

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
 Data File : BF133810.D
 Acq On : 16 Jun 2023 16:58
 Operator : CG\JU
 Sample : 03222-13 2X
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SB-06

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133810.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	23	rVB	258595	377107	30.28%	2.734%
2	2.246	25	27	40	rVB5	17057	30783	2.47%	0.223%
3	5.087	507	510	517	rBV	67835	78535	6.31%	0.569%
4	5.493	574	579	587	rVB	1083017	1065662	85.56%	7.726%
5	6.493	744	749	752	rBV	1161690	1062155	85.28%	7.701%
6	6.863	808	812	818	rBV	753998	577001	46.33%	4.183%
7	7.422	903	907	910	rBV	807115	658843	52.90%	4.777%
8	8.139	1026	1029	1037	rVB	844040	705871	56.67%	5.118%
9	8.851	1148	1150	1158	rVB	16757	16612	1.33%	0.120%
10	9.216	1208	1212	1215	rBV	1668223	1245494	100.00%	9.030%
11	9.757	1301	1304	1307	rBV	31565	26817	2.15%	0.194%
12	9.898	1324	1328	1331	rBV	928768	743408	59.69%	5.390%
13	9.928	1331	1333	1338	rVB	30992	27914	2.24%	0.202%
14	10.098	1359	1362	1366	rVB2	25725	26468	2.13%	0.192%
15	10.445	1418	1421	1427	rVB4	23389	25641	2.06%	0.186%
16	10.610	1442	1449	1453	rBV	278874	244996	19.67%	1.776%
