

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
 Data File : BF122447.D
 Acq On : 23 Nov 2020 15:11
 Operator : JU/CG
 Sample : L4836-08
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-08

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122447.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	5	11	23	rVB	588332	813765	14.22%	1.601%
2	2.257	25	29	35	rVB	62945	85733	1.50%	0.169%
3	3.940	311	315	321	rVB	49831	63806	1.11%	0.126%
4	4.451	397	402	408	rBV	89893	102300	1.79%	0.201%
5	5.081	502	509	519	rVB	1941761	2664310	46.55%	5.242%
6	5.487	573	578	582	rBV	4032867	4290059	74.96%	8.441%
7	5.875	641	644	648	rBV	288423	232957	4.07%	0.458%
8	6.498	744	750	754	rBV	4095293	4734944	82.73%	9.316%
9	6.863	808	812	815	rBV	1453199	1133470	19.80%	2.230%
10	7.428	902	908	911	rBV	2819828	2930470	51.20%	5.766%
11	8.151	1026	1031	1034	rBV	1483357	1446650	25.28%	2.846%
12	9.228	1209	1214	1217	rBV	5726204	5322242	92.99%	10.472%
13	9.622	1277	1281	1285	rBV	170133	171093	2.99%	0.337%
14	9.904	1322	1329	1333	rBV	1833320	1732707	30.27%	3.409%
15	10.698	1458	1464	1475	rBV	3607435	3668909	64.10%	7.219%
16	11.251	1553	1558	1563	rBV5	34718	68679	1.20%	0.135%
17	11.392	1578	1582	1585	rBV	1886014	1815797	31.73%	3.573%
18	11.416	1585	1586	1590	rVV	564429	397043	6.94%	0.781%
