

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080517\
 Data File : BF097409.D
 Acq On : 5 Aug 2017 20:47
 Operator : SJ/JU
 Sample : I4613-01 5X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-05-080317

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-BF072517.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	4.534	464	467	483	rBV	59508	92654	8.87%	0.837%
2	5.028	548	551	571	rBV	245337	401972	38.50%	3.632%
3	6.104	731	734	748	rBV	316014	452333	43.32%	4.087%
4	6.204	748	751	763	rVB	394640	465852	44.61%	4.209%
5	6.428	785	789	798	rBV	523443	529513	50.71%	4.784%
6	6.581	811	815	823	rBV	344253	326801	31.30%	2.953%
7	6.998	883	886	902	rBV	176267	216500	20.73%	1.956%
8	7.710	1003	1007	1018	rBV	675362	599821	57.44%	5.419%
9	8.786	1186	1190	1197	rBV	456987	394078	37.74%	3.560%
10	9.186	1255	1258	1264	rBV	29199	28831	2.76%	0.260%
11	9.316	1277	1280	1286	rVB	25699	22289	2.13%	0.201%
12	9.451	1299	1303	1307	rBV	604336	503973	48.27%	4.553%
13	9.663	1336	1339	1343	rVB	10919	10570	1.01%	0.095%
14	9.998	1393	1396	1403	rVB	24635	24894	2.38%	0.225%
15	10.239	1434	1437	1446	rVB	177699	162607	15.57%	1.469%
16	10.374	1455	1460	1465	rBV3	15508	19162	1.84%	0.173%
17	10.692	1512	1514	1519	rVB	20010	18815	1.80%	0.170%
18	10.922	1550	1553	1556	rBV	540381	483931	46.35%	4.372%
19	10.945	1556	1557	1562	rVV	180628	126746	12.14%	1.145%
