

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
 Data File : BF125665.D
 Acq On : 25 Sep 2021 19:39
 Operator : JU/CG
 Sample : M3941-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 124019

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-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125665.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	19	rBV	1073494	1382654	35.08%	3.650%
2	5.504	576	581	584	rBV	3512304	3295587	83.60%	8.699%
3	6.504	746	751	754	rBV	3068613	3329275	84.46%	8.788%
4	6.886	812	816	819	rBV	1199956	902737	22.90%	2.383%
5	7.445	906	911	914	rBV	2446239	2112315	53.59%	5.576%
6	8.063	1013	1016	1026	rBV	440783	405641	10.29%	1.071%
7	8.169	1030	1034	1036	rVV	1481575	1245093	31.59%	3.287%
8	8.186	1036	1037	1042	rVB	132574	86448	2.19%	0.228%
9	8.880	1151	1155	1158	rVB	64056	51327	1.30%	0.135%
10	9.245	1212	1217	1220	rBV	4466698	3941869	100.00%	10.405%
11	9.922	1328	1332	1335	rBV	1738642	1319460	33.47%	3.483%
12	9.951	1335	1337	1341	rVB	140229	110141	2.79%	0.291%
13	10.122	1362	1366	1370	rBV	124356	106545	2.70%	0.281%
14	10.463	1421	1424	1429	rBV	127383	121395	3.08%	0.320%
15	10.704	1461	1465	1469	rBV	2451340	2272643	57.65%	5.999%
16	10.827	1482	1486	1490	rVB4	33482	51307	1.30%	0.135%
17	11.298	1564	1566	1572	rVB	48414	45226	1.15%	0.119%
18	11.404	1580	1584	1586	rBV	1406795	1160477	29.44%	3.063%
19	11.427	1586	1588	1591	rVV	758128	552637	14.02%	1.459%
20	11.480	1591	1597	1600	rVV	202274	189403	4.80%	0.500%
21	11.510	1600	1602	1606	rVV	54755	47983	1.22%	0.127%
22	11.633	1617	1623	1625	rBV2	77744	83928	2.13%	0.222%
23	11.904	1664	1669	1671	rBV	94066	96113	2.44%	0.254%
24	11.927	1671	1673	1678	rVB2	368536	346389	8.79%	0.914%
25	11.980	1678	1682	1685	rVB2	60325	63234	1.60%	0.167%
26	12.016	1685	1688	1691	rBV	179115	199679	5.07%	0.527%
27	12.198	1717	1719	1721	rBV	72698	65779	1.67%	0.174%
28	12.351	1740	1745	1748	rBV3	42617	50654	1.29%	0.134%
29	12.451	1756	1762	1766	rBV	69650	97230	2.47%	0.257%
30	12.492	1766	1769	1774	rVB3	44556	60793	1.54%	0.160%
31	12.539	1774	1777	1783	rVB	138046	146475	3.72%	0.387%
32	12.616	1786	1790	1794	rBV	1281333	1076325	27.30%	2.841%
33	12.663	1795	1798	1804	rBV2	63004	87876	2.23%	0.232%
34	12.716	1804	1807	1811	rBV	164396	188231	4.78%	0.497%
35	12.845	1823	1829	1832	rBV2	1103335	1109199	28.14%	2.928%
36	12.892	1835	1837	1843	rVB2	56012	66358	1.68%	0.175%

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Max Peaks: 100

Stop Thrs : 0

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Peak separation: 5

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37	12.963	1846	1849	1850	rBV	80017	64027	1.62%	0.169%
38	12.986	1850	1853	1857	rVV	3105850	3012655	76.43%	7.952%
39	13.063	1860	1866	1869	rBV3	95979	162923	4.13%	0.430%
40	13.151	1878	1881	1882	rBV	74837	83158	2.11%	0.220%

41	13.174	1882	1885	1887	rVB	176786	175325	4.45%	0.463%
42	13.239	1892	1896	1898	rBV	164830	139940	3.55%	0.369%
43	13.274	1898	1902	1905	rBV2	131589	136561	3.46%	0.360%
44	13.368	1915	1918	1920	rBV	84012	64708	1.64%	0.171%
45	13.398	1920	1923	1927	rVV2	74307	76458	1.94%	0.202%

46	13.463	1932	1934	1942	rVB6	25568	43534	1.10%	0.115%
47	13.545	1943	1948	1949	rBV3	34579	42528	1.08%	0.112%
48	13.568	1949	1952	1955	rBV4	38720	42780	1.09%	0.113%
49	13.674	1968	1970	1975	rVB	79702	87662	2.22%	0.231%
50	13.792	1985	1990	1992	rBV2	86335	123505	3.13%	0.326%