19	11.469	1592	1595	1599	rVB	157738	139899	2.44%	0.275%
20	11.898	1664	1668	1670	rBV	141434	129064	2.26%	0.254%
21	11.927	1670	1673	1677	rVV	582425	564751	9.87%	1.111%
22	11.974	1678	1681	1683	rVV	81786	97063	1.70%	0.191%
23	12.010	1683	1687	1689	rVV2	189368	240057	4.19%	0.472%
24	12.033	1689	1691	1696	rVB	112420	100319	1.75%	0.197%
25	12.192	1710	1718	1720	rBV	94995	101189	1.77%	0.199%
26	12.374	1746	1749	1752	rBV2	104274	109269	1.91%	0.215%
27	12.445	1756	1761	1764	rBV	127170	140933	2.46%	0.277%
28	12.486	1764	1768	1773	rVB4	76262	125974	2.20%	0.248%
29	12.533	1773	1776	1781	rVB3	103857	117850	2.06%	0.232%
30	12.610	1785	1789	1792	rBV	1122114	957325	16.73%	1.884%
31	12.710	1803	1806	1813	rBV4	128690	196526	3.43%	0.387%
32	12.839	1822	1828	1831	rBV	1140796	1147598	20.05%	2.258%
33	12.886	1834	1836	1842	rVB2	59011	84934	1.48%	0.167%
34	12.986	1849	1853	1857	rVV	5600364	5723420	100.00%	11.261%
35	13.057	1860	1865	1869	rBV3	97852	144804	2.53%	0.285%
36	13.145	1877	1880	1881	rBV2	66797	65864	1.15%	0.130%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	13.169	1881	1884	1887	rVB	187013	181167	3.17%	0.356%
38	13.233	1887	1895	1898	rBV2	147645	183218	3.20%	0.360%
39	13.268	1898	1901	1904	rBV2	147558	151803	2.65%	0.299%
40	13.363	1913	1917	1920	rBV	94885	83287	1.46%	0.164%
41	13.392	1920	1922	1927	rVV	87072	83849	1.47%	0.165%
