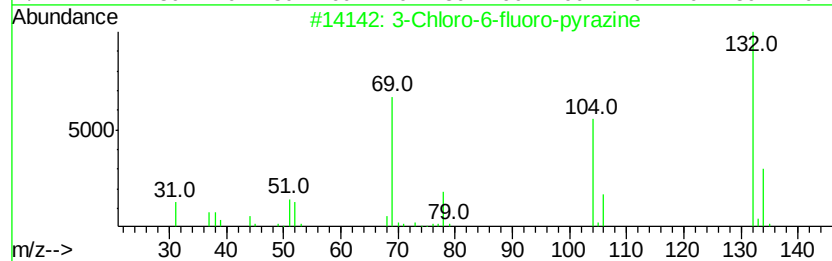
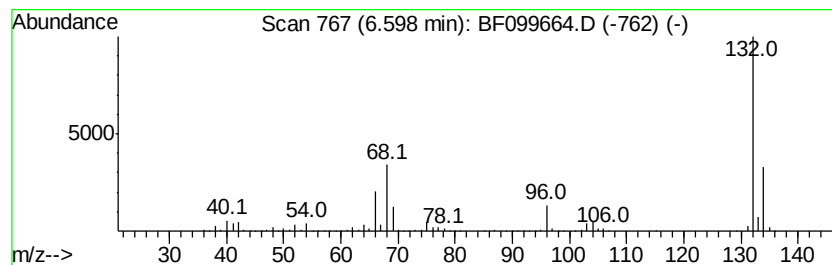
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	82.71 ng	2171090	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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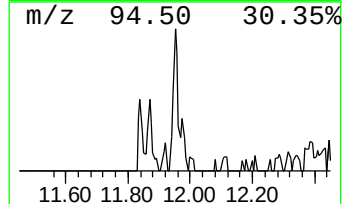
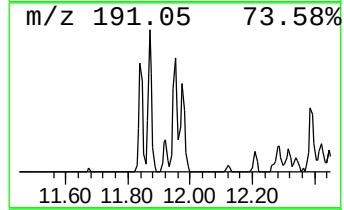
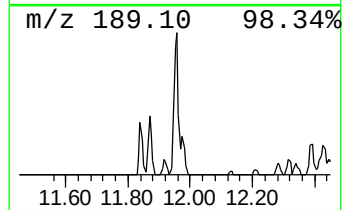
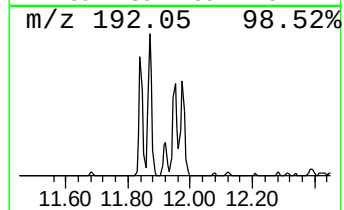
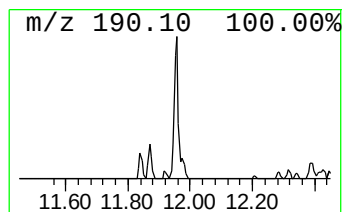
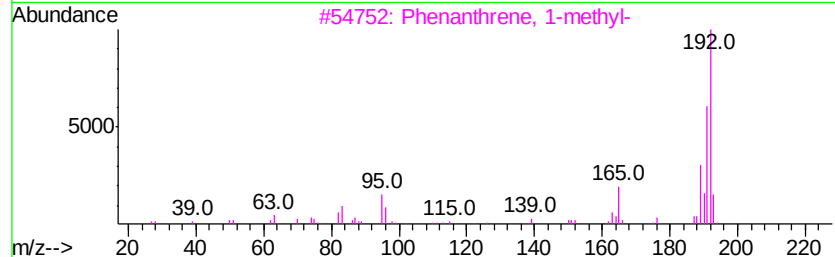
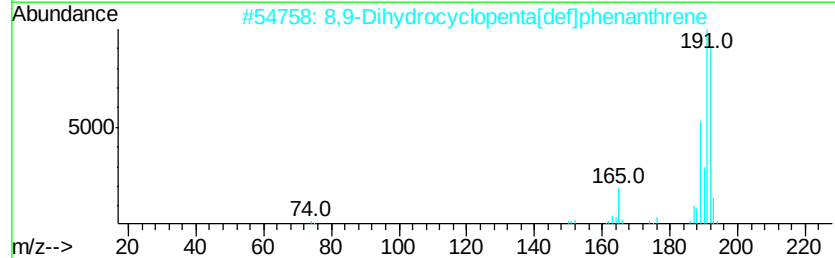
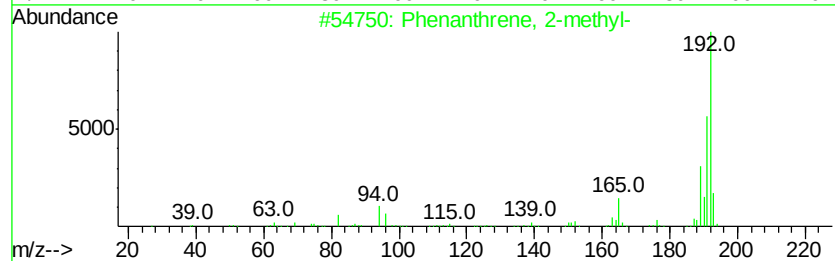
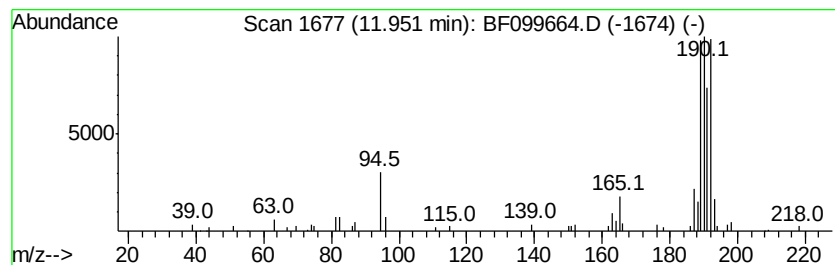
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.95	2.20 ng	83698	Phenanthrene-d10		11.34	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	86
2		8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	83