17	10.686	1458	1462	1474	rVV	844131	733574	58.90%	5.318%
18	10.816	1479	1484	1487	rVB3	20977	29674	2.38%	0.215%
19	10.922	1499	1502	1506	rVB	35413	32362	2.60%	0.235%
20	11.192	1545	1548	1552	rBV2	20115	16988	1.36%	0.123%
21	11.286	1562	1564	1570	rVB	24474	24393	1.96%	0.177%
22	11.392	1578	1582	1584	rBV	775992	727507	58.41%	5.274%
23	11.416	1584	1586	1589	rVV	244902	201633	16.19%	1.462%
24	11.463	1591	1594	1597	rVB	63526	60347	4.85%	0.438%
25	11.622	1618	1621	1628	rVB	24857	26541	2.13%	0.192%
26	11.722	1635	1638	1642	rVB4	14803	16829	1.35%	0.122%
27	11.798	1646	1651	1655	rVB6	21541	29308	2.35%	0.212%
28	11.892	1664	1667	1669	rBV	46837	42448	3.41%	0.308%
29	11.922	1669	1672	1676	rVV	163325	154544	12.41%	1.120%
30	12.004	1683	1686	1689	rBV	67629	79794	6.41%	0.579%
31	12.027	1689	1690	1695	rVB	38035	26420	2.12%	0.192%
32	12.092	1696	1701	1705	rVB6	16959	24100	1.93%	0.175%
33	12.192	1715	1718	1720	rVV	34033	30085	2.42%	0.218%
34	12.216	1720	1722	1725	rVB2	31860	28225	2.27%	0.205%
35	12.445	1758	1761	1764	rBV2	37155	43434	3.49%	0.315%
36	12.486	1764	1768	1770	rVV3	29234	32469	2.61%	0.235%