20	11.004	1562	1567	1571	rVB	42630	41960	4.02%	0.379%
21	11.169	1591	1595	1600	rBV2	15966	18890	1.81%	0.171%
22	11.263	1608	1611	1614	rVB2	34695	32295	3.09%	0.292%
23	11.339	1621	1624	1628	rVB	389980	356586	34.15%	3.222%
24	11.427	1636	1639	1641	rBV	30760	27177	2.60%	0.246%
25	11.451	1641	1643	1646	rVV	35669	29743	2.85%	0.269%
26	11.533	1654	1657	1660	rBV	78252	76225	7.30%	0.689%
27	11.557	1660	1661	1666	rVB	27772	18919	1.81%	0.171%
28	11.721	1686	1689	1691	rBV	21058	17848	1.71%	0.161%
29	11.757	1691	1695	1699	rVB4	19319	24313	2.33%	0.220%
30	11.974	1728	1732	1734	rBV	23426	26543	2.54%	0.240%
31	12.021	1734	1740	1741	rVV	347617	339864	32.55%	3.071%
32	12.039	1741	1743	1754	rVB	1060963	1044168	100.00%	9.434%
33	12.127	1754	1758	1763	rBV	670230	577214	55.28%	5.215%
34	12.198	1765	1770	1773	rBV4	12834	19945	1.91%	0.180%

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 Integrator: RTE
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 Sampling : 1
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35	12.274	1779	1783	1787	rBV3	22968	25865	2.48%	0.234%
36	12.351	1791	1796	1801	rBV	434921	453719	43.45%	4.099%
37	12.404	1803	1805	1811	rVB4	23393	32145	3.08%	0.290%
38	12.480	1815	1818	1819	rBV	22001	21723	2.08%	0.196%
39	12.504	1819	1822	1829	rVB	333520	328725	31.48%	2.970%
40	12.574	1829	1834	1838	rBV2	33065	59917	5.74%	0.541%