3		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	83
4		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	50
5		Anthracene, 1-methyl-	192	C15H12	000610-48-0	50



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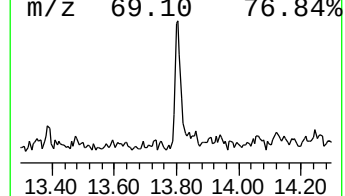
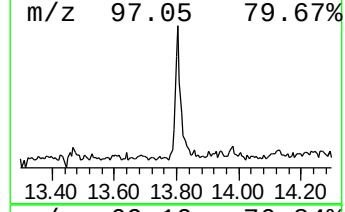
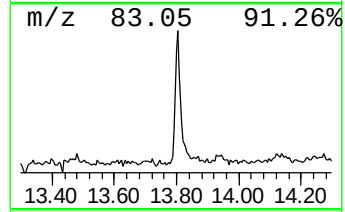
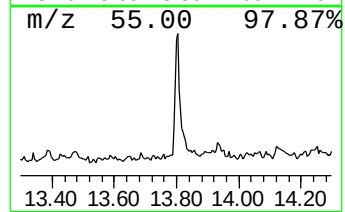
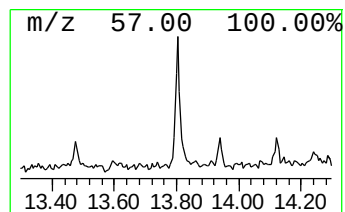
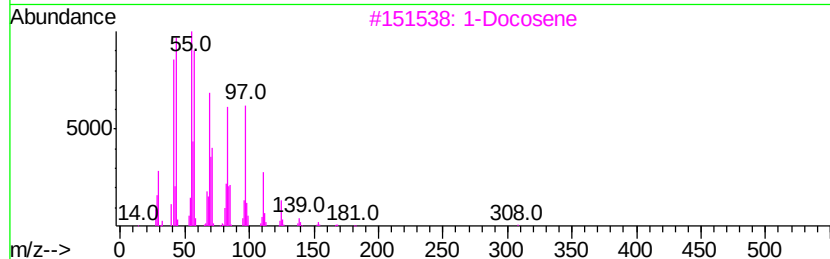
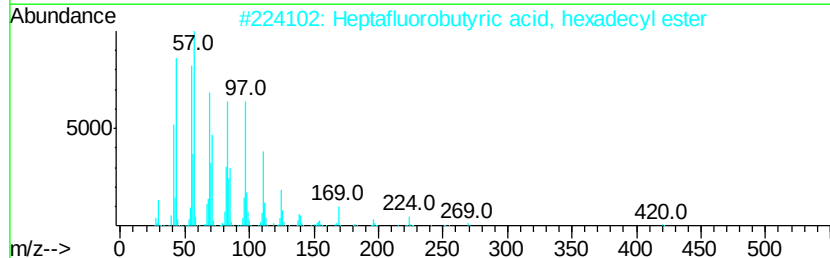
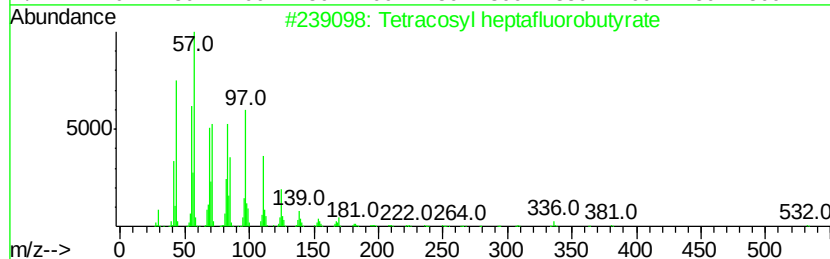
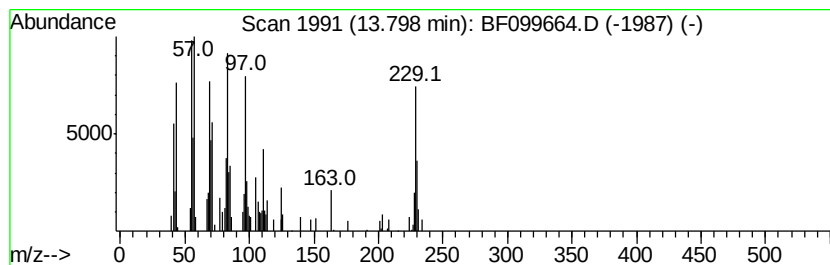
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetracosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.80	4.07 ng	119575	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	76
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	76