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37	12.533	1773	1776	1781	rBV	34326	43607	3.50%	0.316%
38	12.610	1785	1789	1794	rVV	531359	439541	35.29%	3.187%
39	12.710	1803	1806	1808	rBV2	47302	50314	4.04%	0.365%
40	12.839	1822	1828	1834	rBV	516140	528934	42.47%	3.835%
41	12.892	1834	1837	1841	rVB3	27400	33852	2.72%	0.245%
42	12.986	1849	1853	1860	rVB	1224167	1112568	89.33%	8.066%
43	13.057	1863	1865	1869	rVB3	29185	38839	3.12%	0.282%
44	13.145	1877	1880	1881	rBV3	23720	25671	2.06%	0.186%
45	13.169	1882	1884	1887	rVB	67746	58481	4.70%	0.424%
46	13.233	1893	1895	1899	rVB	44775	42608	3.42%	0.309%
47	13.274	1899	1902	1905	rBV2	44060	38015	3.05%	0.276%
48	13.369	1915	1918	1921	rBV2	28571	26163	2.10%	0.190%
49	13.398	1921	1923	1926	rBV	31712	27863	2.24%	0.202%
50	13.680	1968	1971	1977	rBV	45918	67936	5.45%	0.493%
51	13.821	1993	1995	1997	rBV	33188	24834	1.99%	0.180%
52	13.845	1997	1999	2003	rBV2	31398	33659	2.70%	0.244%
53	13.898	2005	2008	2015	rVB3	65711	96354	7.74%	0.699%
54	14.045	2028	2033	2036	rBV2	654830	777032	62.39%	5.634%
55	14.074	2036	2038	2046	rVB	201814	184892	14.84%	1.340%
56	14.151	2049	2051	2054	rVB2	50522	39959	3.21%	0.290%