41	12.686	1846	1853	1855	rBV	79181	115954	11.10%	1.048%
42	12.721	1855	1859	1861	rVV5	15408	23186	2.22%	0.209%
43	12.751	1861	1864	1866	rVV2	65844	68764	6.59%	0.621%
44	12.786	1867	1870	1877	rVB	54202	70194	6.72%	0.634%
45	12.851	1877	1881	1882	rBV3	20938	17443	1.67%	0.158%
46	12.880	1882	1886	1888	rVB	21747	21001	2.01%	0.190%
47	12.910	1888	1891	1894	rBV	25666	26093	2.50%	0.236%
48	13.004	1905	1907	1910	rVB3	20506	21088	2.02%	0.191%
49	13.039	1910	1913	1914	rBV3	12132	12708	1.22%	0.115%
50	13.092	1920	1922	1923	rBV2	13046	11849	1.13%	0.107%
51	13.168	1932	1935	1937	rBV3	15436	17744	1.70%	0.160%
52	13.198	1937	1940	1943	rVB	30508	30210	2.89%	0.273%
53	13.298	1954	1957	1959	rBV	31925	27632	2.65%	0.250%
54	13.321	1959	1961	1963	rVB	25047	18187	1.74%	0.164%
55	13.345	1963	1965	1967	rBV	27888	21174	2.03%	0.191%
56	13.404	1973	1975	1977	rBV	24074	21917	2.10%	0.198%
57	13.427	1977	1979	1984	rVB4	28920	35156	3.37%	0.318%
58	13.545	1991	1999	2002	rBV2	609346	808766	77.46%	7.307%
59	13.568	2002	2003	2010	rVV	195373	166285	15.93%	1.502%
60	13.651	2013	2017	2019	rBV	41924	42559	4.08%	0.385%
61	13.710	2023	2027	2029	rBV4	18770	32163	3.08%	0.291%
62	14.127	2096	2098	2101	rBV4	21337	19763	1.89%	0.179%
63	14.539	2164	2168	2176	rVB	169295	275783	26.41%	2.492%
64	14.780	2207	2209	2215	rVB	84285	89473	8.57%	0.808%
65	14.839	2215	2219	2223	rBV	121117	137939	13.21%	1.246%