42	13.674	1964	1970	1975	rVB2	87235	134290	2.35%	0.264%
43	13.786	1984	1989	1992	rBV2	79610	119309	2.08%	0.235%
44	13.816	1992	1994	1996	rVV	99121	81519	1.42%	0.160%
45	13.839	1996	1998	2002	rVV2	69993	82657	1.44%	0.163%
46	13.898	2003	2008	2017	rVV2	239814	467689	8.17%	0.920%
47	14.039	2025	2032	2035	rBV2	2035666	2427180	42.41%	4.776%
48	14.063	2035	2036	2042	rVB	543318	440547	7.70%	0.867%
49	14.145	2048	2050	2053	rVB	106235	74739	1.31%	0.147%
50	14.427	2094	2098	2101	rVV	128555	121521	2.12%	0.239%
51	14.463	2101	2104	2107	rVB	79053	77019	1.35%	0.152%
52	14.515	2107	2113	2116	rBV5	95492	153106	2.68%	0.301%
53	14.551	2116	2119	2121	rVV	73876	83259	1.45%	0.164%
54	14.574	2121	2123	2126	rVB3	65216	62868	1.10%	0.124%
55	14.827	2162	2166	2169	rBV3	52956	73345	1.28%	0.144%
56	15.086	2205	2210	2213	rBV	398710	624688	10.91%	1.229%
57	15.192	2226	2228	2233	rVB	79189	82558	1.44%	0.162%
58	15.304	2240	2247	2251	rBV3	32950	76119	1.33%	0.150%
59	15.392	2257	2262	2267	rBV	243336	306130	5.35%	0.602%
60	15.451	2268	2272	2278	rVV	351810	433089	7.57%	0.852%
61	15.521	2278	2284	2287	rVV	1099203	1425758	24.91%	2.805%
62	15.551	2287	2289	2296	rVB3	124658	179286	3.13%	0.353%
63	16.004	2362	2366	2371	rBV4	39044	60343	1.05%	0.119%
64	16.821	2497	2505	2511	rBV6	25956	76733	1.34%	0.151%