57	15.110	2210	2214	2217	rBV	165307	244502	19.63%	1.773%
58	15.427	2265	2268	2273	rVB	81485	100372	8.06%	0.728%
59	15.486	2275	2278	2285	rVB	109850	144235	11.58%	1.046%
60	15.557	2286	2290	2294	rBV	274002	338806	27.20%	2.456%

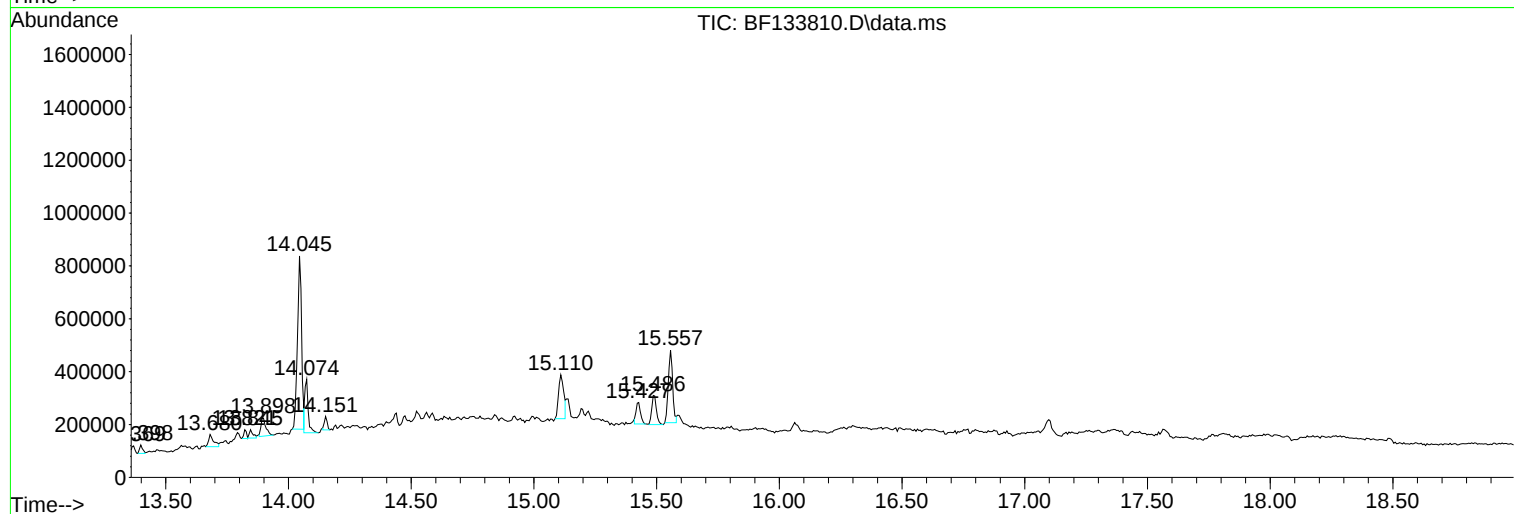
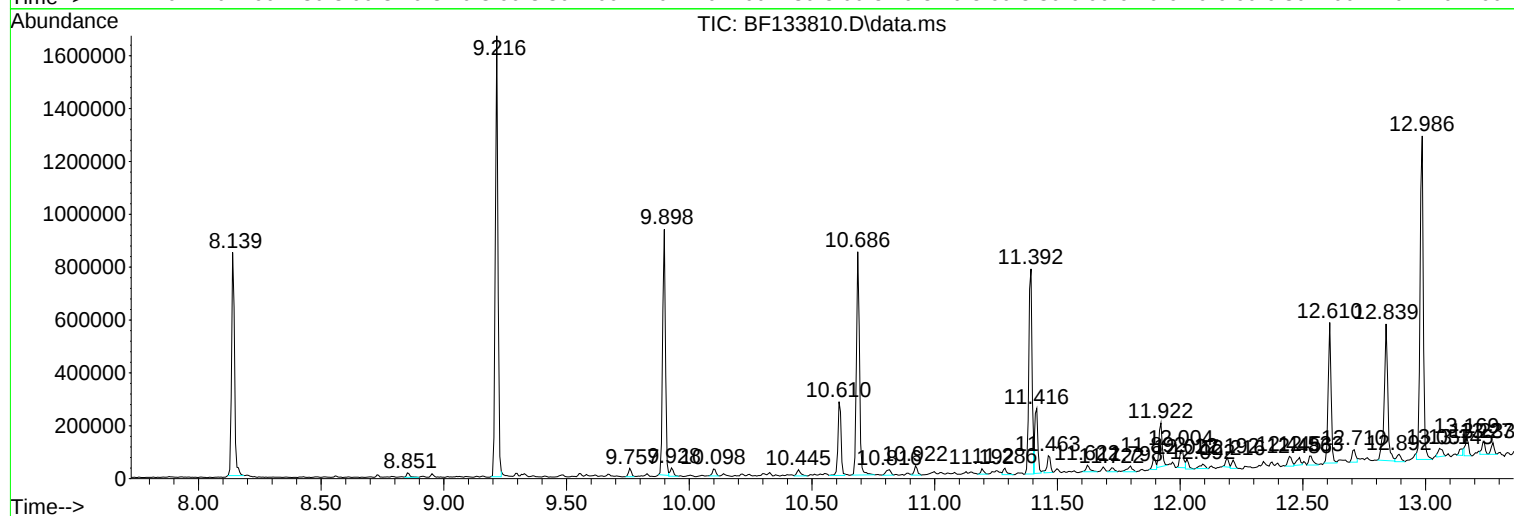
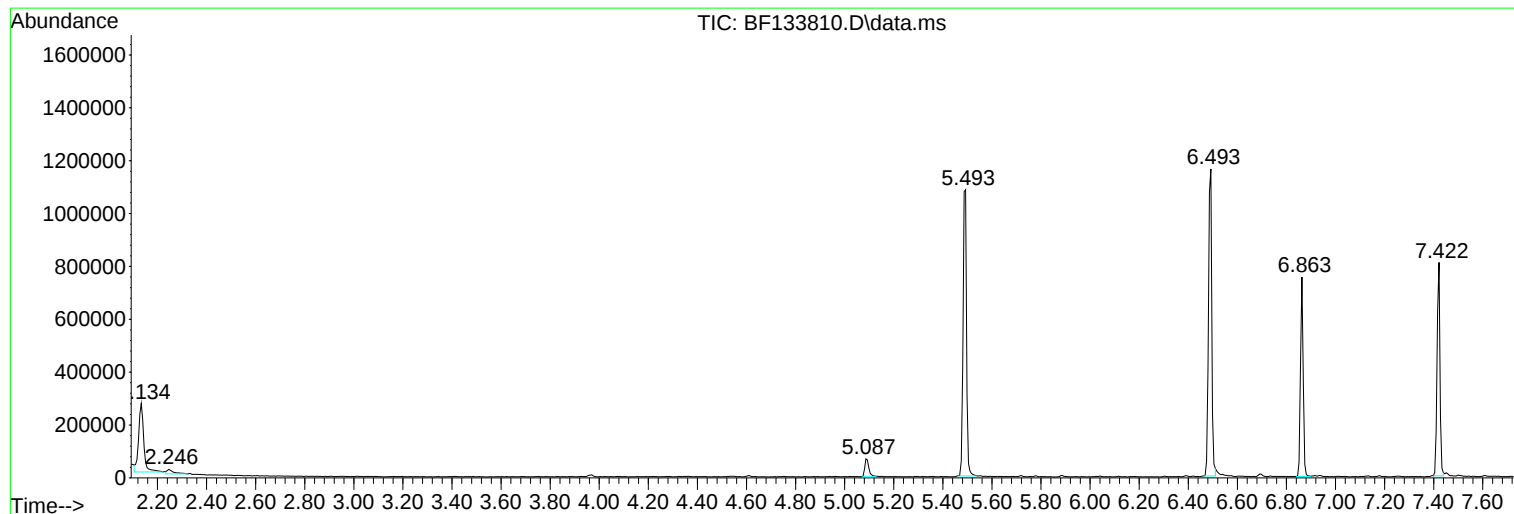
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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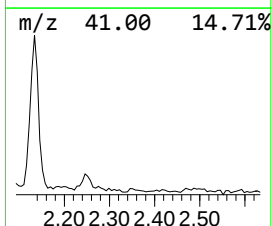
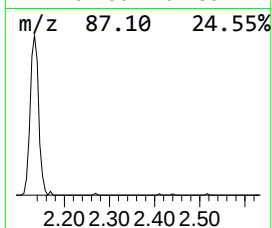
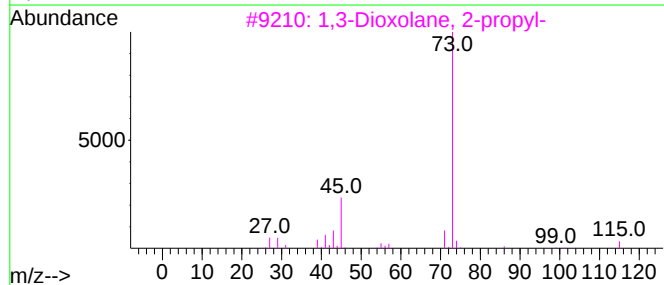
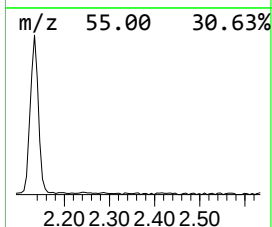
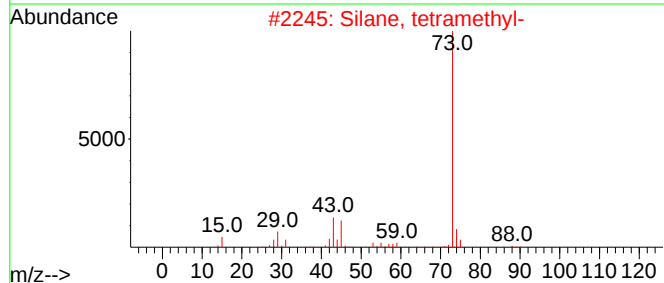
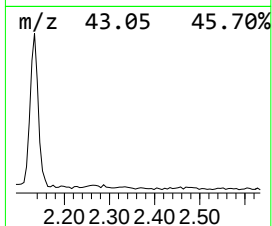
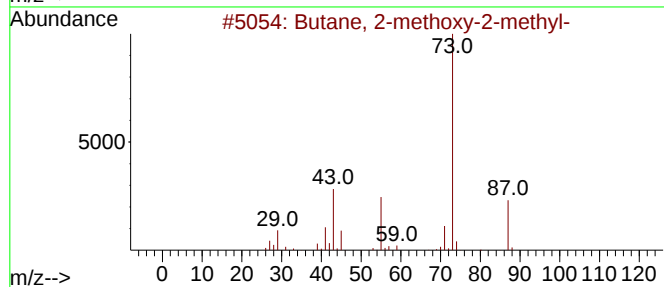
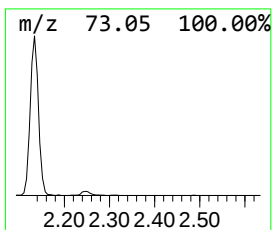
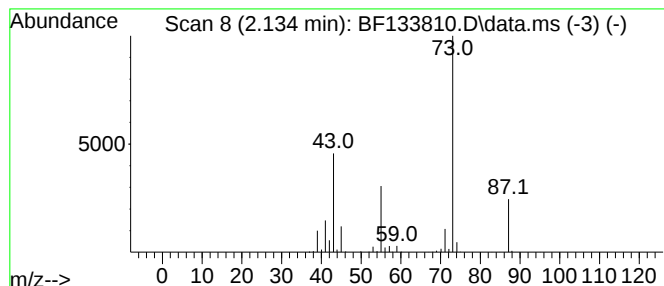
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	13.07 ng	377107	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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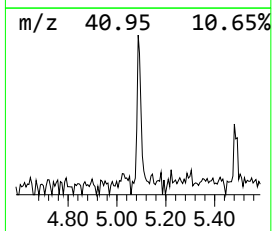
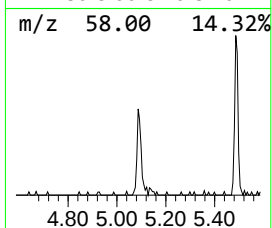
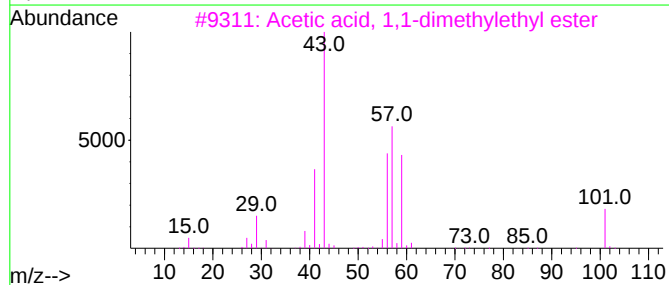
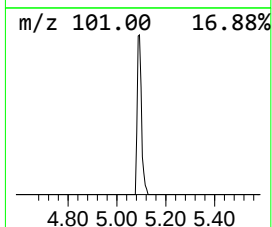