66	14.886	2223	2227	2230	rBV	276788	287942	27.58%	2.601%
67	16.080	2428	2430	2436	rVB	45296	60029	5.75%	0.542%
68	17.092	2600	2602	2607	rVB6	23442	23722	2.27%	0.214%
69	17.362	2646	2648	2649	rBV	33452	21074	2.02%	0.190%
70	18.627	2861	2863	2864	rBV2	26284	18345	1.76%	0.166%
71	18.827	2896	2897	2901	rBV4	29019	28639	2.74%	0.259%

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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

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72	18.950	2916	2918	2920	rBV3	19264	17703	1.70%	0.160%
73	19.174	2954	2956	2957	rBV2	27221	22841	2.19%	0.206%

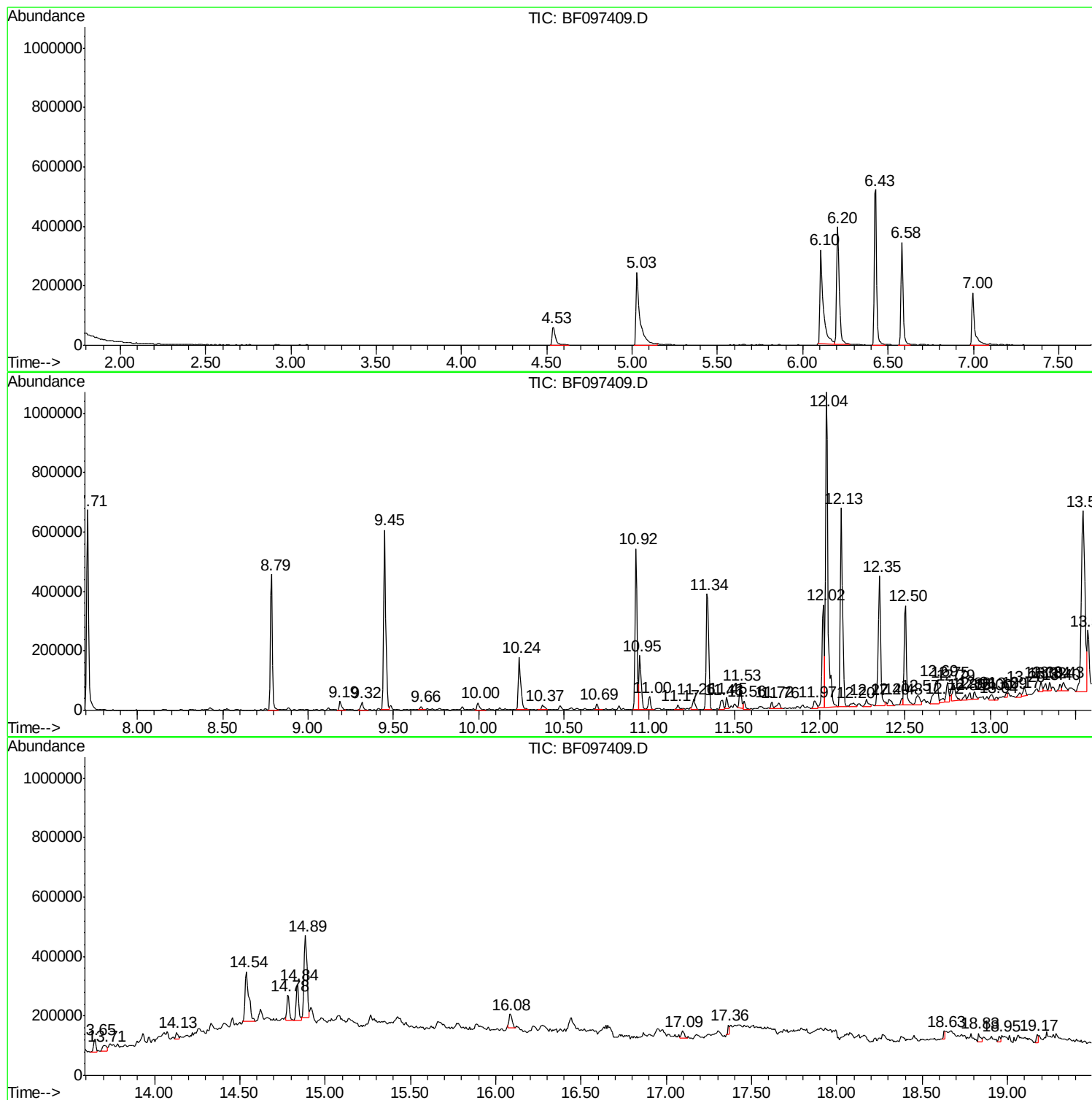
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : SJ/JU
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ALS Vial : 20 Sample Multiplier: 1

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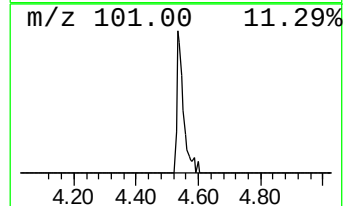
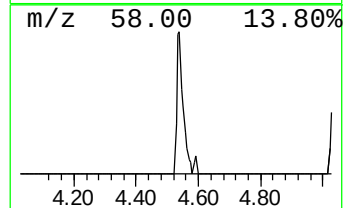
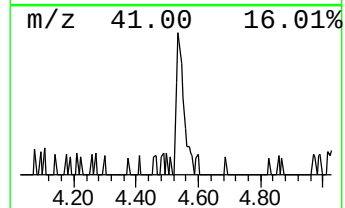
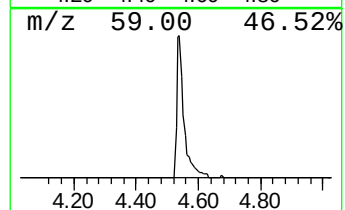
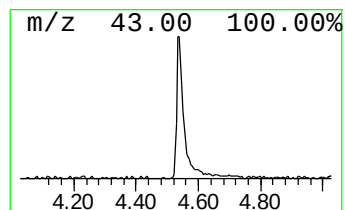
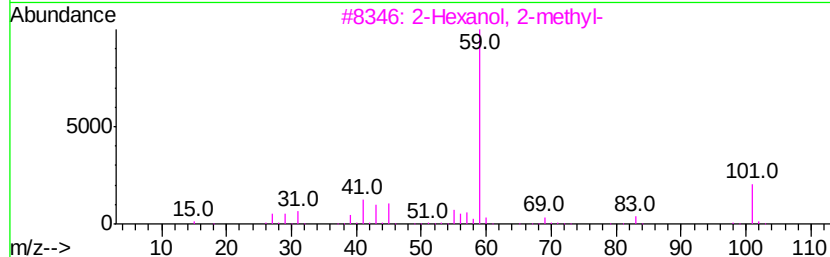
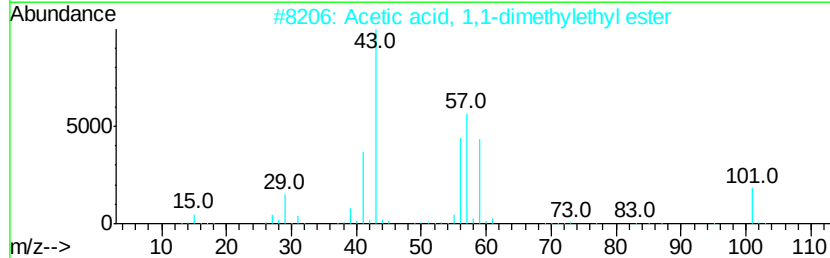
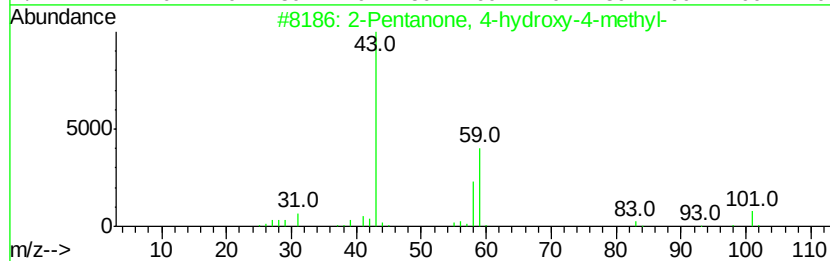
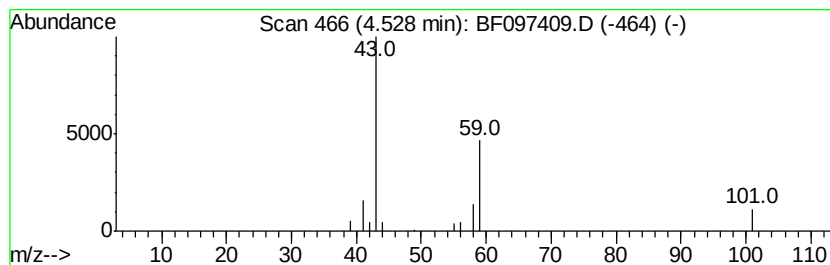
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.50 ng	92654	1,4-Dichlorobenzene-d4	6.43

