

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF093021\
 Data File : BF125739.D
 Acq On : 30 Sep 2021 18:11
 Operator : JU/CG
 Sample : M3988-01 5X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-03-092921

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125739.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	5	10	16	rVB	209648	270626	15.17%	1.561%
2	5.492	575	579	590	rBV	784407	689393	38.64%	3.976%
3	6.498	746	750	759	rBV	811415	685101	38.40%	3.951%
4	6.886	812	816	819	rBV	1518167	1211343	67.89%	6.987%
5	7.439	906	910	915	rBV	525250	412805	23.14%	2.381%
6	8.069	1013	1017	1027	rBV	45340	73642	4.13%	0.425%
7	8.169	1030	1034	1037	rBV	1950559	1690489	94.75%	9.750%
8	9.239	1212	1216	1225	rBV	1071405	869122	48.71%	5.013%
9	9.922	1328	1332	1336	rBV	2067711	1784191	100.00%	10.291%
10	9.951	1336	1337	1347	rVB	80745	77473	4.34%	0.447%
11	10.121	1362	1366	1371	rBV	27110	29236	1.64%	0.169%
12	10.469	1421	1425	1429	rBV	55352	58163	3.26%	0.335%
13	10.704	1461	1465	1480	rVB	426859	416783	23.36%	2.404%
14	10.827	1482	1486	1494	rBV5	15865	27430	1.54%	0.158%
15	11.016	1512	1518	1520	rBV2	15135	20966	1.18%	0.121%
16	11.298	1564	1566	1572	rVB	37561	39132	2.19%	0.226%
17	11.404	1580	1584	1586	rBV	1932580	1585626	88.87%	9.145%