51	13.821	1992	1995	1996	rVV	103259	98207	2.49%	0.259%
52	13.839	1996	1998	2003	rVV2	103205	129691	3.29%	0.342%
53	13.880	2003	2005	2011	rVV2	57590	106066	2.69%	0.280%
54	14.039	2024	2032	2035	rBV3	1410290	2108754	53.50%	5.566%
55	14.063	2035	2036	2042	rVB	469539	410122	10.40%	1.083%

56	14.145	2048	2050	2052	rBV	87903	73105	1.85%	0.193%
57	14.257	2066	2069	2073	rBV2	47995	72862	1.85%	0.192%
58	14.362	2081	2087	2089	rBV2	46722	63705	1.62%	0.168%
59	14.427	2093	2098	2101	rVV	120490	159742	4.05%	0.422%
60	14.462	2101	2104	2107	rVV2	75925	81579	2.07%	0.215%

61	14.515	2110	2113	2116	rVV2	96661	115938	2.94%	0.306%
62	14.551	2116	2119	2121	rVV2	94532	103790	2.63%	0.274%
63	14.574	2121	2123	2126	rVV2	66098	62061	1.57%	0.164%
64	14.621	2127	2131	2136	rVB6	45811	84391	2.14%	0.223%
65	14.674	2137	2140	2144	rBV4	40520	48522	1.23%	0.128%

66	14.727	2146	2149	2153	rBV4	46872	58877	1.49%	0.155%
67	14.821	2161	2165	2168	rVB4	53917	69301	1.76%	0.183%
68	14.904	2175	2179	2185	rBV4	76512	124536	3.16%	0.329%
69	15.080	2205	2209	2213	rBV	380451	607338	15.41%	1.603%
70	15.162	2220	2223	2226	rBV	63800	77837	1.97%	0.205%

71	15.192	2226	2228	2232	rVB	76272	69854	1.77%	0.184%
72	15.386	2257	2261	2267	rVB	200853	266936	6.77%	0.705%
73	15.451	2268	2272	2278	rVV	269731	336180	8.53%	0.887%
74	15.515	2278	2283	2287	rVV2	906863	1164645	29.55%	3.074%
75	15.551	2287	2289	2296	rVB3	127857	170056	4.31%	0.449%

76	15.686	2306	2312	2316	rBV7	33398	61395	1.56%	0.162%
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ClientSampleId :
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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.998	2361	2365	2371	rBV4	67613	109124	2.77%	0.288%
78	16.515	2448	2453	2456	rBV4	41527	74206	1.88%	0.196%
79	16.986	2528	2533	2541	rVB2	71029	135592	3.44%	0.358%
80	17.427	2604	2608	2624	rVB2	49285	115785	2.94%	0.306%