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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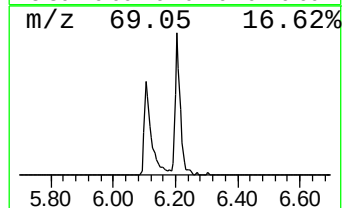
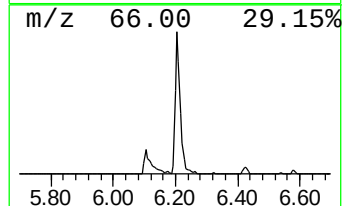
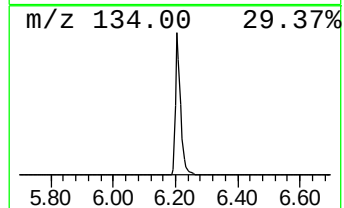
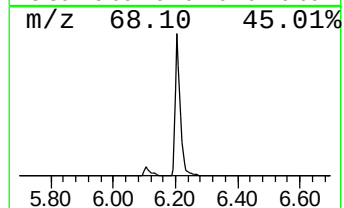
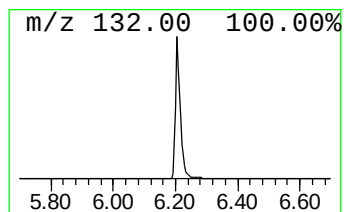
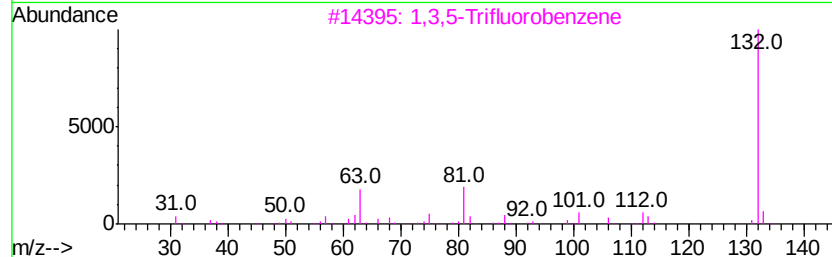
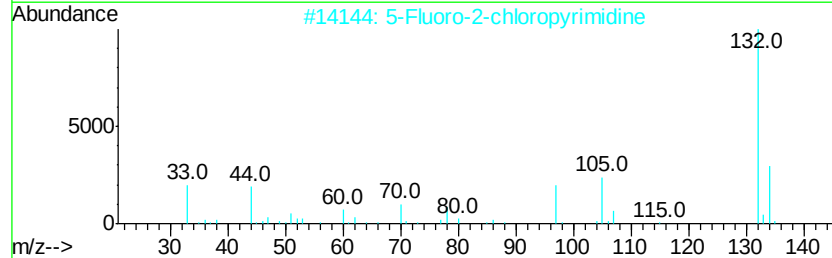
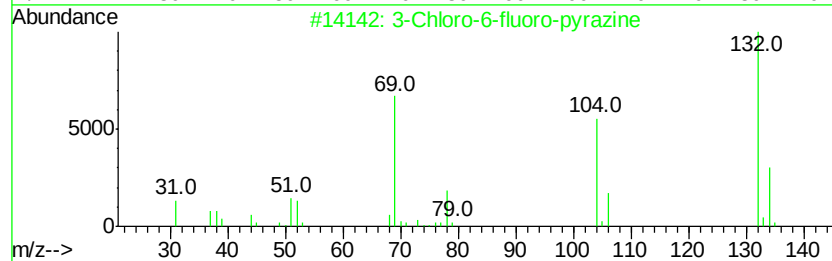
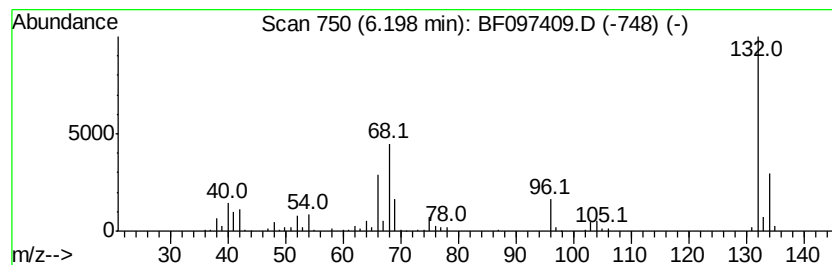
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.20 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.20	17.60 ng	465852	1,4-Dichlorobenzene-d4	6.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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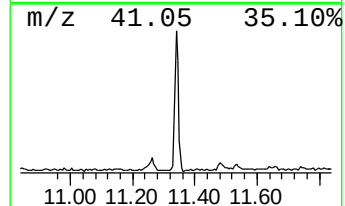
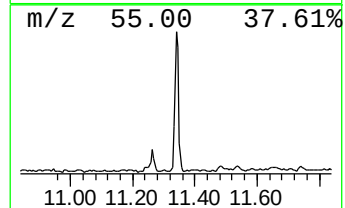
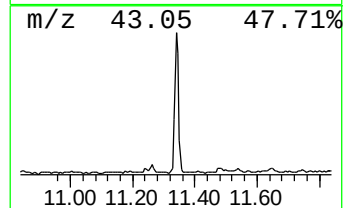
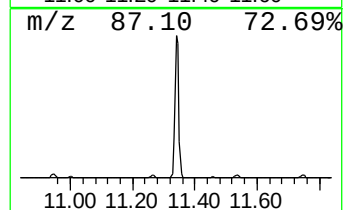
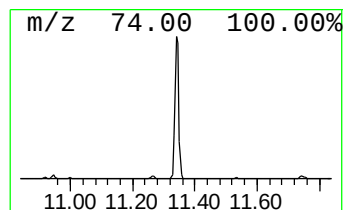
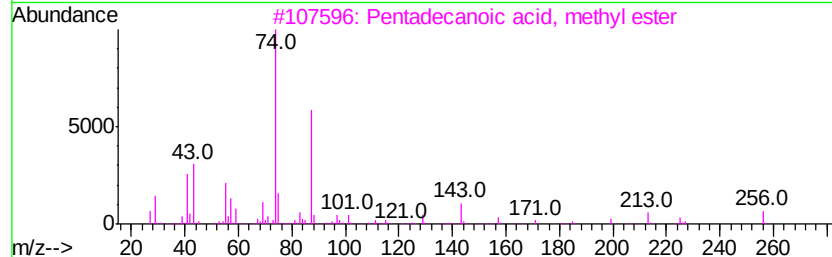
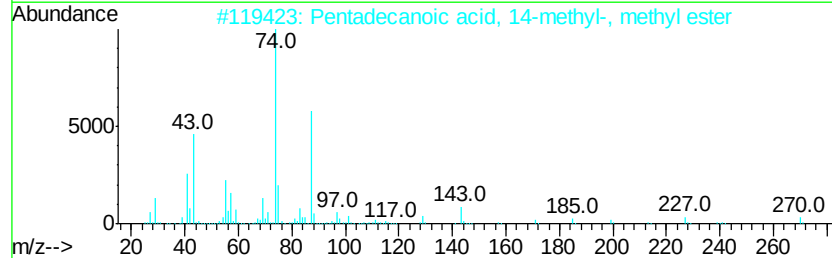
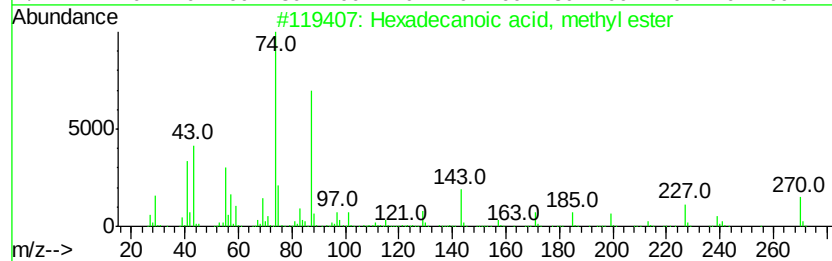
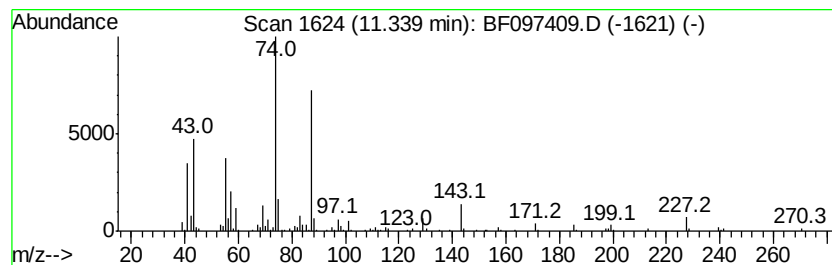
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.34	14.74 ng	356586	Phenanthrene-d10	10.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
5		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87



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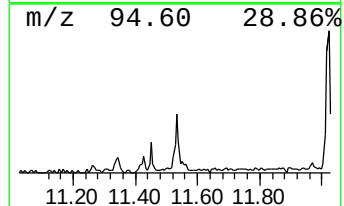