65	16.986	2527	2533	2542	rVB2	145216	294334	5.14%	0.579%
66	17.168	2559	2564	2569	rBV2	28198	58220	1.02%	0.115%
67	17.427	2602	2608	2621	rVB	117947	261930	4.58%	0.515%

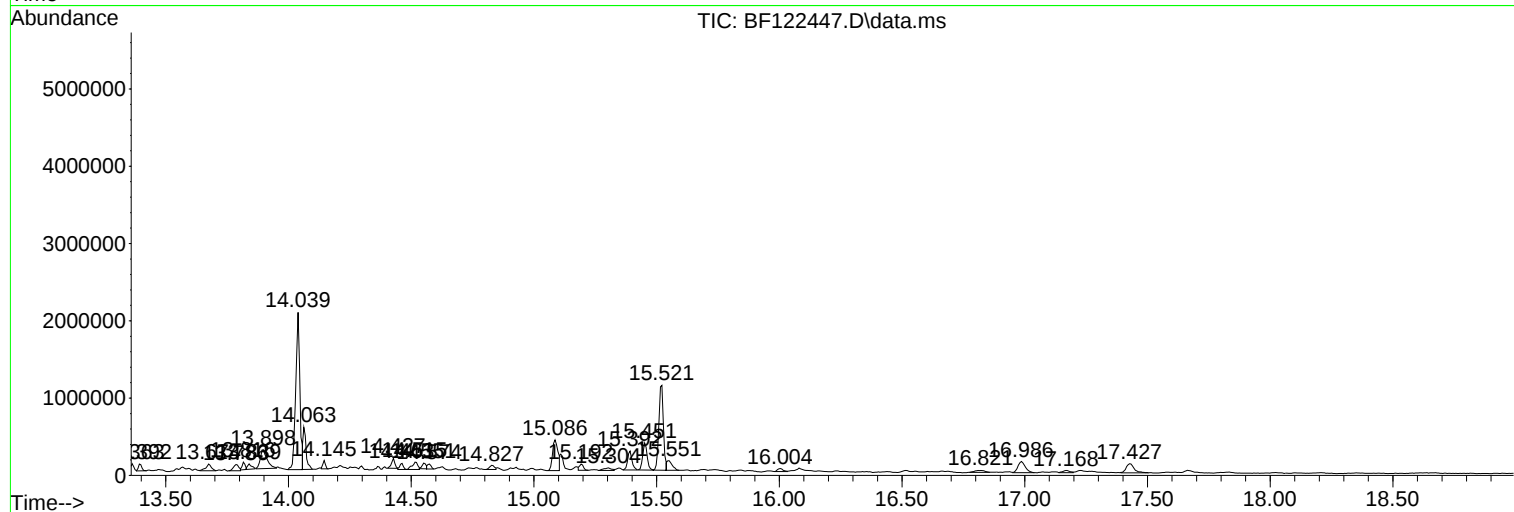
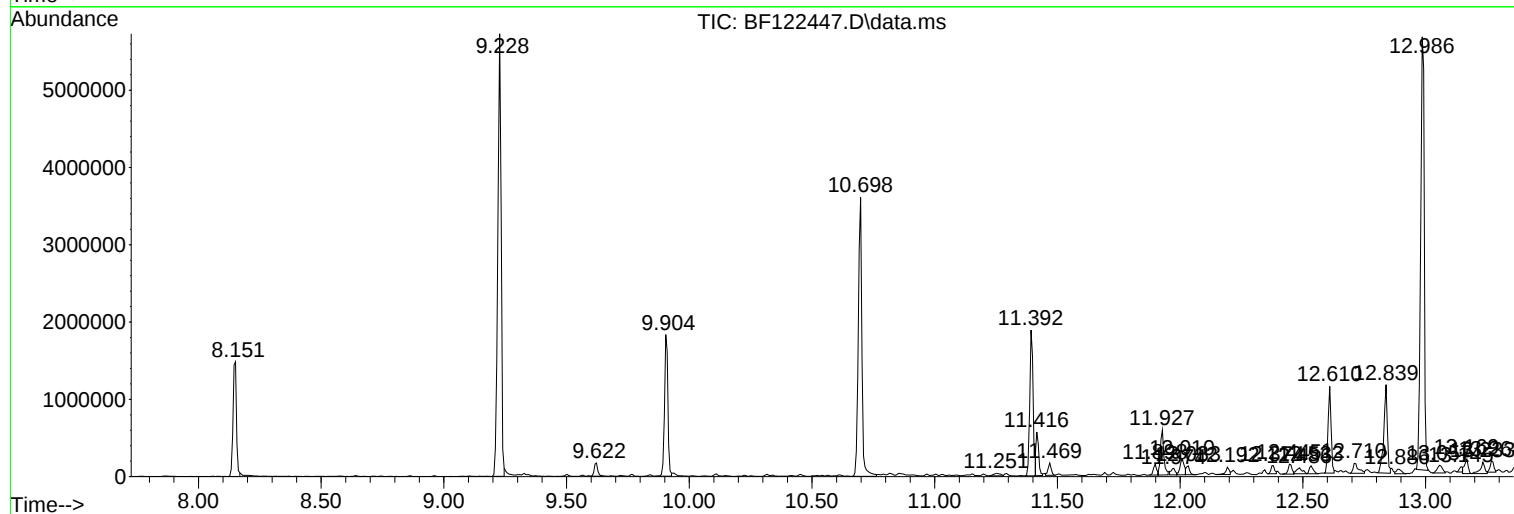
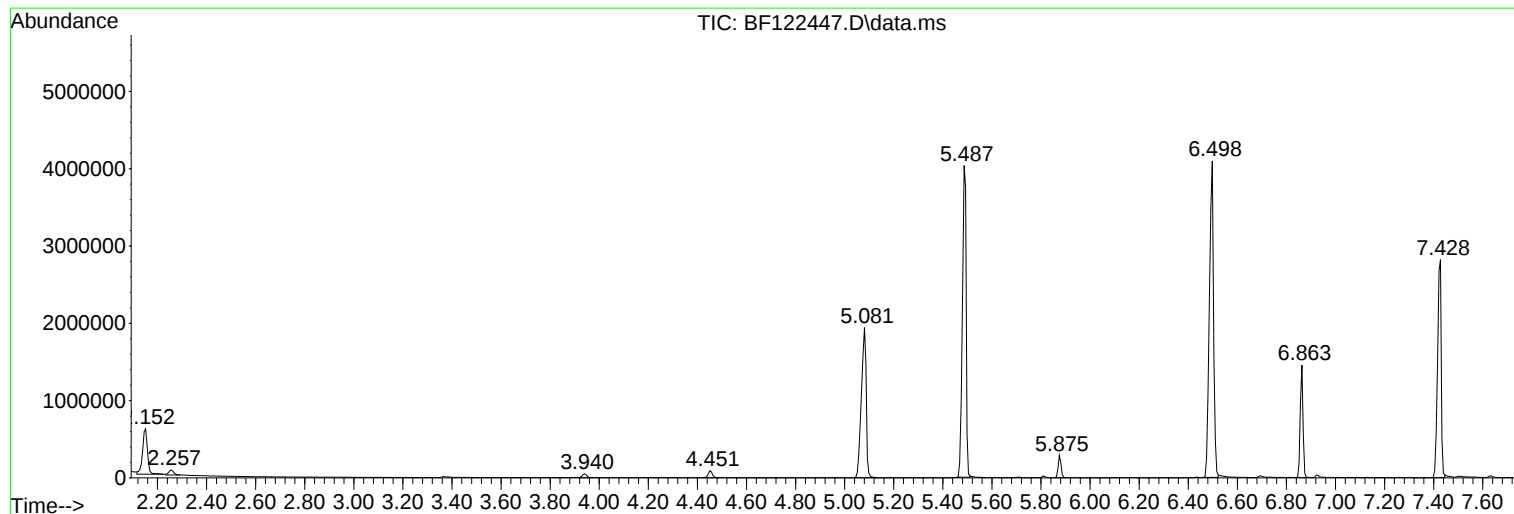
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF122447.D
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Operator : JU/CG
Sample : L4836-08
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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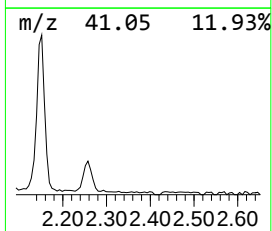
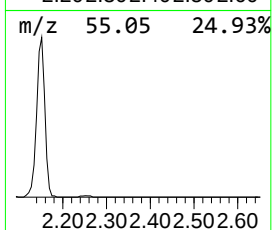
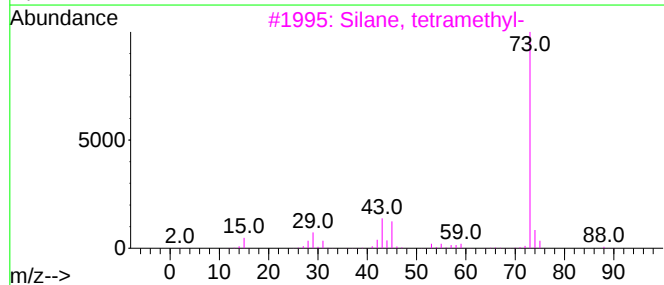
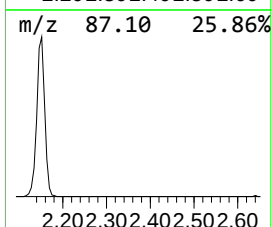
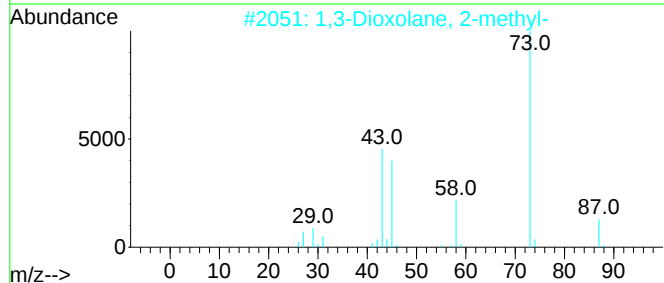
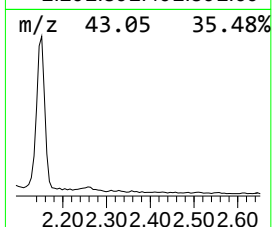
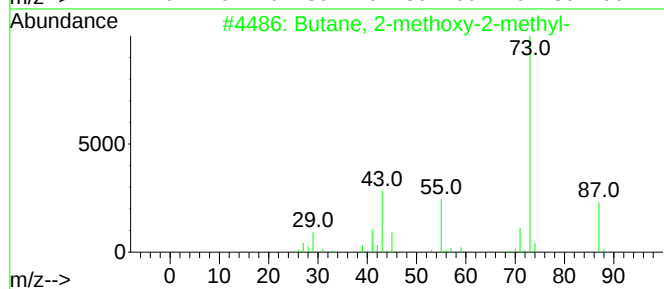
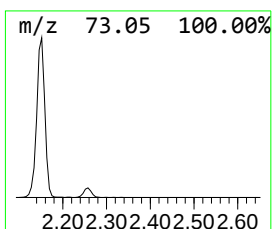
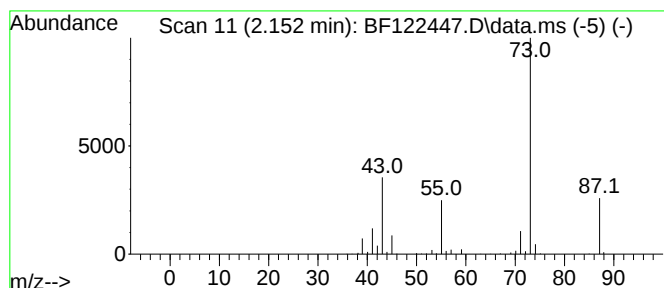
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	14.36 ng	813765	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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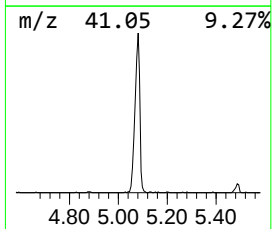
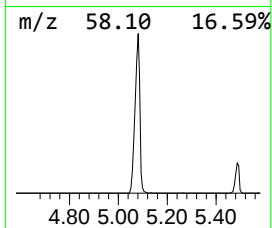
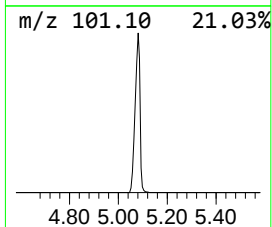
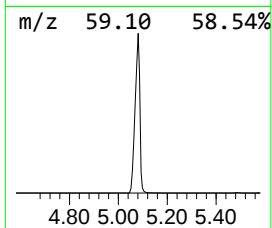
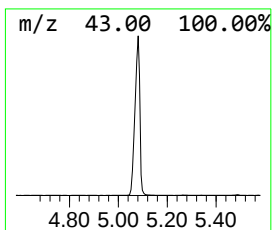