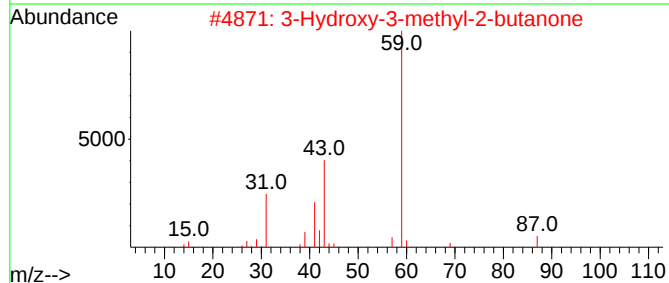
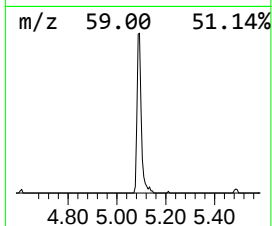
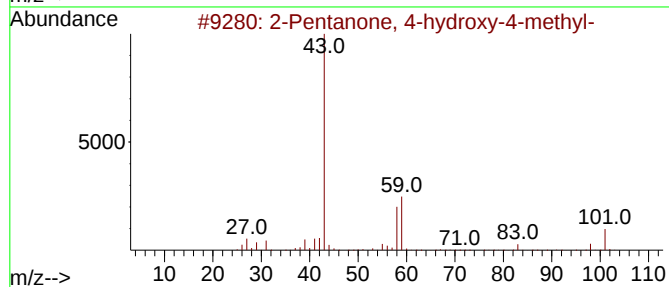
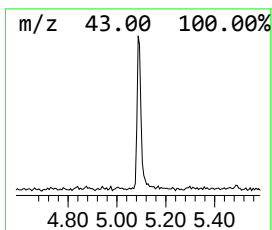
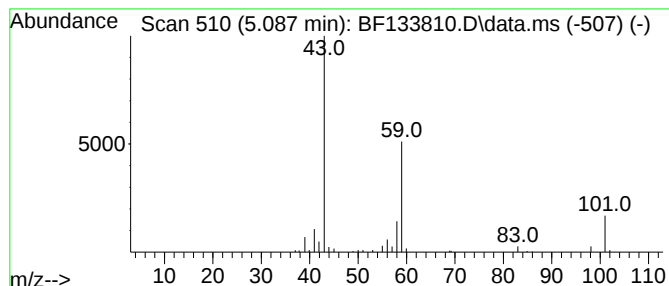
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	2.72 ng	78535	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	64		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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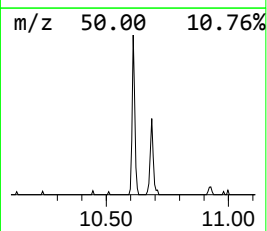
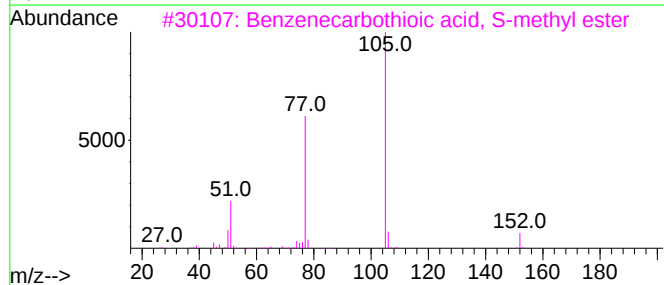
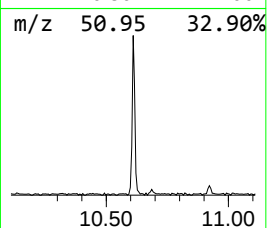
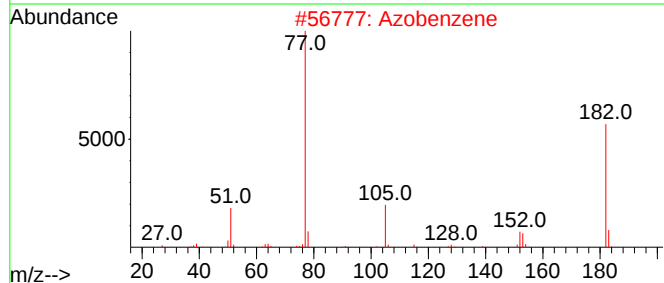
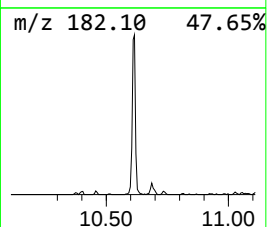
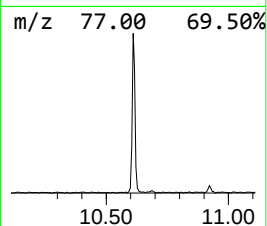
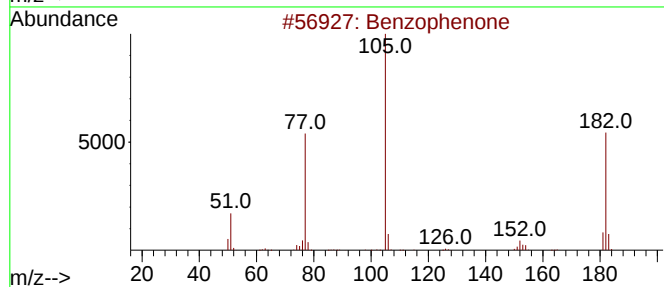
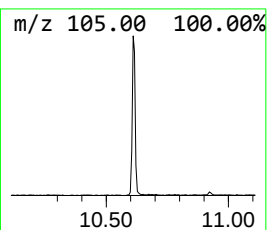
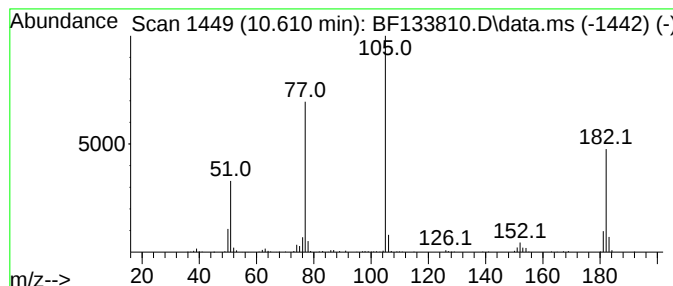
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	6.59 ng	244996	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	50
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Benzoylformic acid	150	C8H6O3	000611-73-4	49
5			Propan-1-one, 3-nitro-1-phenyl-	179	C9H9NO3	062847-52-3	47