3	1-Docosene	308	C22H44	001599-67-3	76
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	76
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	70



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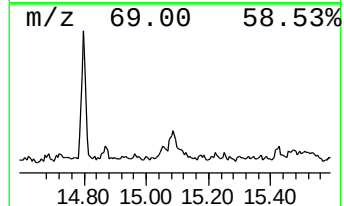
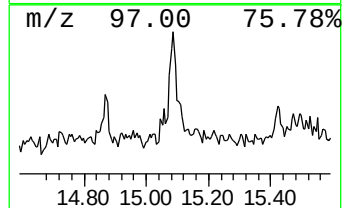
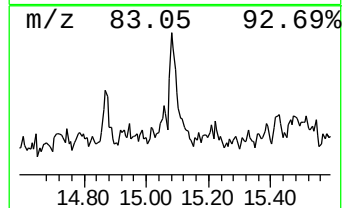
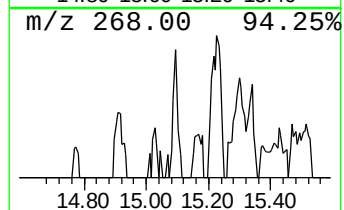
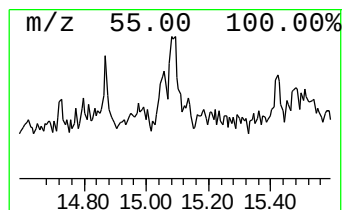
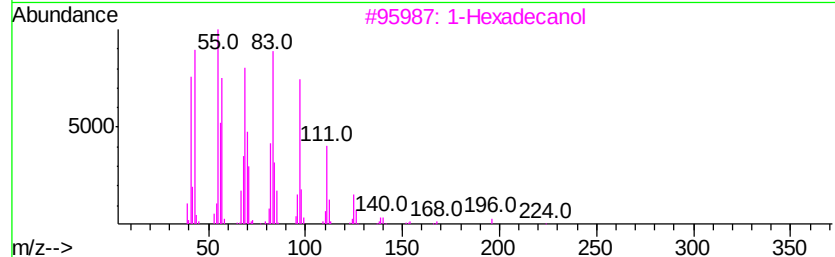
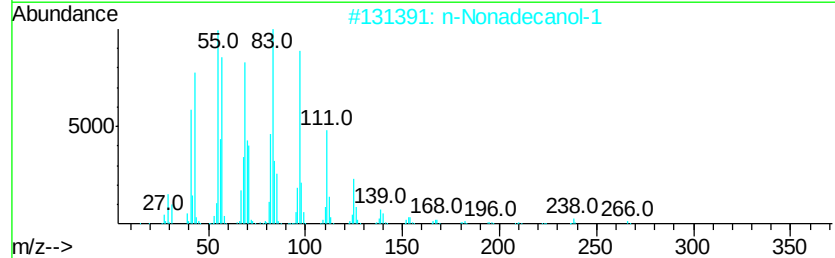
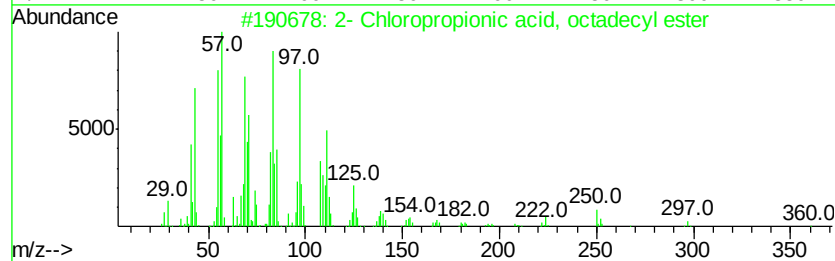
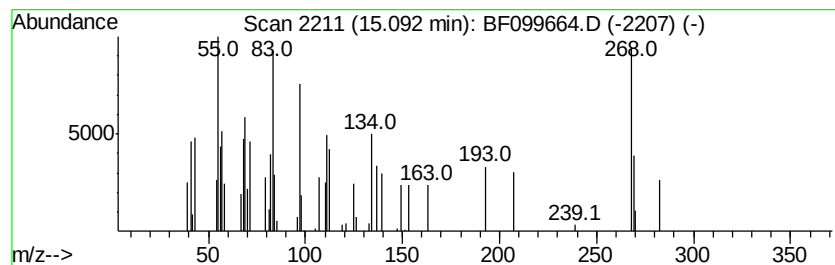
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ClientSampleId :
TP-1(6-8)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2- Chloropropionic acid, oc... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.09	2.20 ng	54388	Perylene-d12	15.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	70