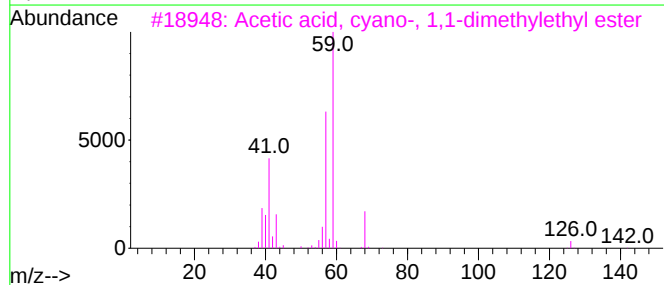
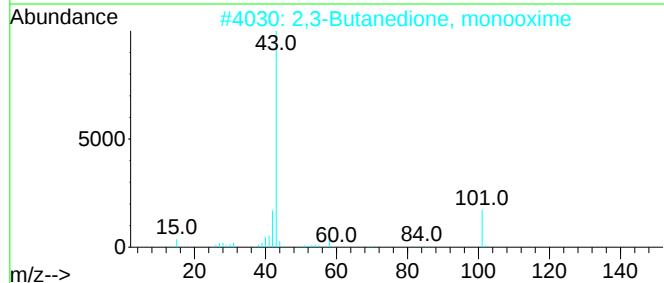
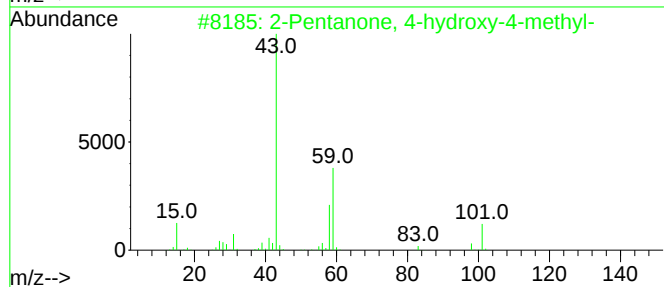
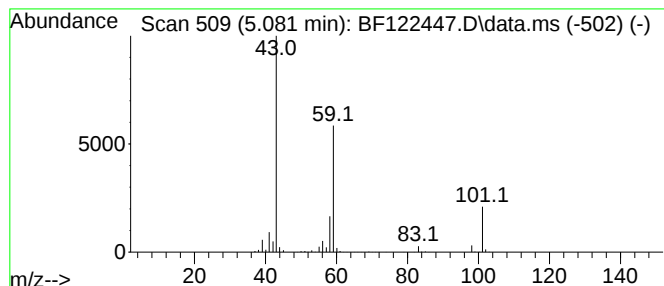
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.081	47.01 ng	2664310	1,4-Dichlorobenzene-d4	6.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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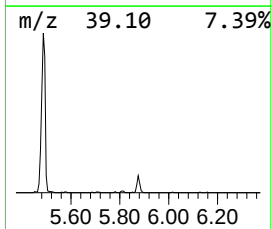
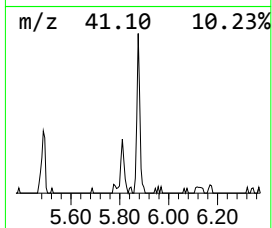
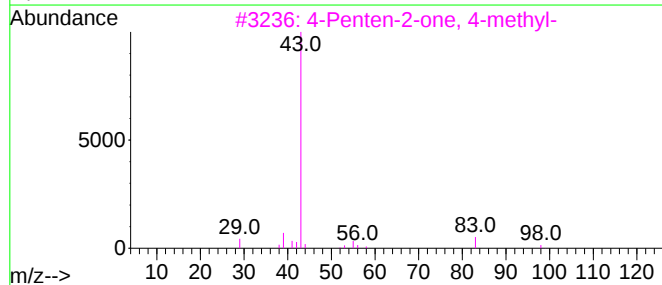
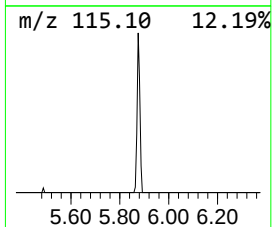
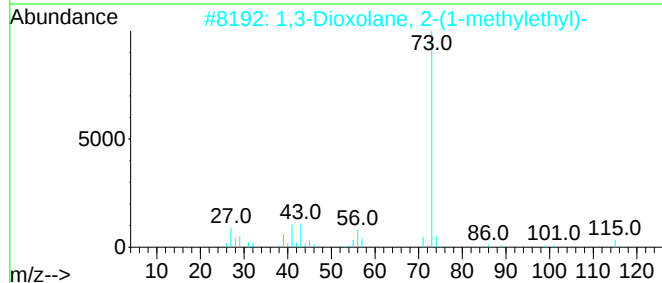
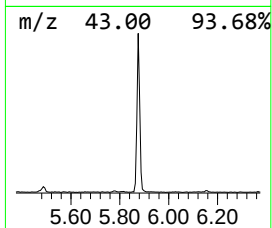
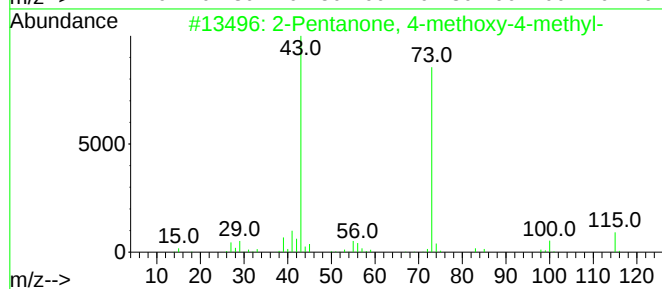
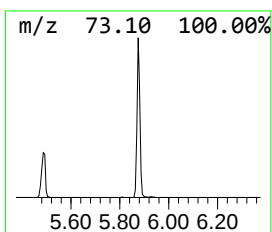
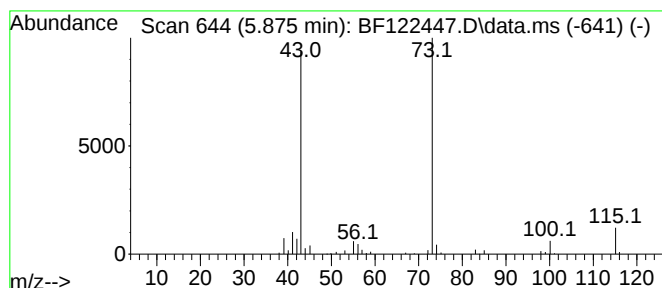
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.875	4.11 ng	232957	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
3			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5			N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



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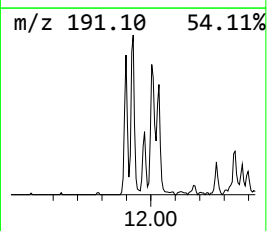
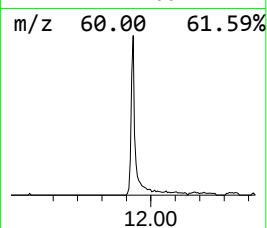
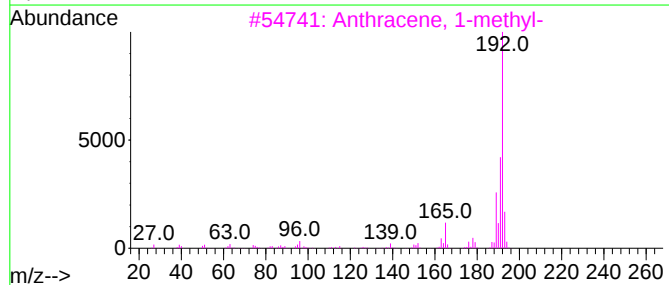
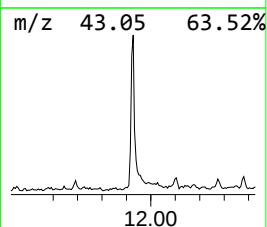
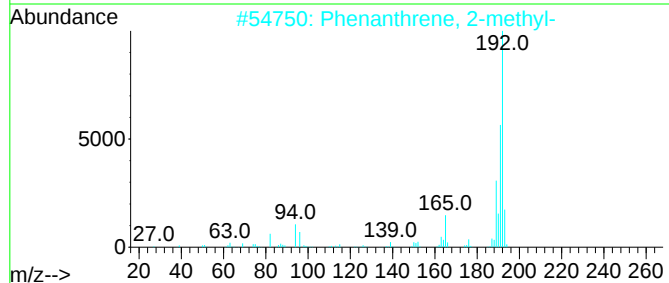
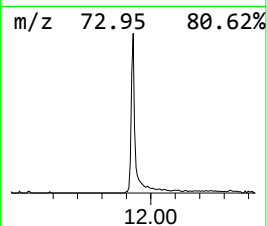
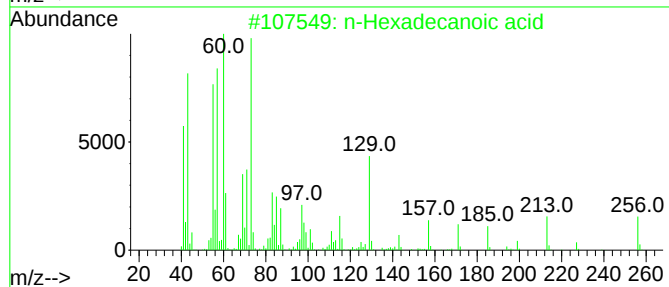