18	11.427	1586	1588	1591	rVV	444409	349945	19.61%	2.018%
19	11.480	1594	1597	1600	rVB	61898	56414	3.16%	0.325%
20	11.633	1618	1623	1629	rBV2	21368	33765	1.89%	0.195%
21	11.733	1638	1640	1646	rVB	24402	27201	1.52%	0.157%
22	11.904	1666	1669	1671	rBV	54217	49723	2.79%	0.287%
23	11.933	1671	1674	1677	rVB	73348	71496	4.01%	0.412%
24	12.015	1684	1688	1690	rBV	94077	96583	5.41%	0.557%
25	12.039	1690	1692	1696	rVB	45219	37902	2.12%	0.219%
26	12.198	1716	1719	1721	rBV	35068	31813	1.78%	0.183%
27	12.221	1721	1723	1727	rVB3	32603	36822	2.06%	0.212%
28	12.380	1747	1750	1753	rBV3	22770	28326	1.59%	0.163%
29	12.457	1759	1763	1765	rBV	57053	61528	3.45%	0.355%
30	12.492	1765	1769	1774	rVB5	54427	93632	5.25%	0.540%
31	12.539	1774	1777	1781	rBV4	28171	35645	2.00%	0.206%
32	12.615	1787	1790	1793	rBV	490170	398463	22.33%	2.298%
33	12.710	1803	1806	1808	rBV2	21782	25619	1.44%	0.148%
34	12.768	1813	1816	1819	rVV2	37765	40943	2.29%	0.236%
35	12.845	1823	1829	1831	rVV	401459	424039	23.77%	2.446%
36	12.904	1835	1839	1842	rVB3	28755	35557	1.99%	0.205%

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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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37	12.962	1846	1849	1850	rBV2	23977	25232	1.41%	0.146%