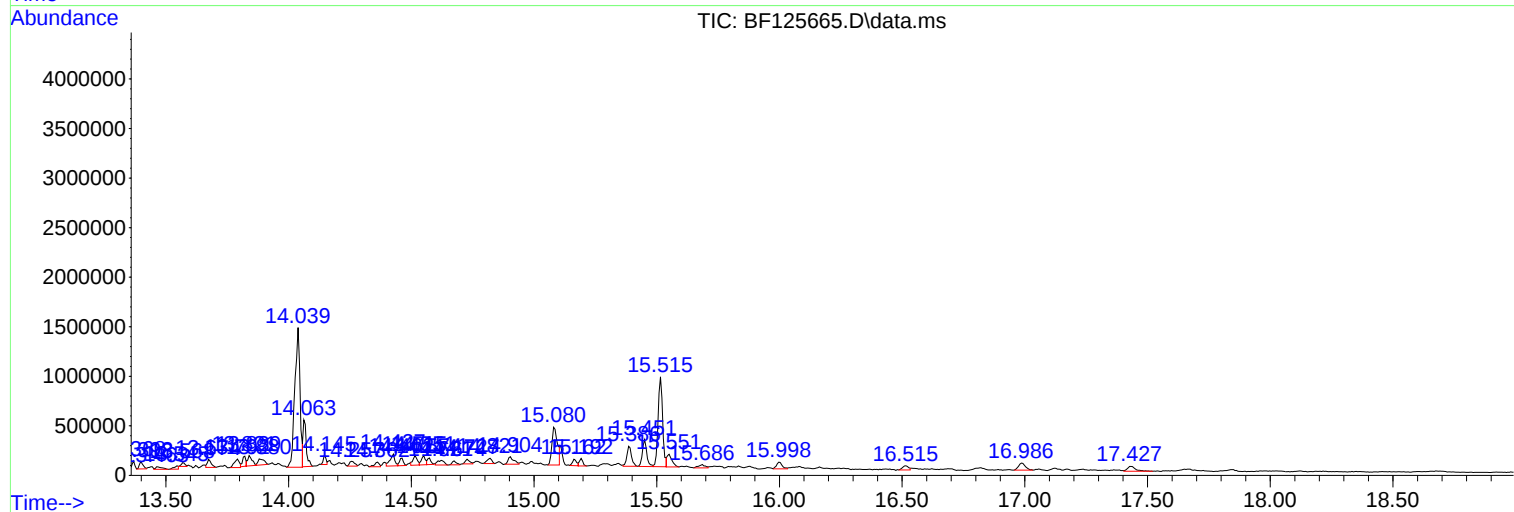
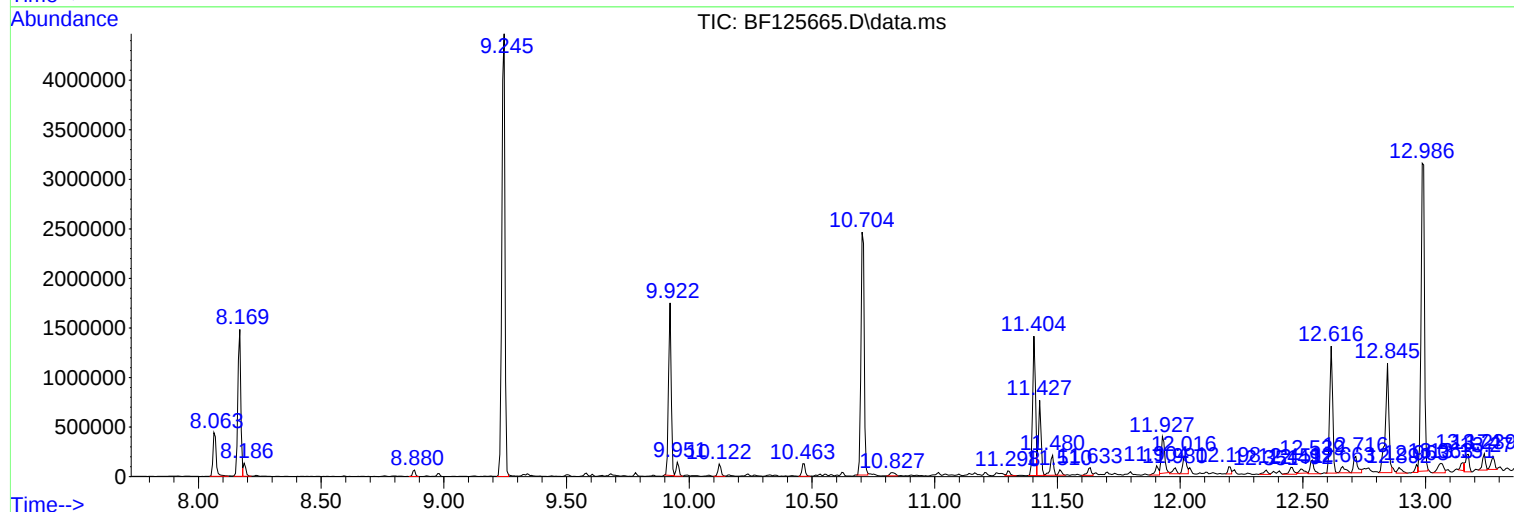
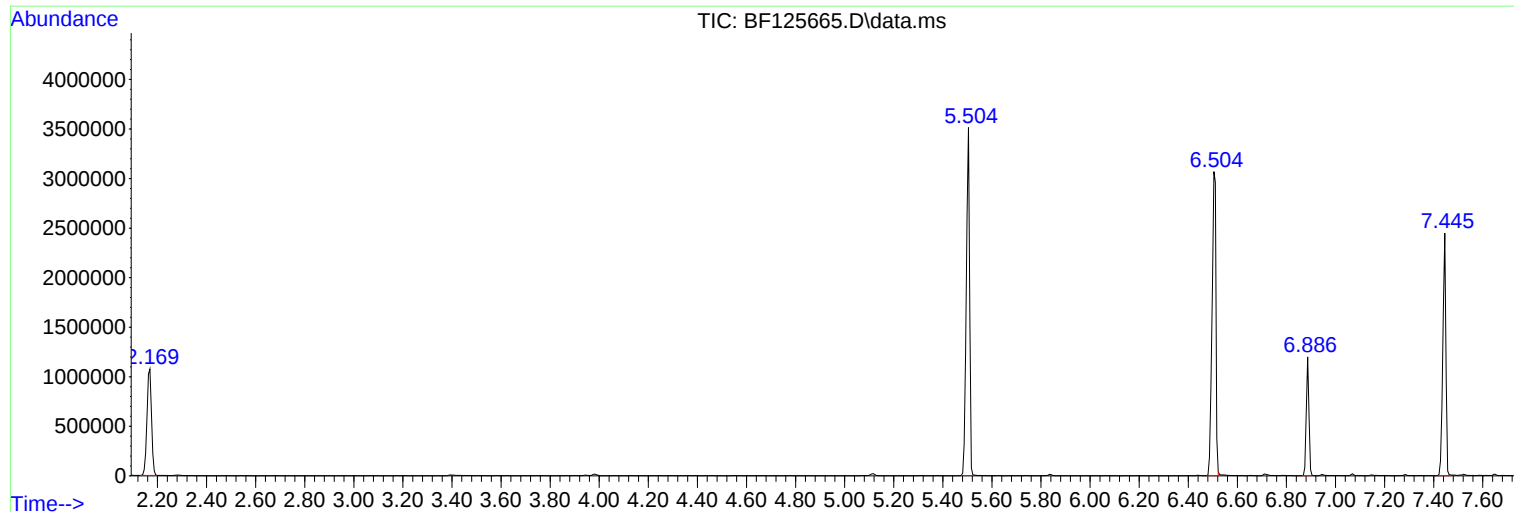
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Instrument :
BNA_F
ClientSampled :
124019