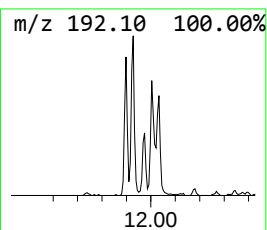
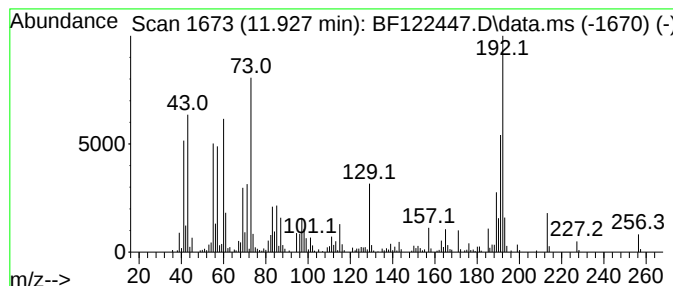
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	6.22 ng	564751	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	94
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122447.D
Acq On : 23 Nov 2020 15:11
Operator : JU/CG
Sample : L4836-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08

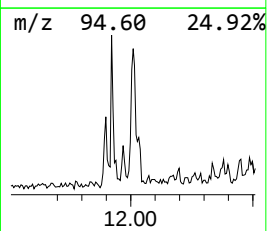
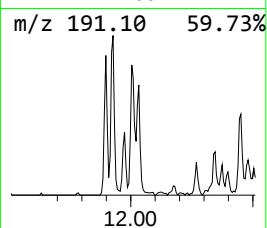
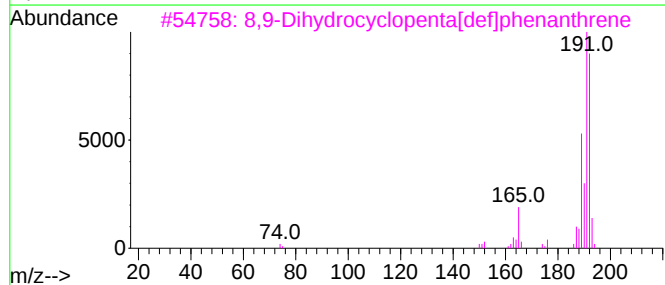
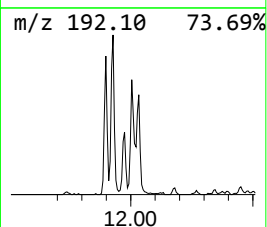
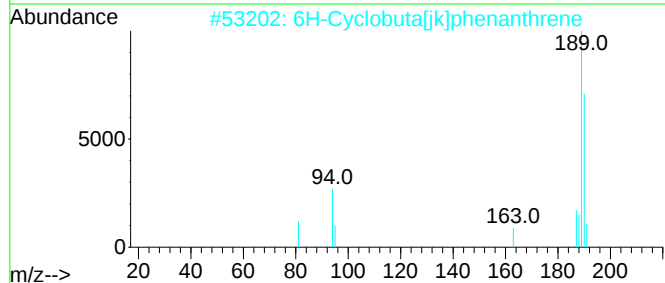
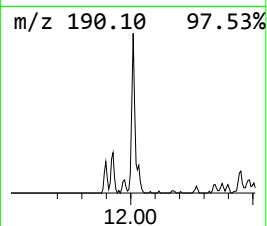
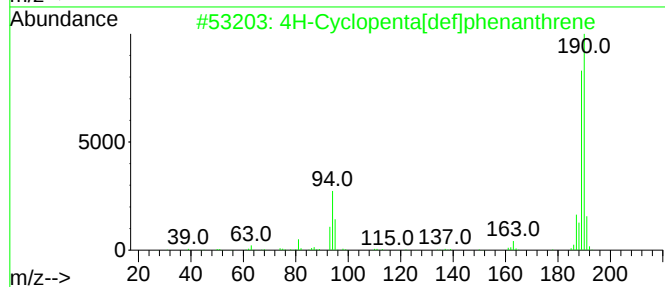
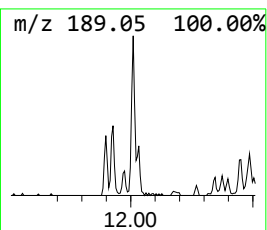
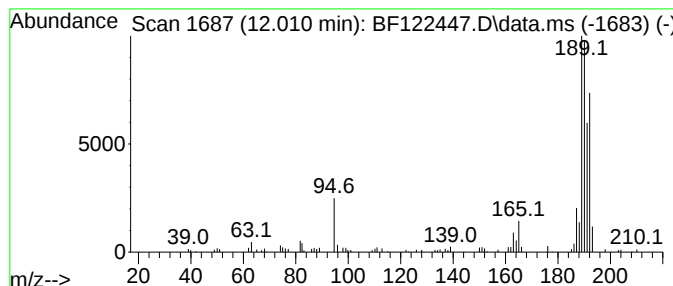
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.64 ng	240057	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3			8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	42
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122447.D
Acq On : 23 Nov 2020 15:11
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Sample : L4836-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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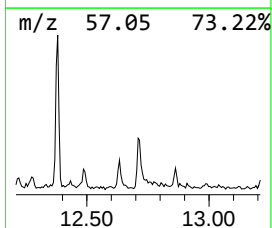
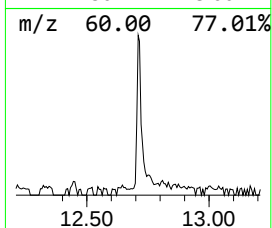
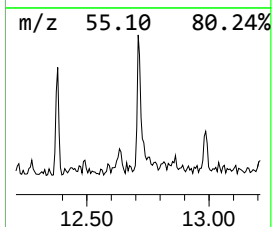