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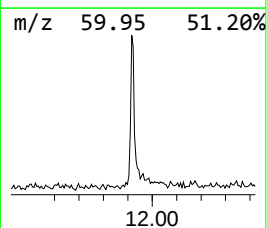
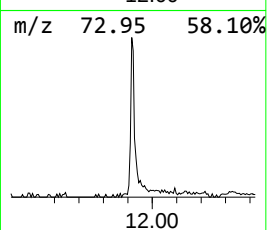
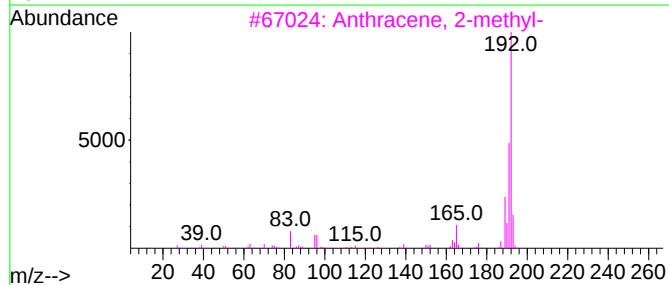
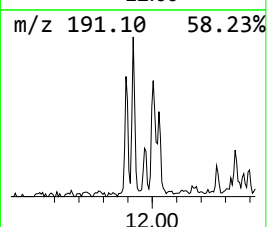
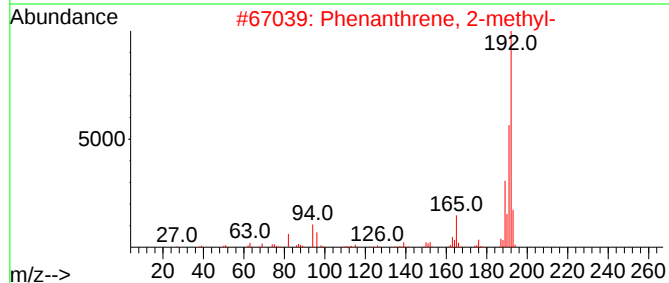
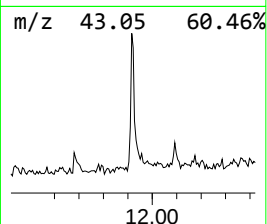
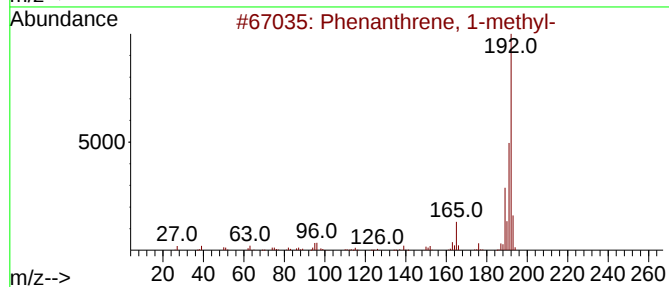
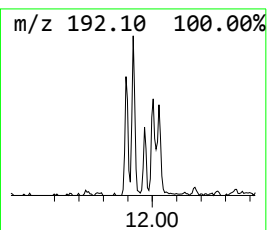
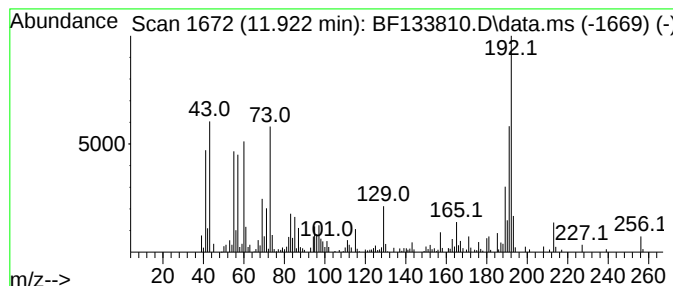
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	4.25 ng	154544	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5			1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	91



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ClientSampleId :
COMPOSITE-SB-06

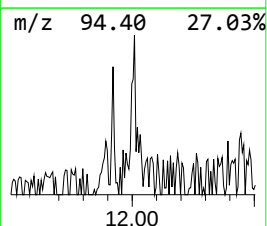
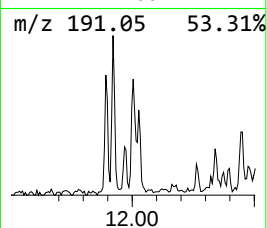
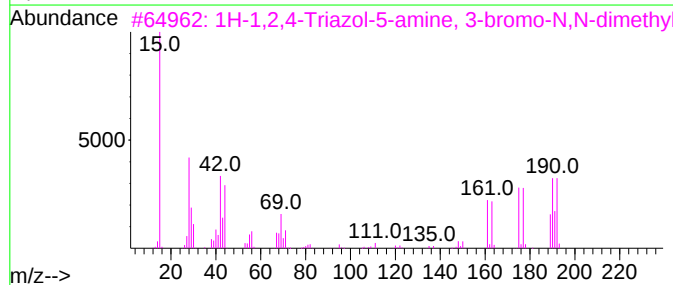
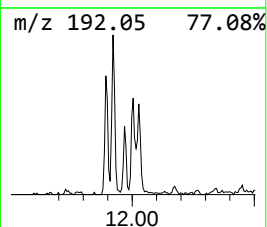
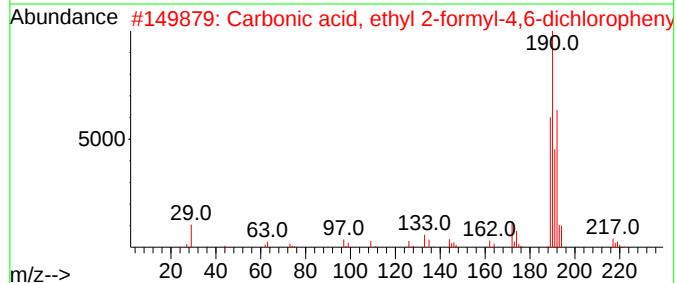
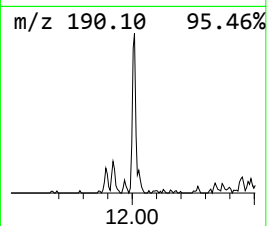
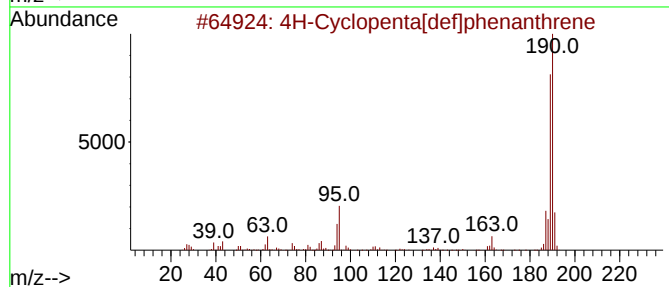
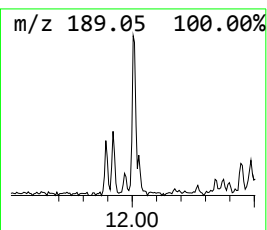
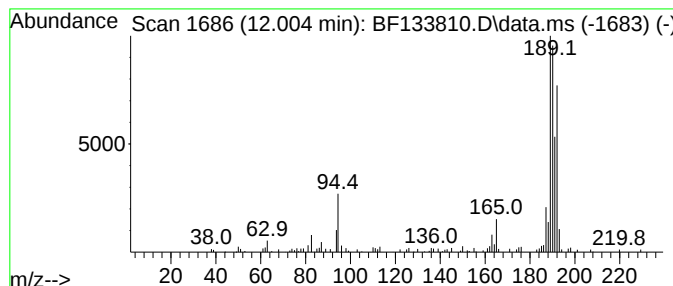
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
12.004	2.19 ng	79794	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