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
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Instrument :
BNA_F
ClientSampleId :
124019

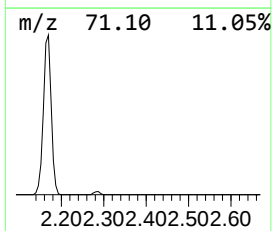
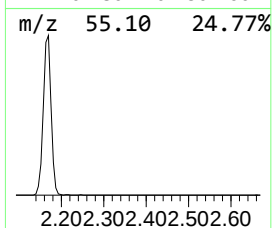
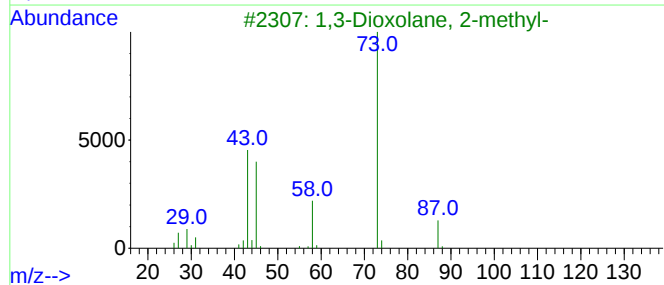
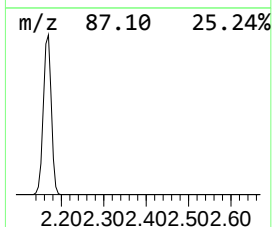
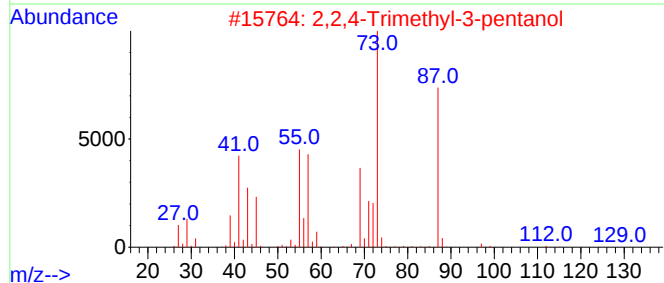
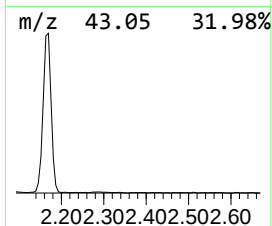
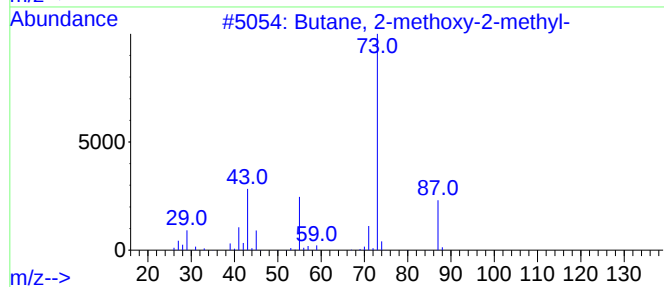
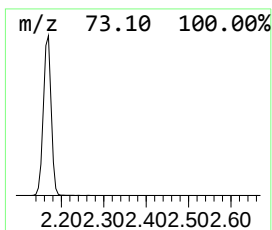
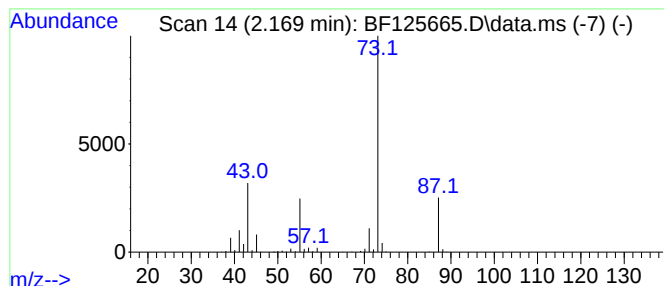
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	30.63 ng	1382650	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	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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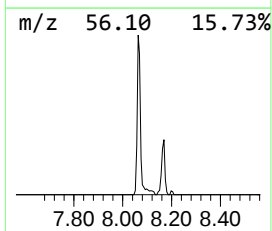
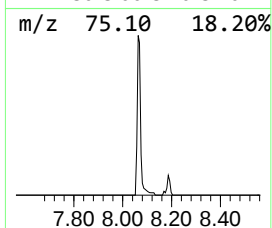
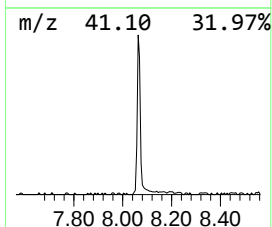
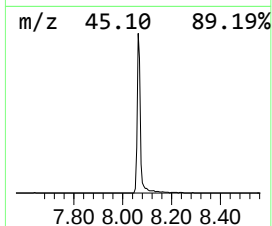
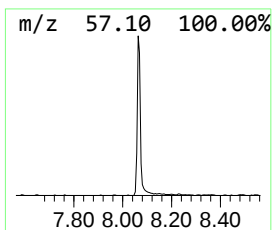
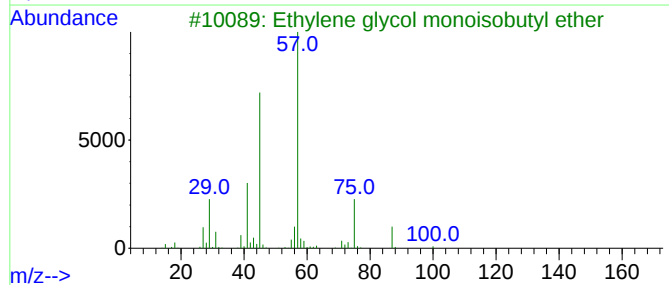
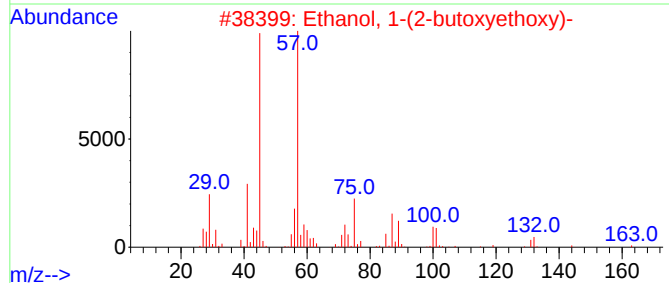
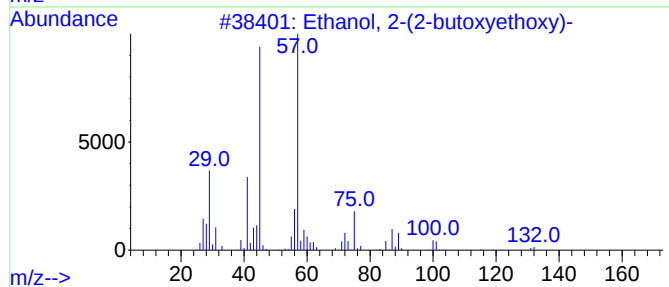
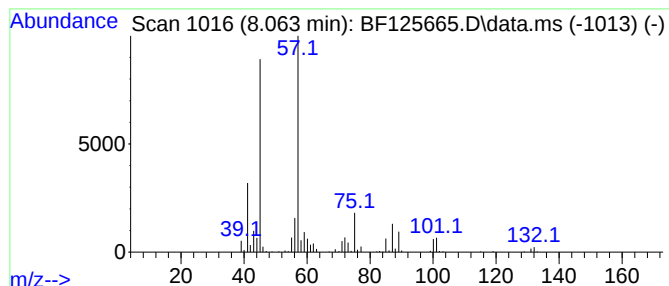
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.063	6.52 ng	405641	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	56