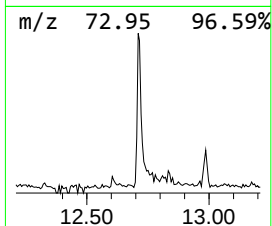
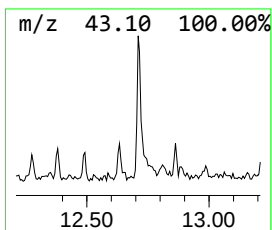
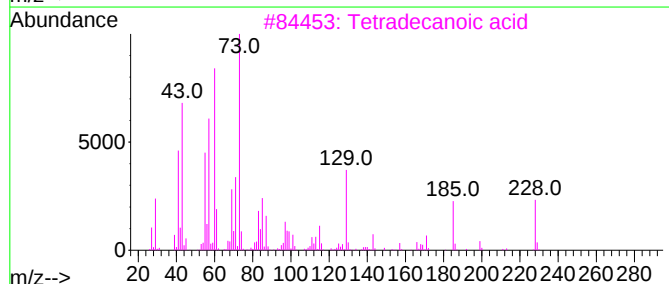
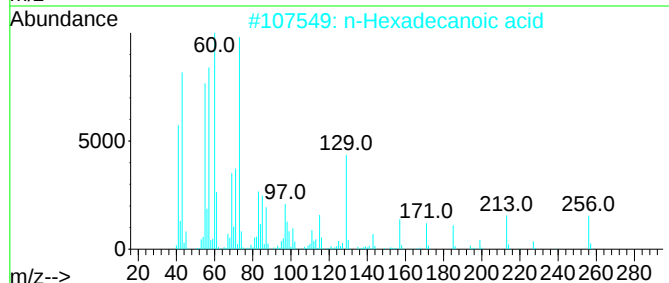
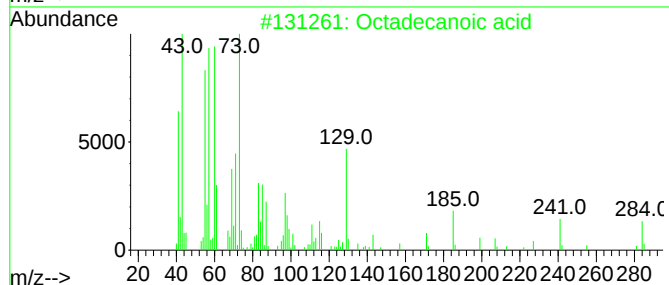
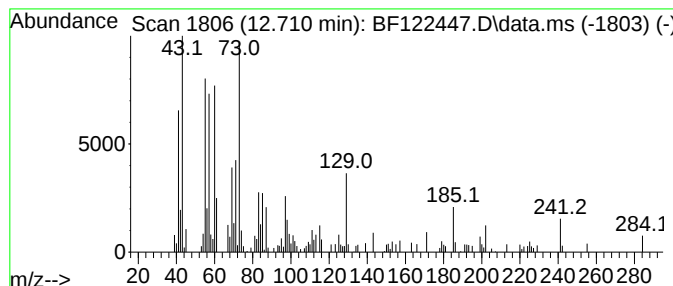
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	2.16 ng	196526	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122447.D
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Operator : JU/CG
Sample : L4836-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-08

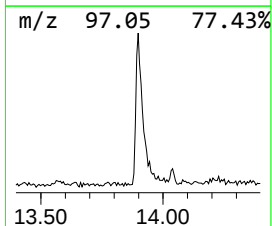
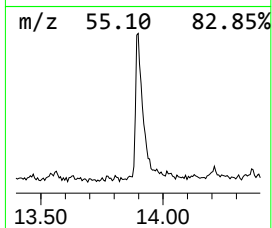
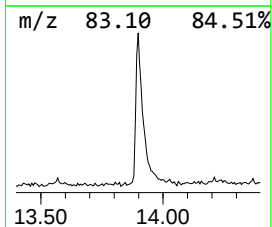
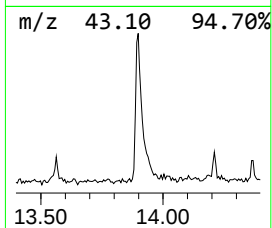
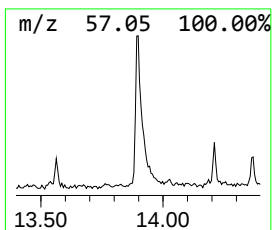
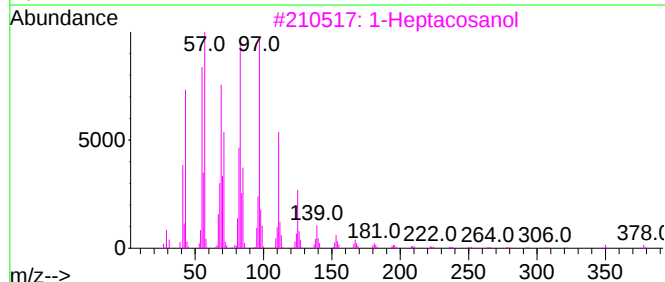
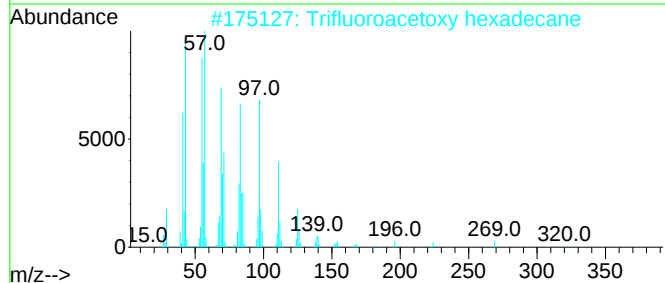
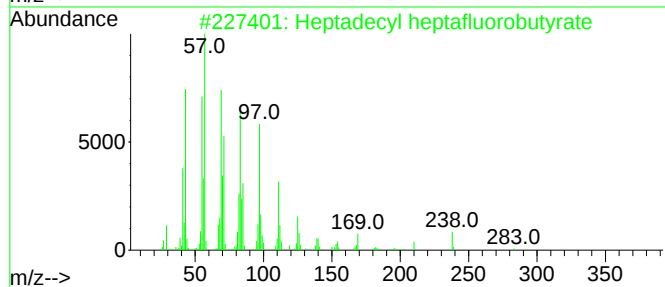
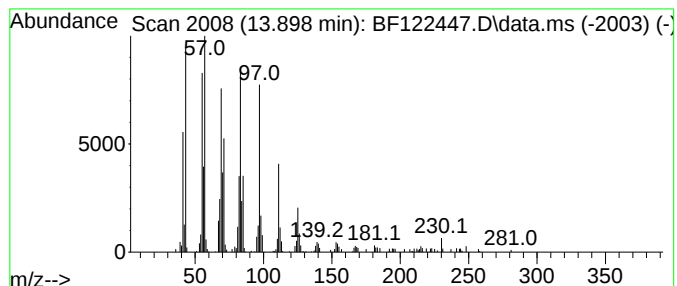
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.85 ng	467689	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122447.D
Acq On : 23 Nov 2020 15:11
Operator : JU/CG
Sample : L4836-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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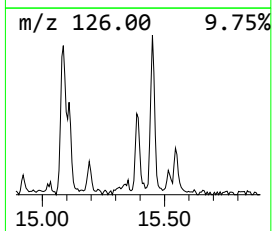
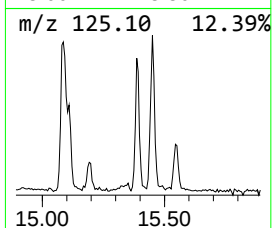
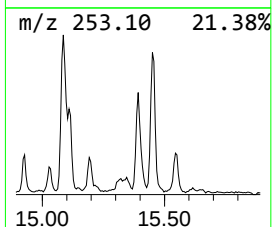