2			Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	53
3			1H-1,2,4-Triazol-5-amine, 3-brom...	190	C4H7BrN4	1000460-85-7	50
4			Methyl diselenide	190	C2H6Se2	007101-31-7	38
5			Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133810.D
Acq On : 16 Jun 2023 16:58
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

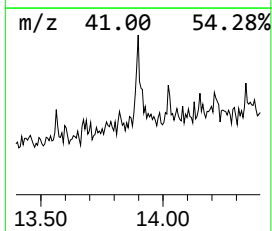
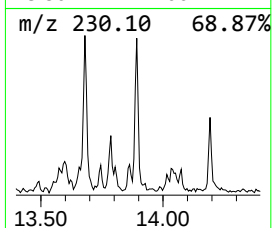
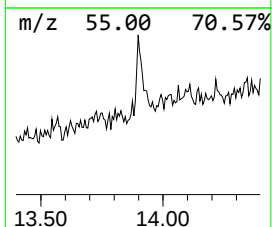
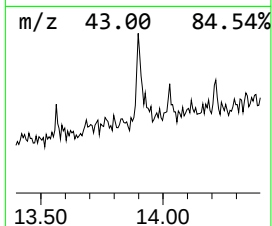
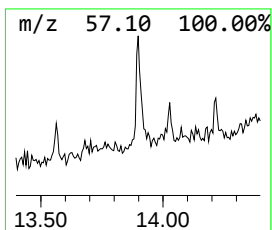
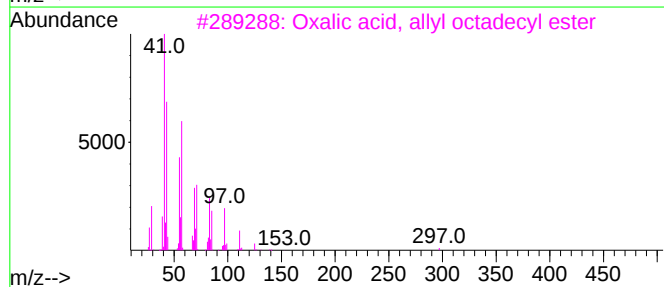
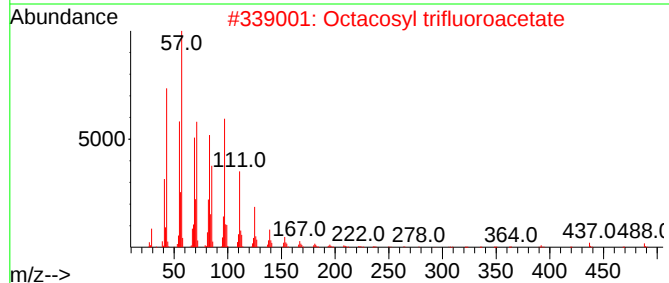
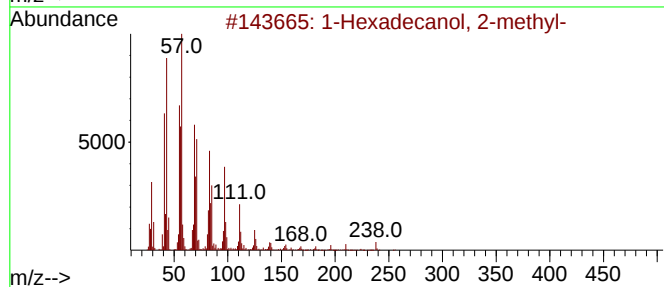
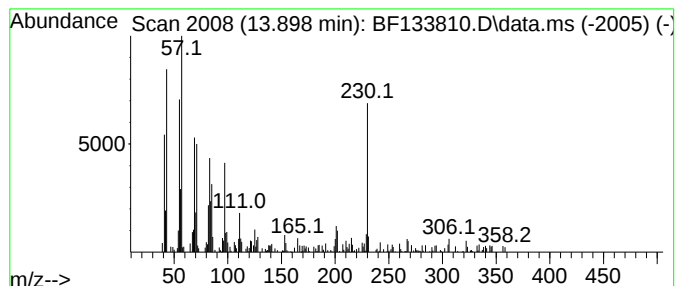
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Hexadecanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.48 ng	96354	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	70
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	58
3			Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	58
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	58
5			1-Tricosene	322	C23H46	018835-32-0	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133810.D