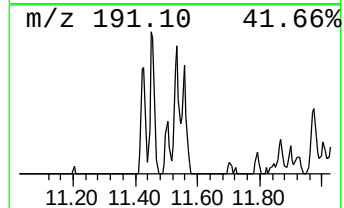
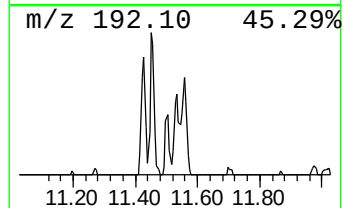
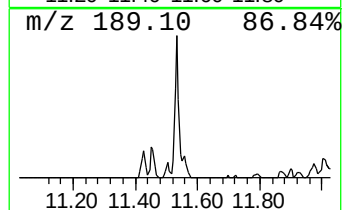
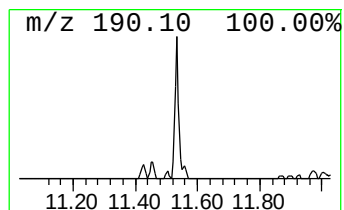
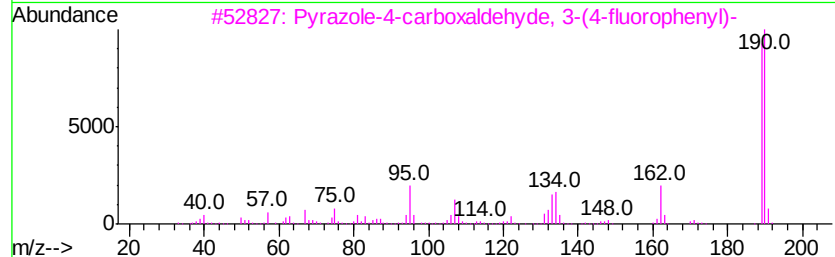
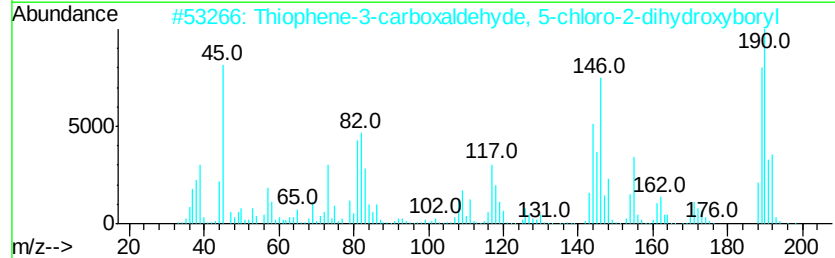
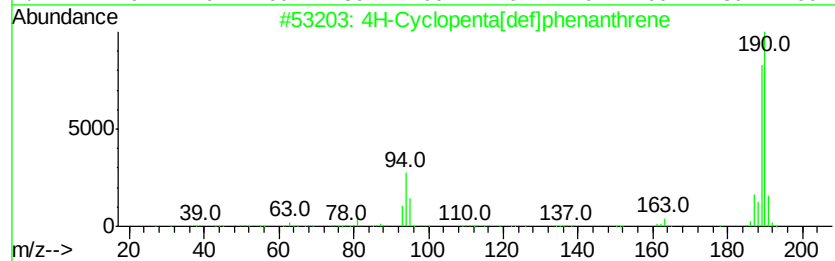
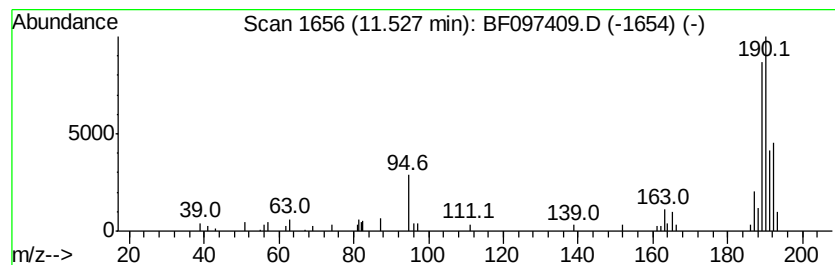
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	3.15 ng	76225	Phenanthrene-d10	10.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	95
2		Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
3		Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	50
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	28
5		Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
Data File : BF097409.D
Acq On : 5 Aug 2017 20:47
Operator : SJ/JU
Sample : I4613-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

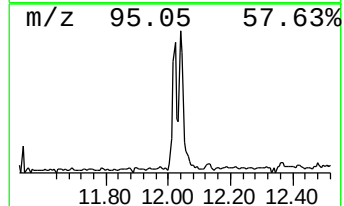
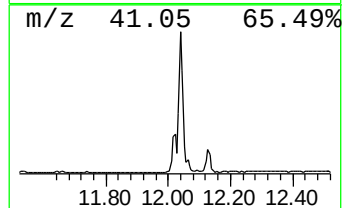
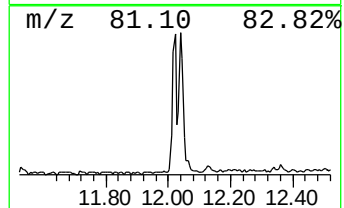
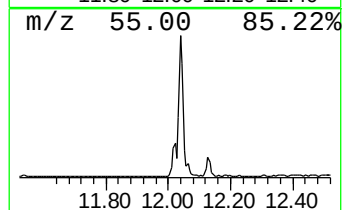
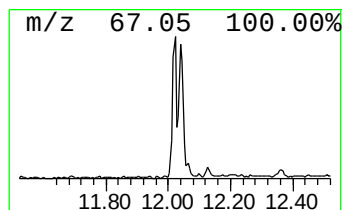
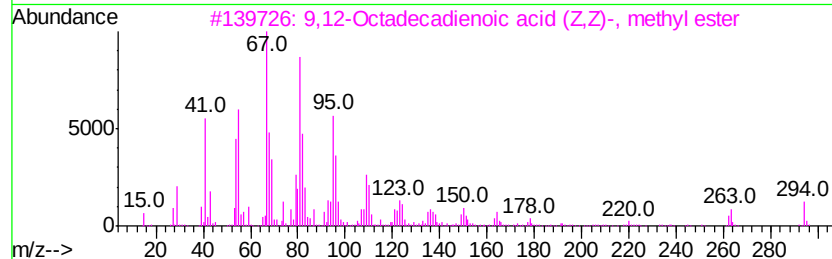
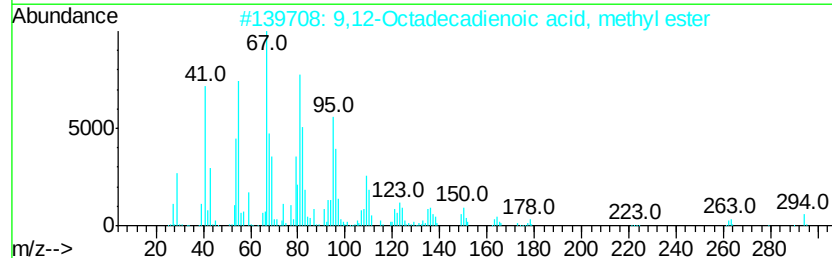
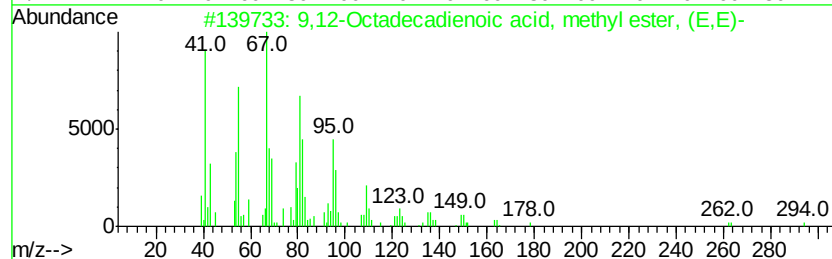
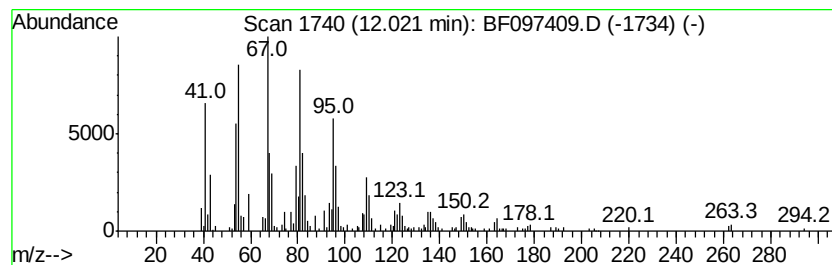
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.02	14.05 ng	339864	Phenanthrene-d10	10.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	97	