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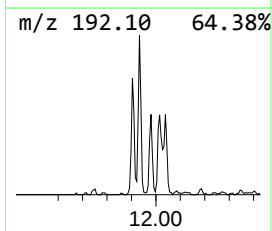
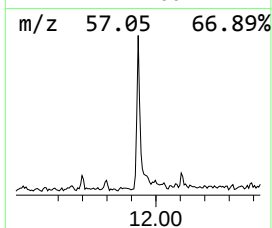
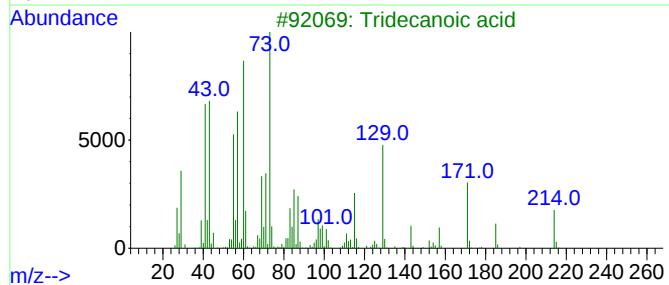
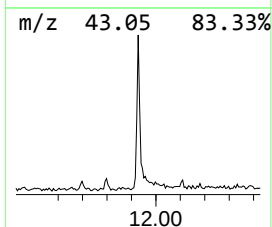
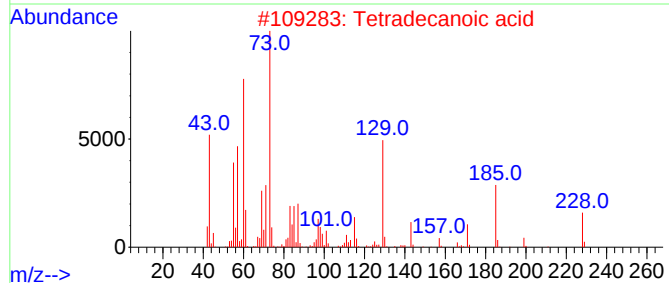
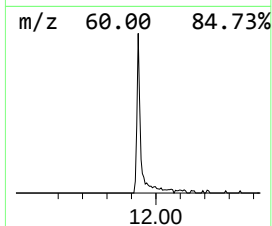
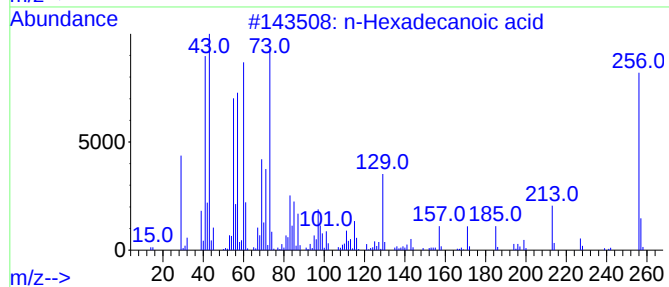
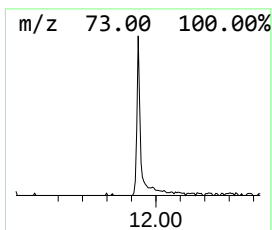
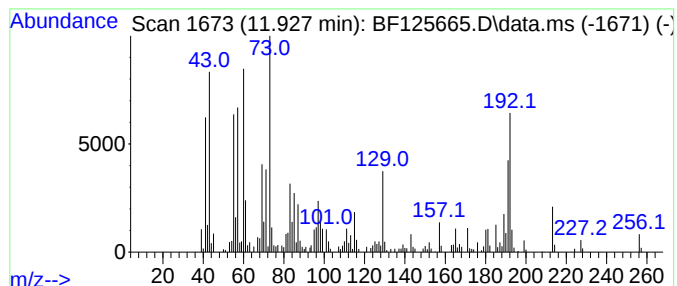
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	5.97 ng	346389	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	59