Acq On : 16 Jun 2023 16:58
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

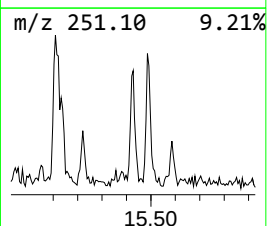
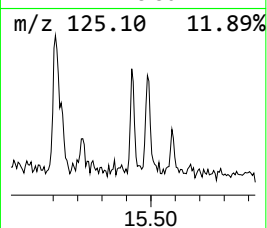
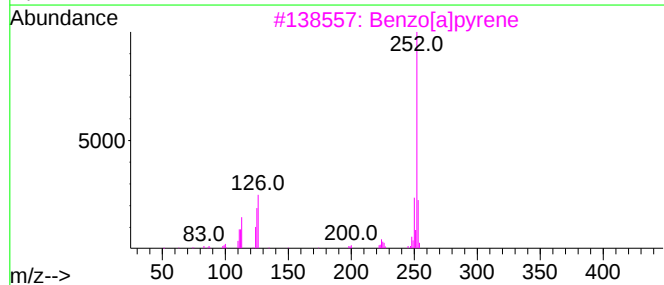
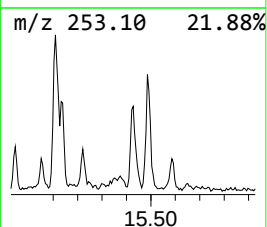
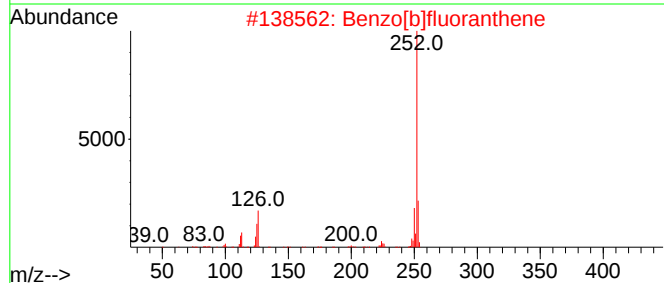
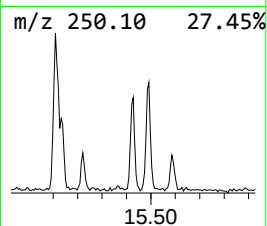
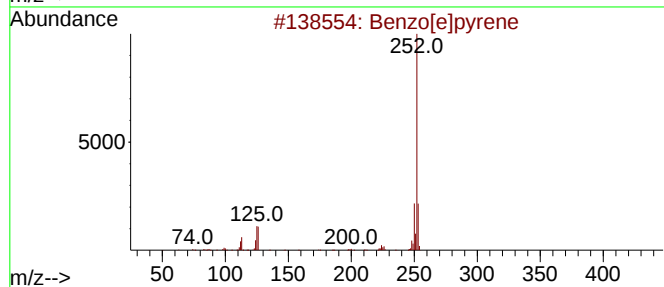
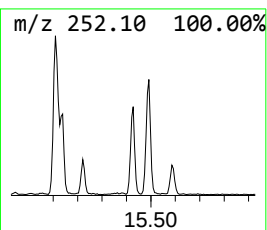
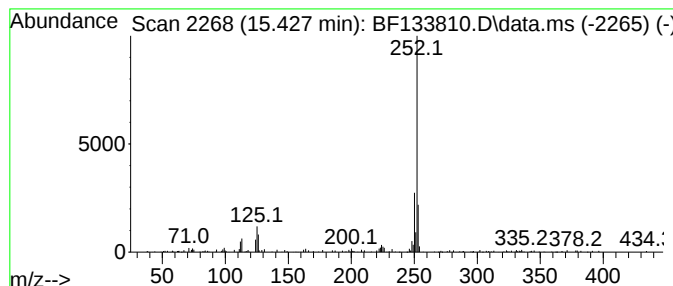
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	5.93 ng	100372	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	90
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061623\
Data File : BF133810.D
Acq On : 16 Jun 2023 16:58
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.134	13.1	ng	377107	1	6.863	577001	20.0
2-Pentanone, 4-...	5.087	2.7	ng	78535	1	6.863	577001	20.0
Benzophenone	10.610	6.6	ng	244996	3	9.898	743408	20.0
Phenanthrene, 1...	11.922	4.3	ng	154544	4	11.392	727507	20.0
4H-Cyclopenta[d...	12.004	2.2	ng	79794	4	11.392	727507	20.0
1-Hexadecanol, ...	13.898	2.5	ng	96354	5	14.045	777032	20.0
Benzo[e]pyrene	15.427	5.9	ng	100372	6	15.557	338806	20.0