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	93	
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	91	
4	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	90	
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	90	



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Data File : BF097409.D
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Operator : SJ/JU
Sample : I4613-01 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-05-080317

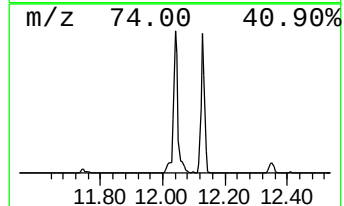
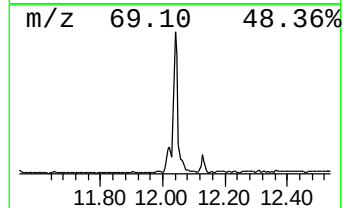
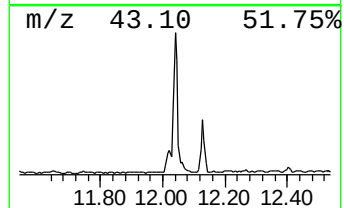
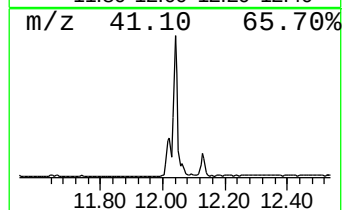
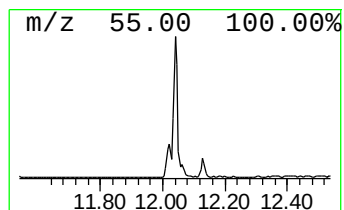
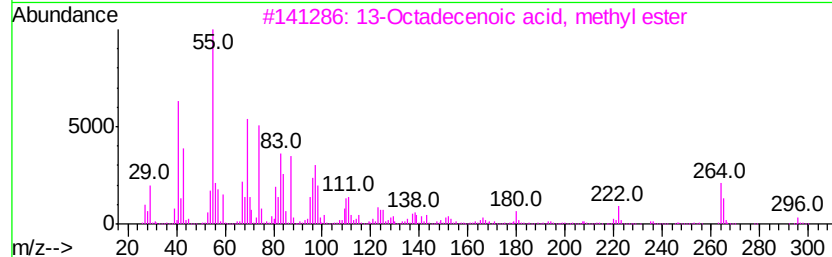
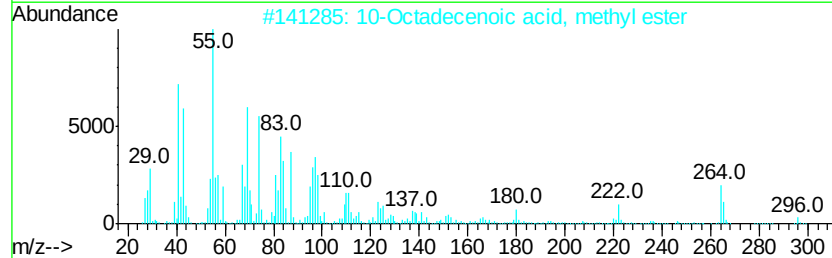
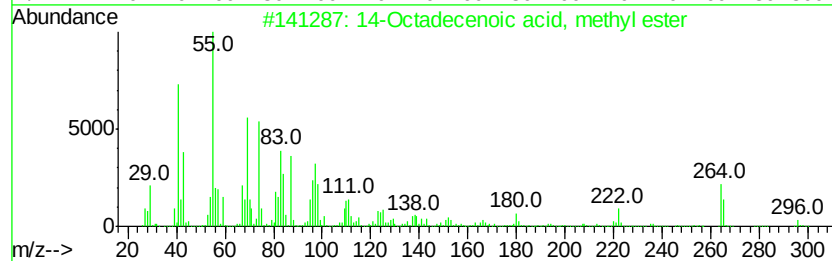
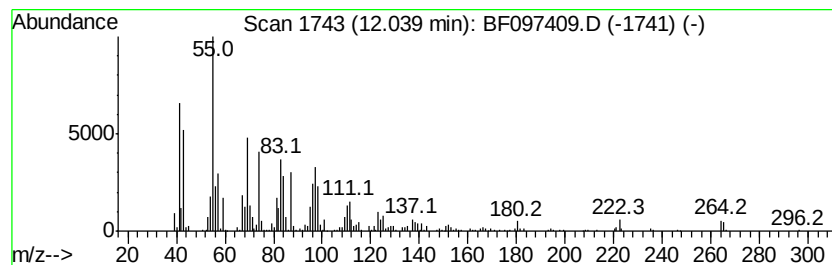
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 14-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	43.15 ng	1044170	Phenanthrene-d10	10.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
2		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	98
3		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	97
4		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	94
5		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	93



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080517\
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Misc :