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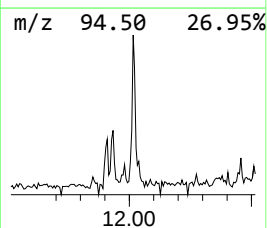
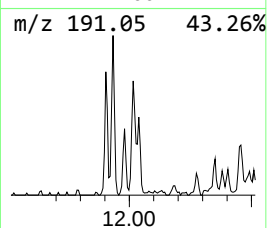
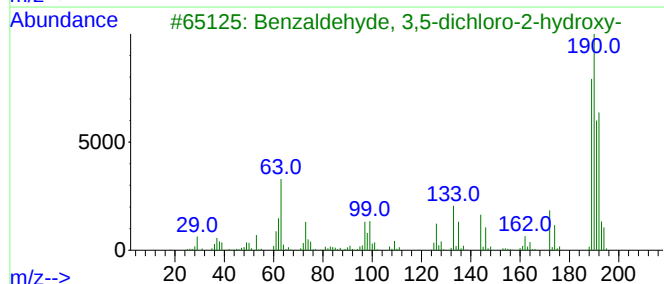
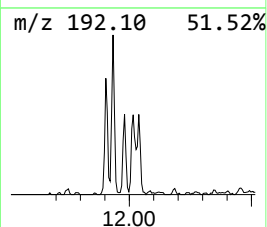
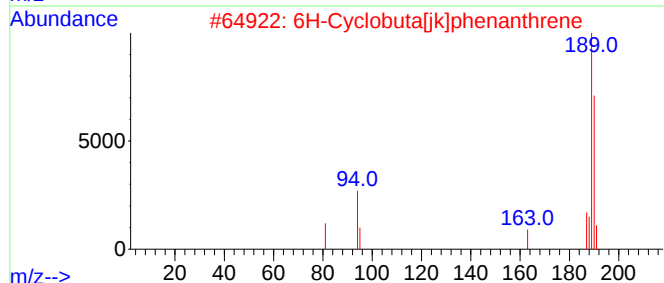
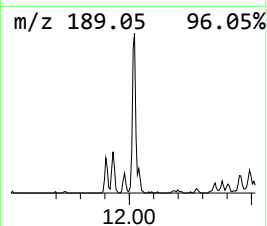
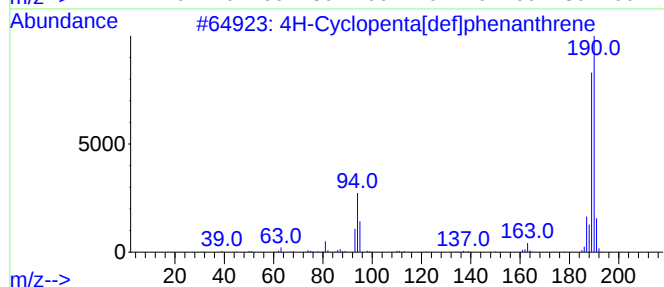
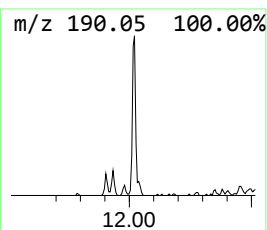
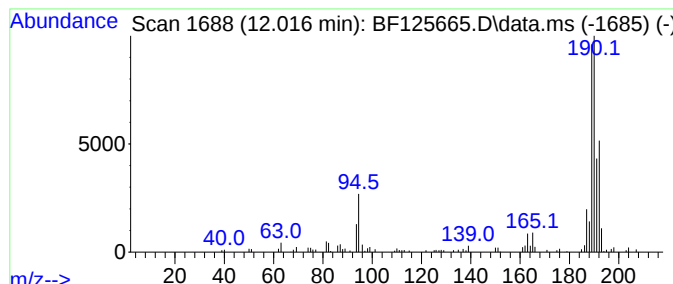
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	3.44 ng	199679	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
4			2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	32
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125665.D
Acq On : 25 Sep 2021 19:39
Operator : JU/CG
Sample : M3941-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
124019