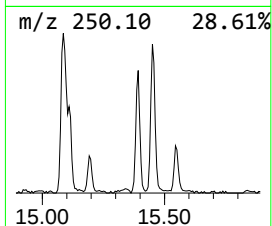
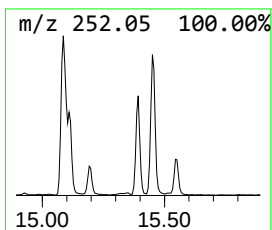
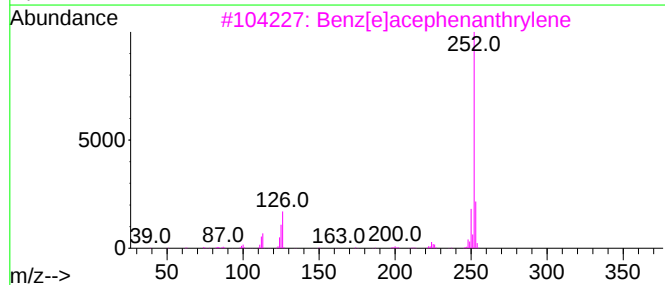
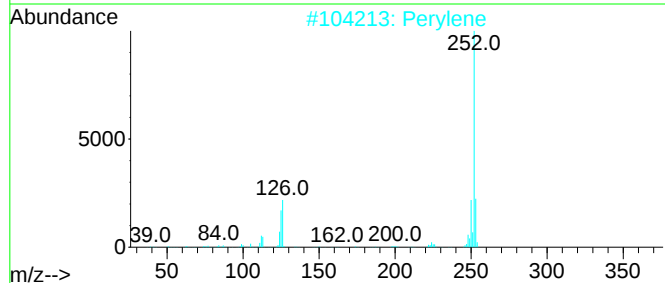
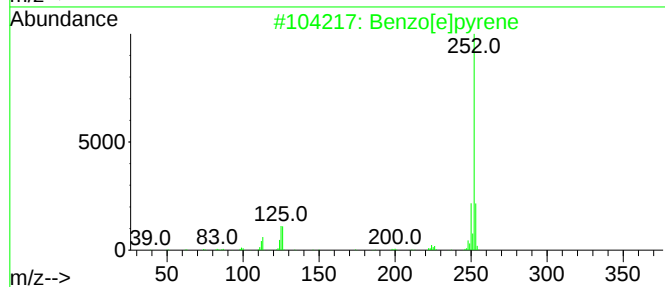
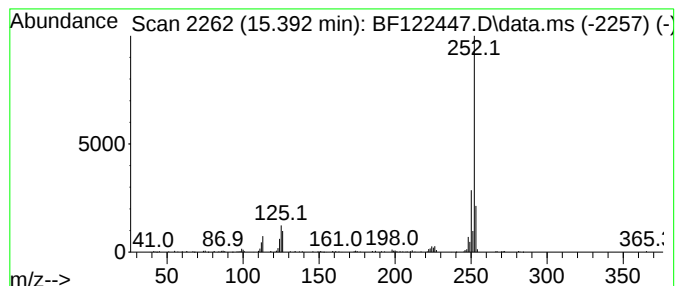
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	4.29 ng	306130	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	95
2			Perylene	252	C20H12	000198-55-0	93
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5			Benzo[a]pyrene	252	C20H12	000050-32-8	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
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Acq On : 23 Nov 2020 15:11
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Sample : L4836-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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
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2-Pentanone, 4-...	5.081	47.0	ng	2664310	1	6.863	1133470	20.0
2-Pentanone, 4-...	5.875	4.1	ng	232957	1	6.863	1133470	20.0
n-Hexadecanoic ...	11.927	6.2	ng	564751	4	11.392	1815800	20.0
4H-Cyclopenta[d...]	12.010	2.6	ng	240057	4	11.392	1815800	20.0
Octadecanoic acid	12.710	2.2	ng	196526	4	11.392	1815800	20.0
Heptadecyl hept...	13.898	3.9	ng	467689	5	14.039	2427180	20.0
Benzo[e]pyrene	15.392	4.3	ng	306130	6	15.521	1425760	20.0