ALS Vial : 20 Sample Multiplier: 1

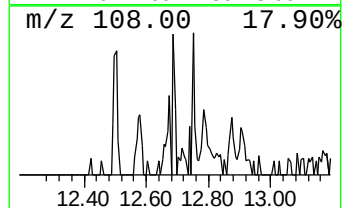
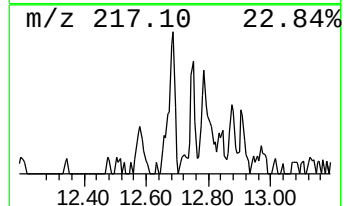
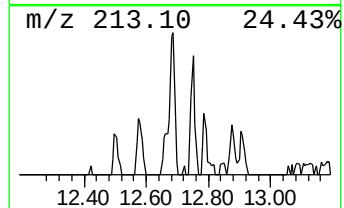
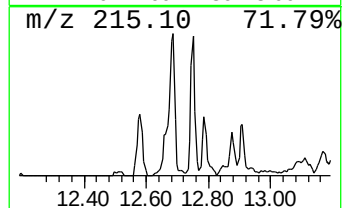
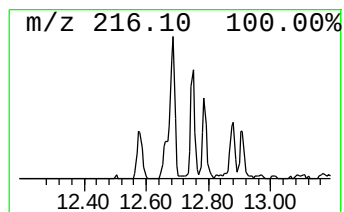
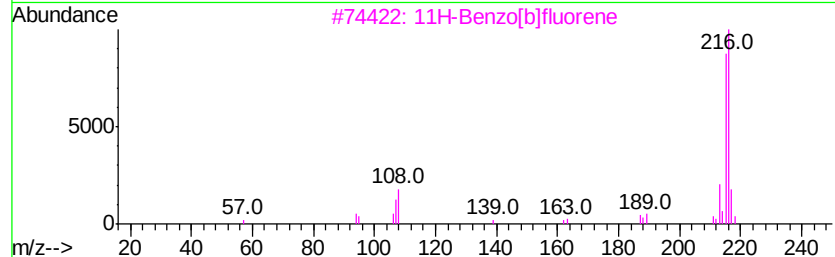
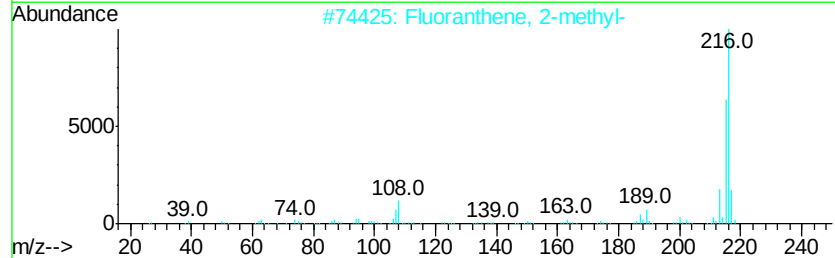
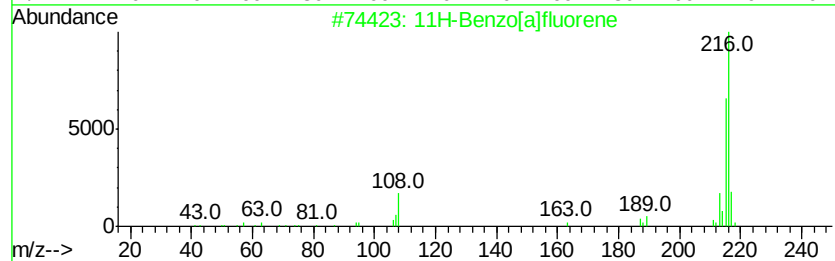
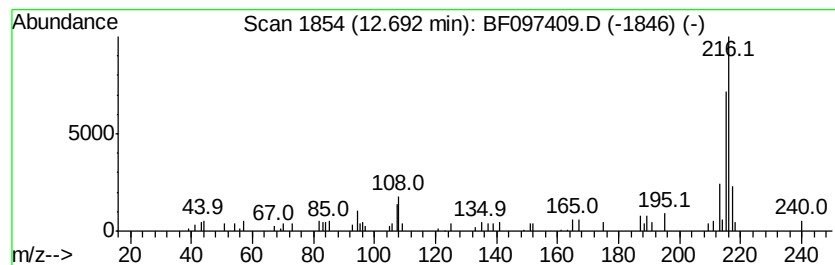
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 11H-Benzo[a]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.87 ng	115954	Chrysene-d12	13.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	11H-Benzo[a]fluorene	216 C17H12	000238-84-6	95
2	Fluoranthene, 2-methyl-	216 C17H12	033543-31-6	94
3	11H-Benzo[b]fluorene	216 C17H12	000243-17-4	93
4	Pyrene, 2-methyl-	216 C17H12	003442-78-2	93
5	Pyrene, 1-methyl-	216 C17H12	002381-21-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080517\
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.53	3.5	ng	92654	1	6.43	529513	20.0
unknown6.20	6.20	17.6	ng	465852	1	6.43	529513	20.0
Hexadecanoic acid...	11.34	14.7	ng	356586	4	10.92	483931	20.0
4H-Cyclopenta[def...	11.53	3.1	ng	76225	4	10.92	483931	20.0
9,12-Octadecadien...	12.02	14.1	ng	339864	4	10.92	483931	20.0
14-Octadecenoic a...	12.04	43.1	ng	1044170	4	10.92	483931	20.0
11H-Benzo[a]fluorene	12.69	2.9	ng	115954	5	13.54	808766	20.0