38	12.986	1850	1853	1861	rVB	810646	725418	40.66%	4.184%
39	13.057	1862	1865	1869	rBV3	32567	48677	2.73%	0.281%
40	13.115	1873	1875	1878	rBV3	17728	20341	1.14%	0.117%
41	13.168	1882	1884	1887	rVB	80780	70058	3.93%	0.404%
42	13.239	1890	1896	1899	rBV2	50257	79682	4.47%	0.460%
43	13.274	1899	1902	1906	rBV3	51546	64808	3.63%	0.374%
44	13.368	1916	1918	1920	rVB2	33012	25950	1.45%	0.150%
45	13.398	1920	1923	1925	rBV2	39644	37231	2.09%	0.215%
46	13.433	1927	1929	1933	rVB4	29207	30944	1.73%	0.178%
47	13.562	1948	1951	1954	rBV4	38628	42994	2.41%	0.248%
48	13.792	1985	1990	1993	rBV2	52047	82063	4.60%	0.473%
49	13.821	1993	1995	1997	rVV	29319	24049	1.35%	0.139%
50	13.892	2004	2007	2010	rVB3	35399	33716	1.89%	0.194%
51	14.039	2027	2032	2035	rBV	1602922	1552313	87.00%	8.953%
52	14.062	2035	2036	2039	rVB	161214	106715	5.98%	0.615%
53	14.204	2058	2060	2063	rBV	41142	38235	2.14%	0.221%
54	14.515	2110	2113	2116	rVB2	66464	67652	3.79%	0.390%
55	14.821	2162	2165	2168	rBV	71240	77643	4.35%	0.448%
56	15.086	2206	2210	2218	rVB	136798	275655	15.45%	1.590%
57	15.162	2221	2223	2226	rVB	63820	59690	3.35%	0.344%
58	15.386	2258	2261	2268	rVB	93853	125743	7.05%	0.725%
59	15.451	2269	2272	2276	rVV	114913	141571	7.93%	0.817%