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	62
3	1-Hexadecanol	242	C16H34O	036653-82-4	62
4	Cyclohexadecane	224	C16H32	000295-65-8	58
5	Cyclopentadecane	210	C15H30	000295-48-7	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101917\
Data File : BF099664.D
Acq On : 19 Oct 2017 18:36
Operator : SJ/JU
Sample : I5879-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

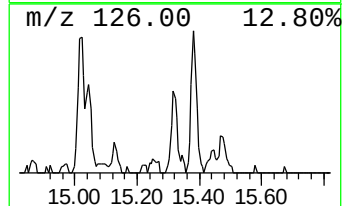
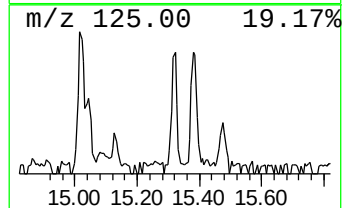
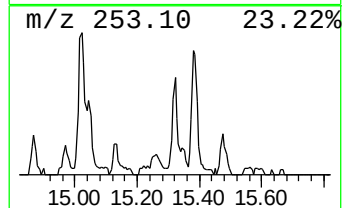
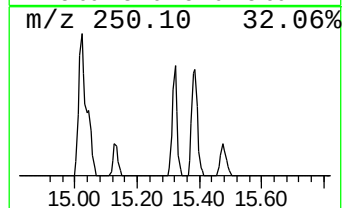
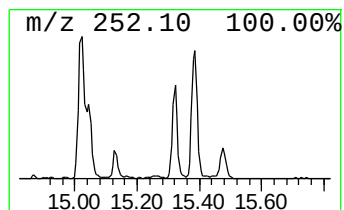
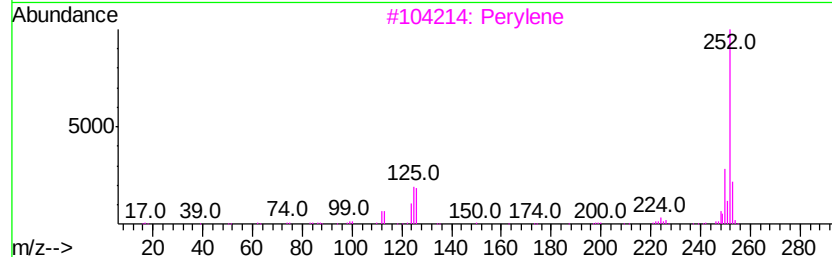
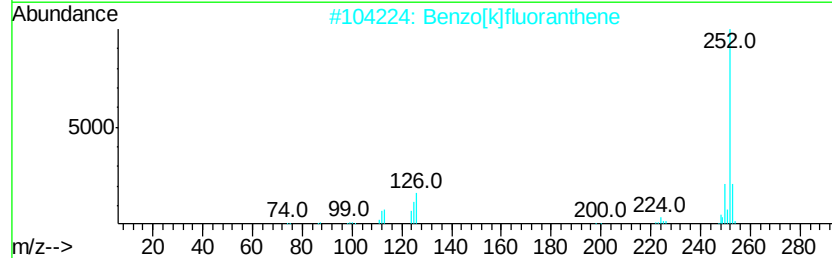
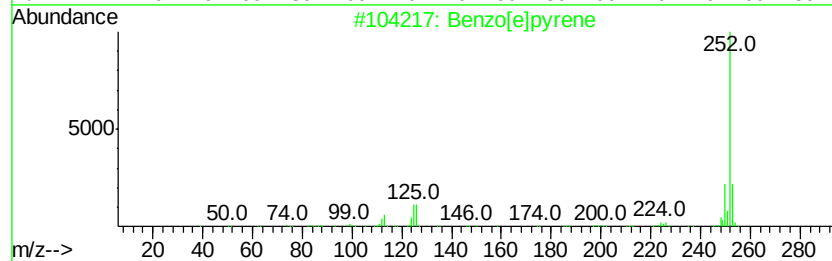
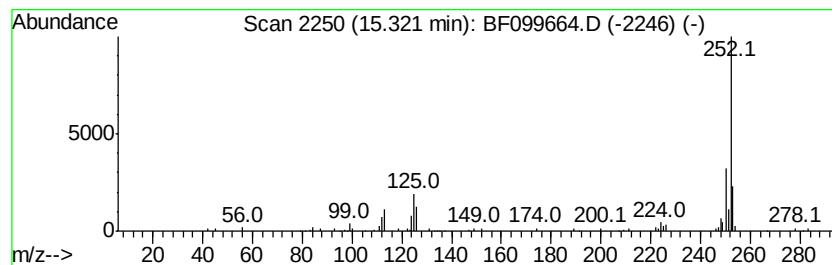
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.32	3.11 ng	76967	Perylene-d12		15.44