60	15.515	2279	2283	2287	rVV	983433	1246294	69.85%	7.188%
61	15.551	2287	2289	2295	rVB3	147867	182105	10.21%	1.050%
62	15.998	2362	2365	2370	rBV	65172	95963	5.38%	0.553%
63	16.239	2404	2406	2414	rVB3	103052	180505	10.12%	1.041%

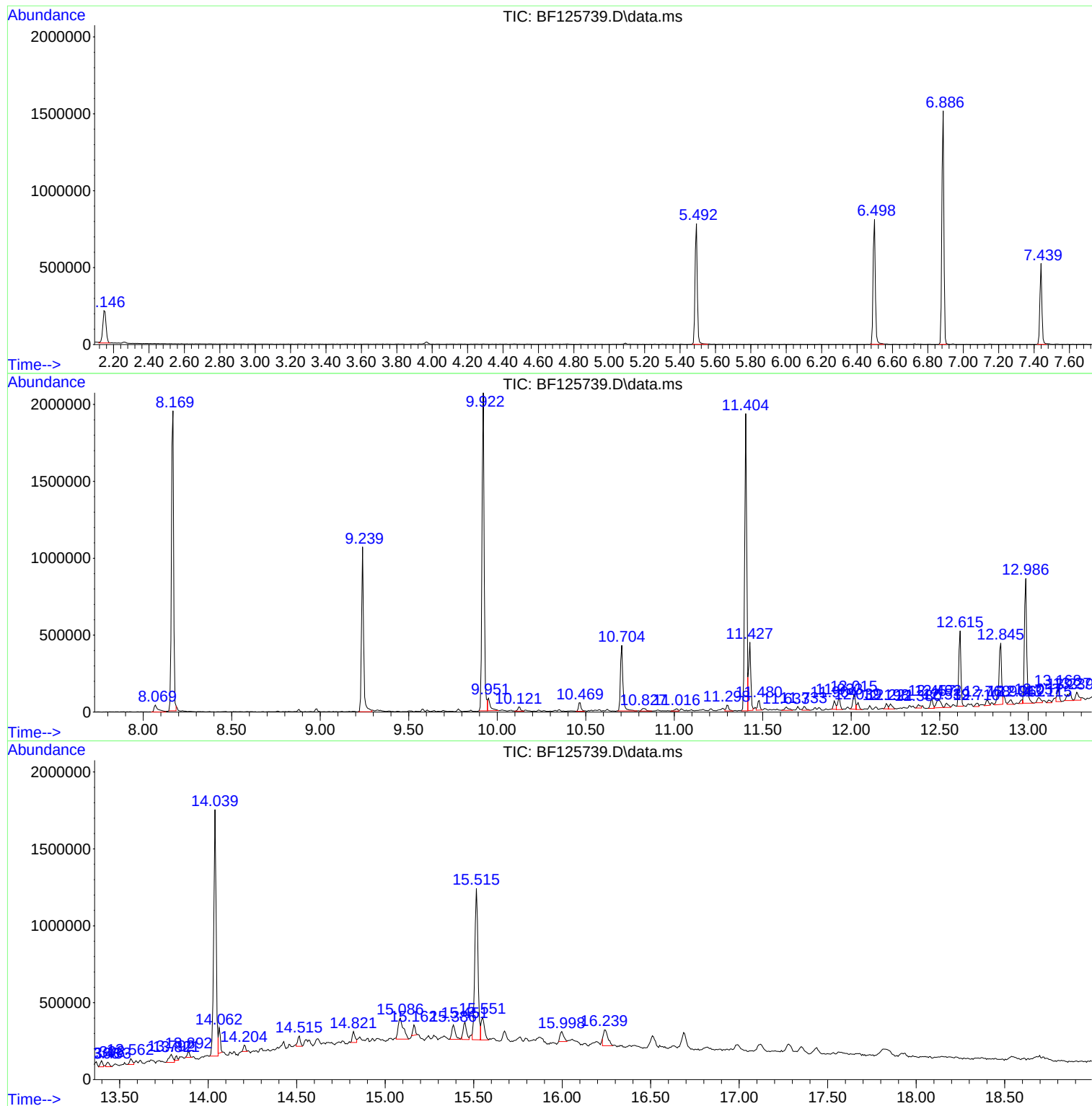
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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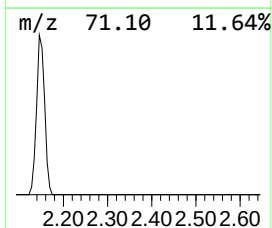
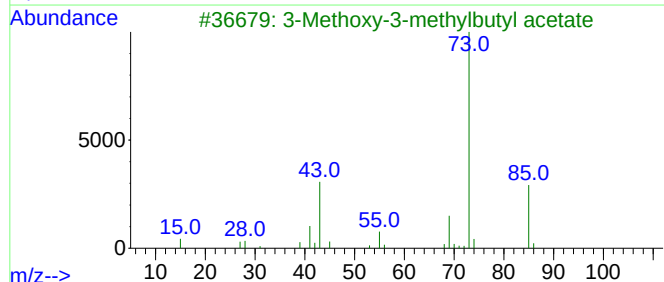
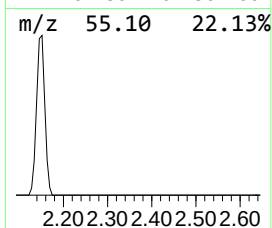
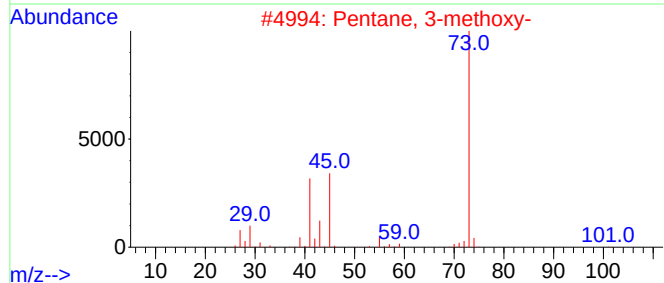
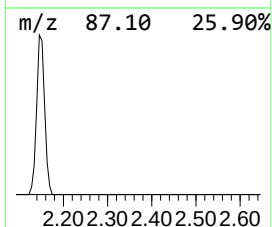
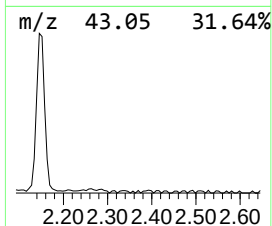
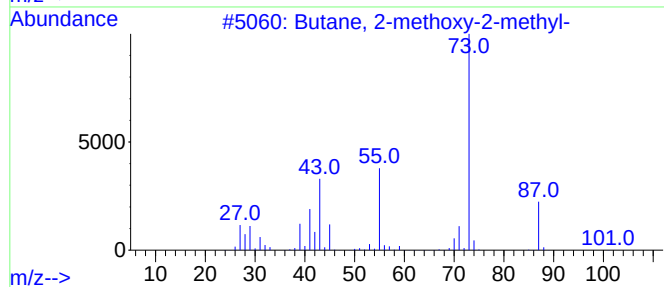
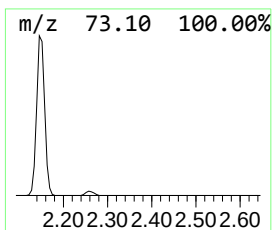
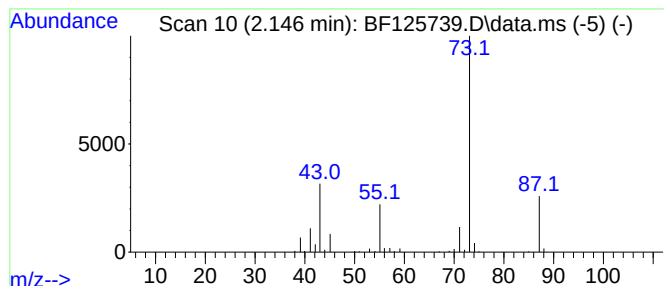
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	4.47 ng	270626	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3			3-Methoxy-3-methylbutyl acetate	160	C8H16O3	1010430-01-2	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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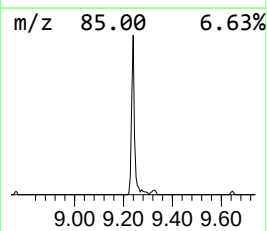
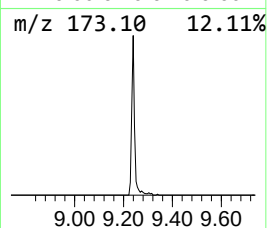
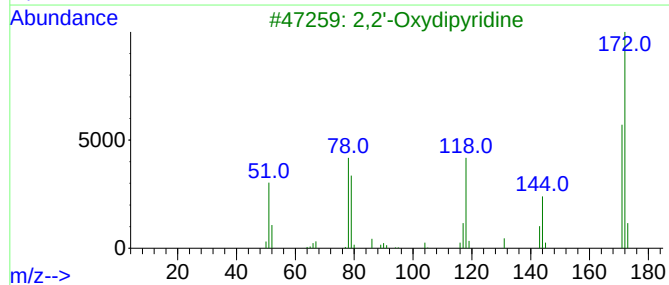
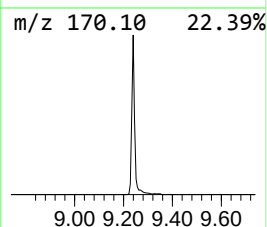
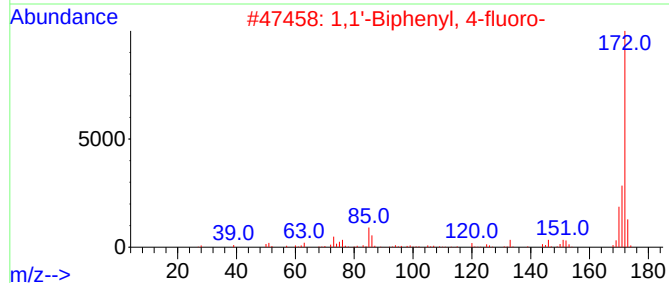
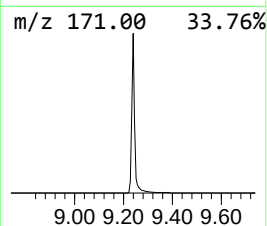
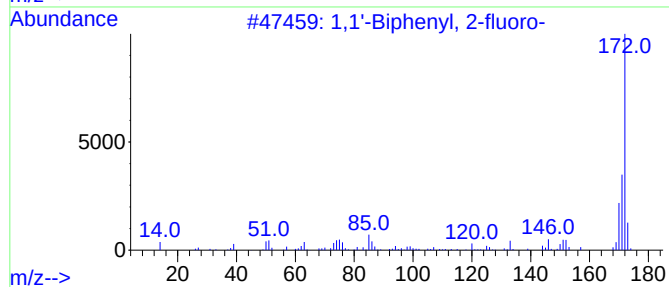
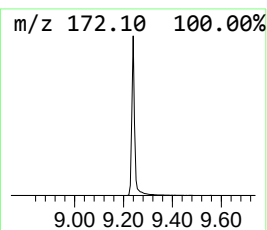
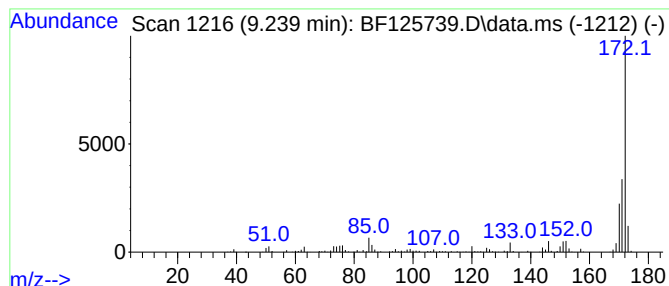
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,1'-Biphenyl, 2-fluoro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.239	9.74 ng	869122	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1'-Biphenyl, 2-fluoro-	172	C12H9F	000321-60-8	96
2			1,1'-Biphenyl, 4-fluoro-	172	C12H9F	000324-74-3	93
3			2,2'-Oxydipyridine	172	C10H8N2O	053258-94-9	52
4			Thiourea, N-cyclohexyl-N'-methyl-	172	C8H16N2S	013120-04-2	47
5			4-Pyrimidinol, 5-phenyl-	172	C10H8N2O	022433-69-8	42



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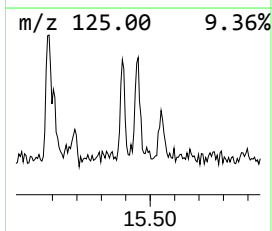
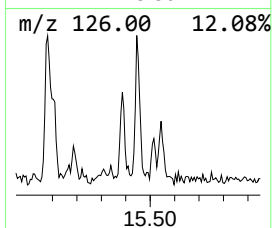
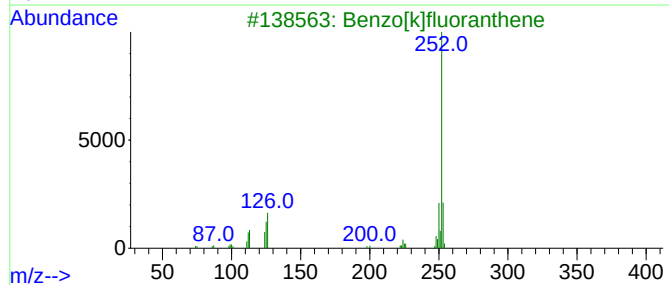
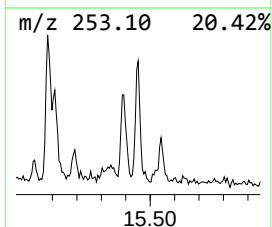
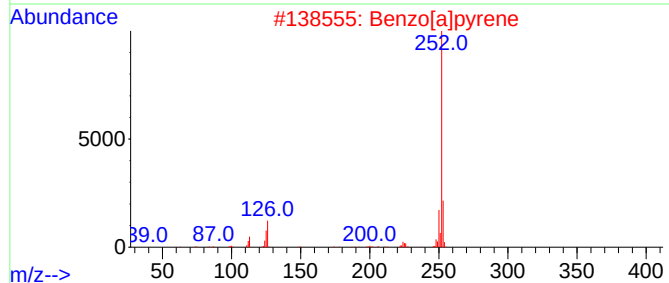
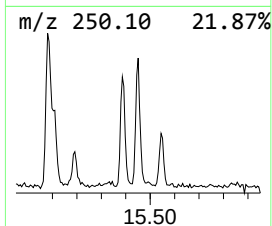
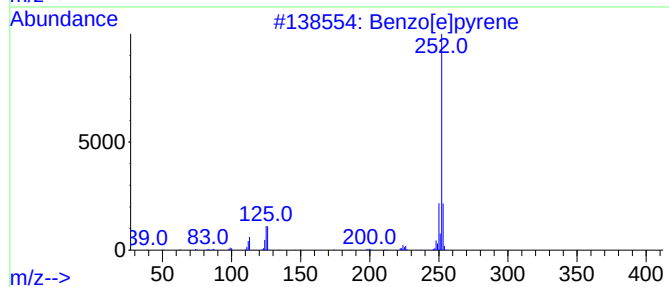
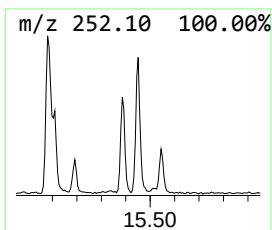
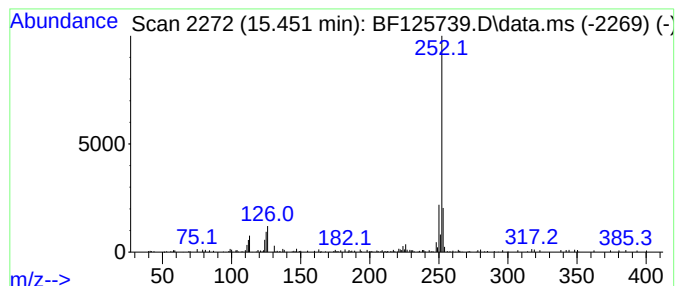
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.451	2.27 ng	141571	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[a]pyrene	252	C20H12	000050-32-8	90