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Perylene	252	C20H12	000198-55-0	97
4	Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101917\
Data File : BF099664.D
Acq On : 19 Oct 2017 18:36
Operator : SJ/JU
Sample : I5879-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1(6-8)

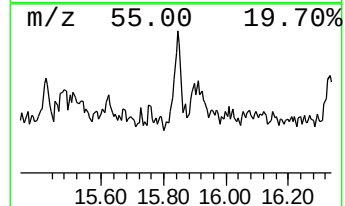
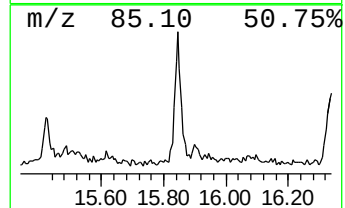
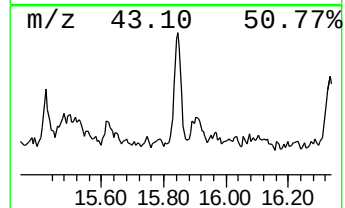
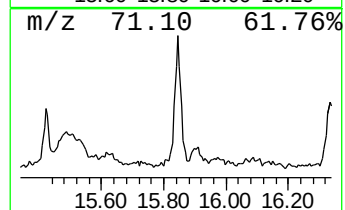
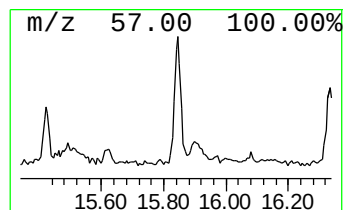
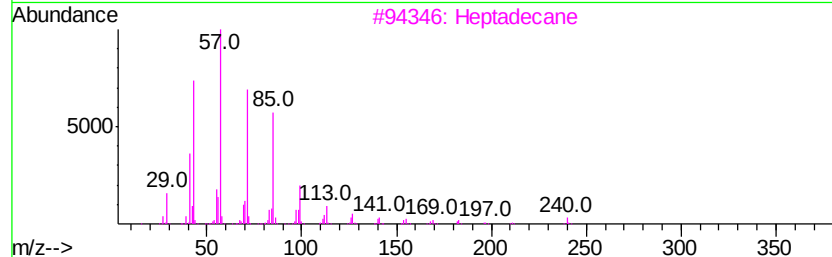
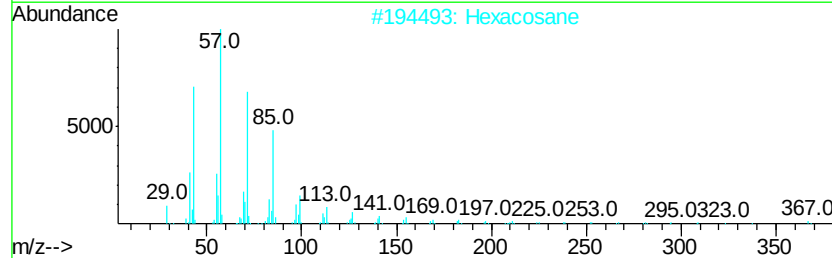
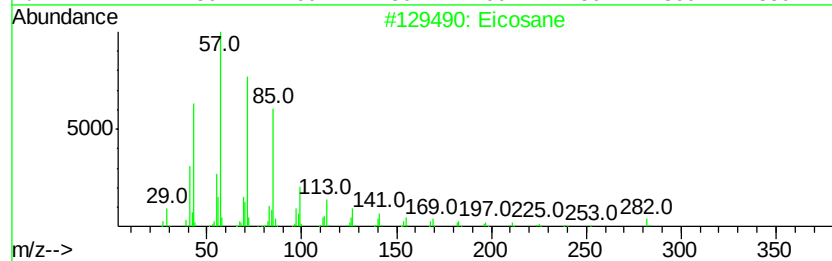
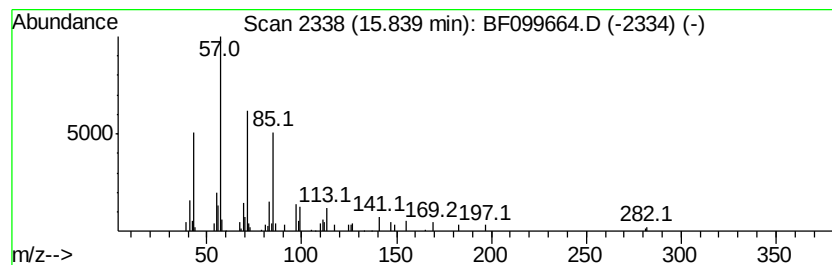
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	3.18 ng	78597	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptadecane	240	C17H36	000629-78-7	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	87