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	81
5			Perylene	252	C20H12	000198-55-0	81



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ALS Vial : 18 Sample Multiplier: 1

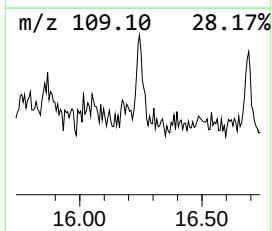
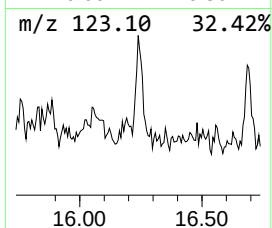
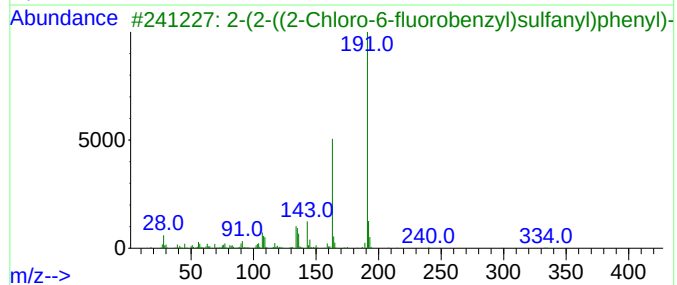
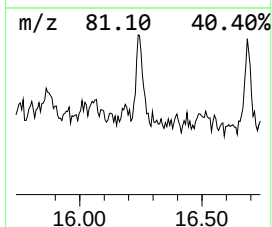
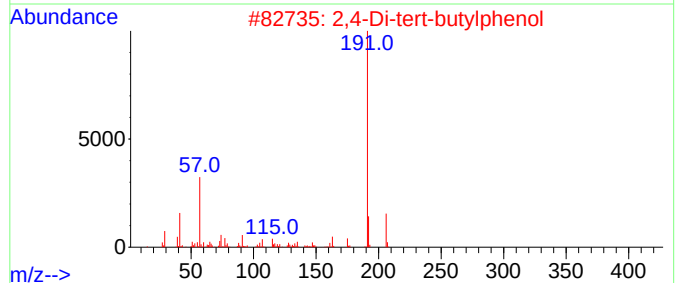
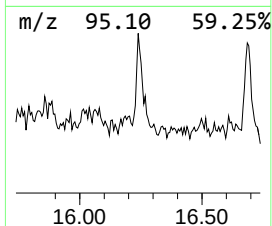
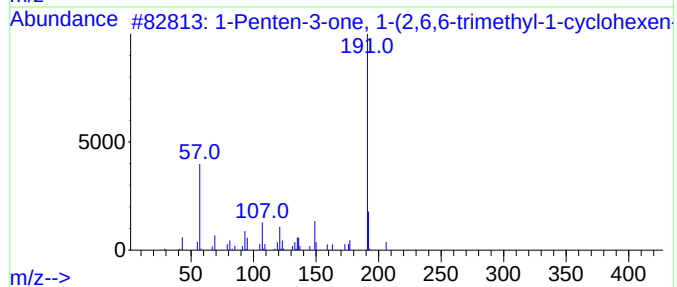
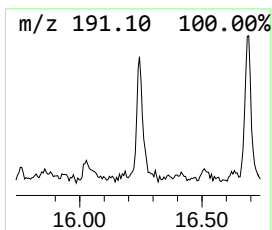
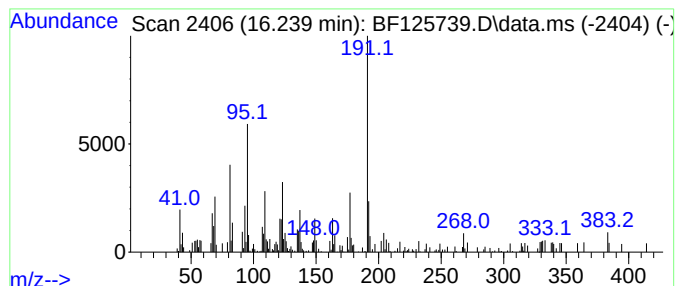
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.239 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.239	2.90 ng	180505	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	46
2	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	30
3	2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	27
4	Anthracene, 1-(3-butenyl)-	232	C18H16	1000156-51-8	27
5	Benzamide, 2-fluoro-3-trifluorom...	333	C17H23F4NO	1000438-42-0	22



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	4.5	ng	270626	1	6.886	1211340	20.0
1,1'-Biphenyl, ...	9.239	9.7	ng	869122	3	9.922	1784190	20.0
Benzo[e]pyrene	15.451	2.3	ng	141571	6	15.515	1246290	20.0
unknown16.239	16.239	2.9	ng	180505	6	15.515	1246290	20.0