5		Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101917\
Data File : BF099664.D
Acq On : 19 Oct 2017 18:36
Operator : SJ/JU
Sample : I5879-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1(6-8)

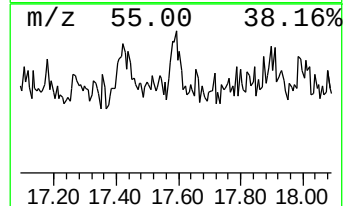
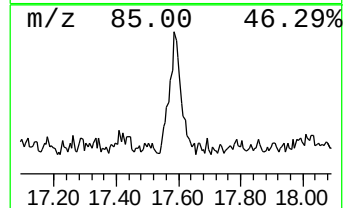
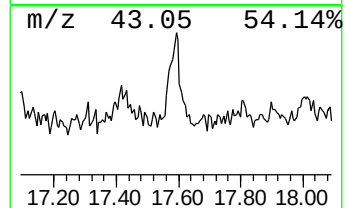
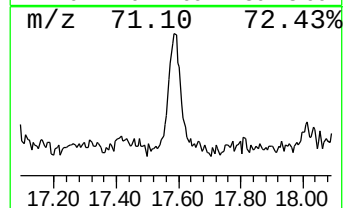
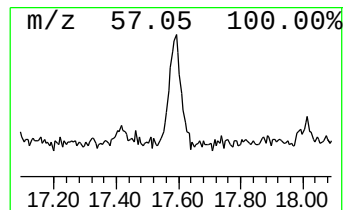
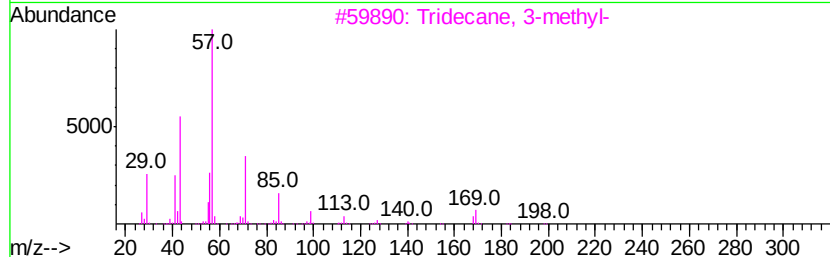
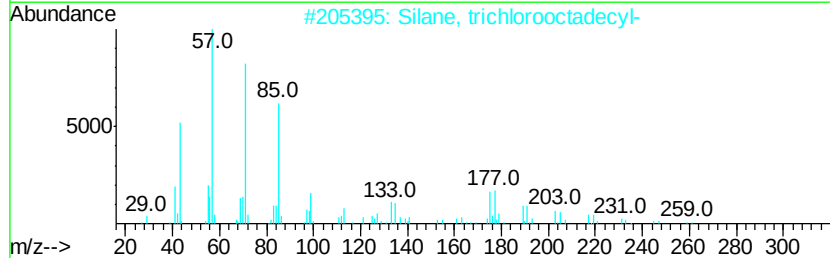
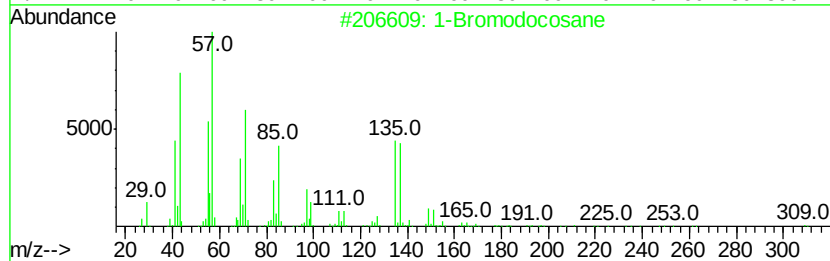
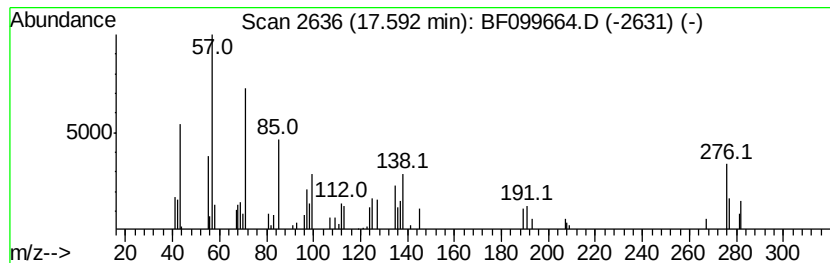
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.59 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.59	3.06 ng	75596	Perylene-d12	15.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Bromodocosane	388	C22H45Br	006938-66-5	47
2			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	35
3			Tridecane, 3-methyl-	198	C14H30	006418-41-3	35
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	27
5			Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101917\
Data File : BF099664.D
Acq On : 19 Oct 2017 18:36
Operator : SJ/JU
Sample : I5879-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1(6-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.05	14.4	ng	376817	1	6.82	524974	20.0
unknown6.60	6.60	82.7	ng	2171090	1	6.82	524974	20.0
Phenanthrene, 2-m...	11.95	2.2	ng	83698	4	11.34	762433	20.0
Tetracosyl heptaf...	13.80	4.1	ng	119575	5	13.98	588069	20.0
2- Chloropropioni...	15.09	2.2	ng	54388	6	15.44	494817	20.0
Benzo[e]pyrene	15.32	3.1	ng	76967	6	15.44	494817	20.0
Eicosane	15.84	3.2	ng	78597	6	15.44	494817	20.0
unknown17.59	17.59	3.1	ng	75596	6	15.44	494817	20.0