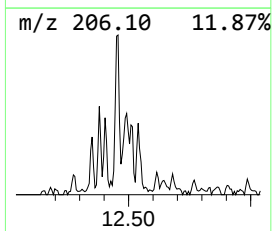
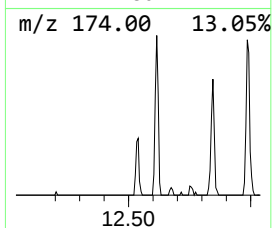
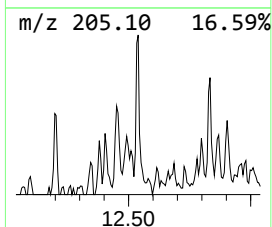
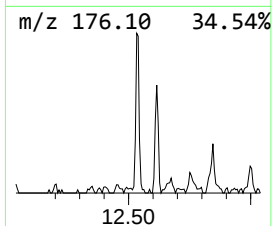
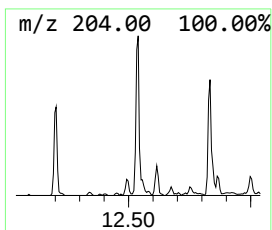
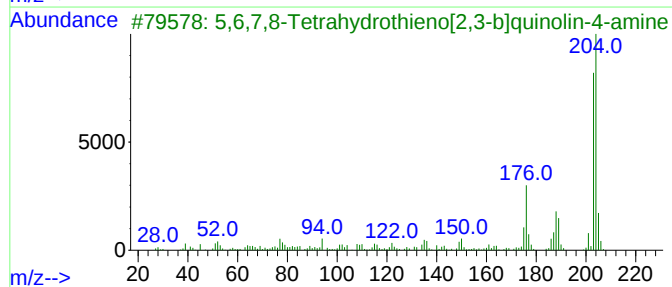
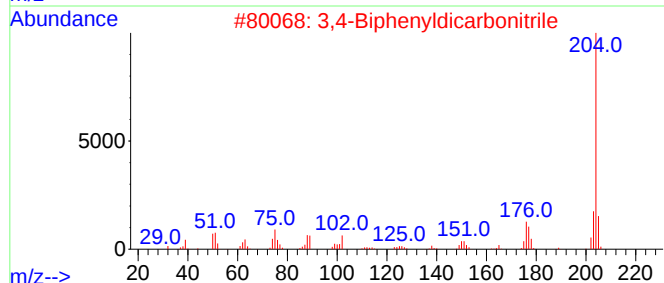
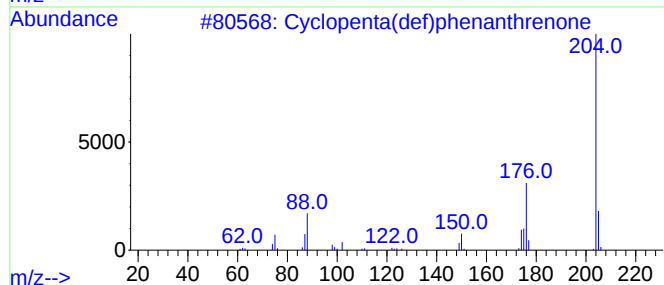
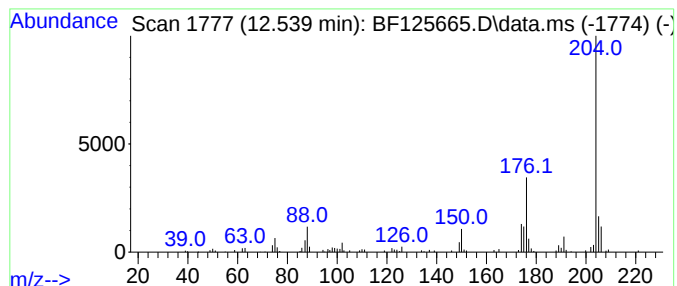
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclopenta(def)phenanthrenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	2.52 ng	146475	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	94
2			3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	72
3			5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	59
4			N-(4-Chloro-phenyl)-2-(3,4-dihyd...	330	C17H15ClN2OS	1010296-34-3	53
5			4,5,6,7-Tetrafluoro-2-methyl-1H...	204	C8H4F4N2	081430-75-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125665.D
Acq On : 25 Sep 2021 19:39
Operator : JU/CG
Sample : M3941-01
Misc :
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Instrument :
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ClientSampleId :
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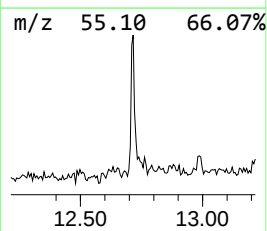
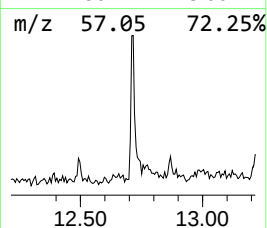
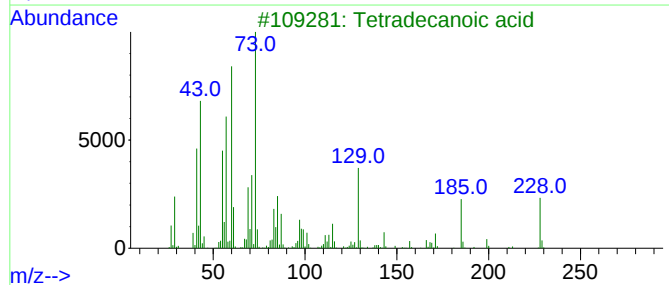
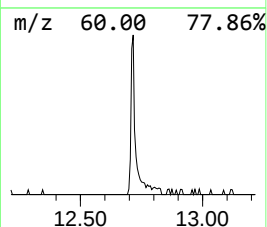
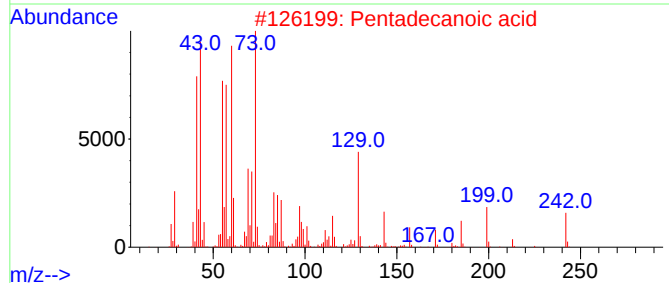
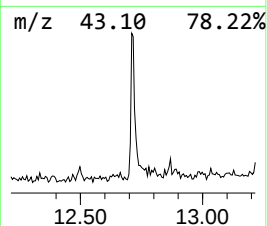
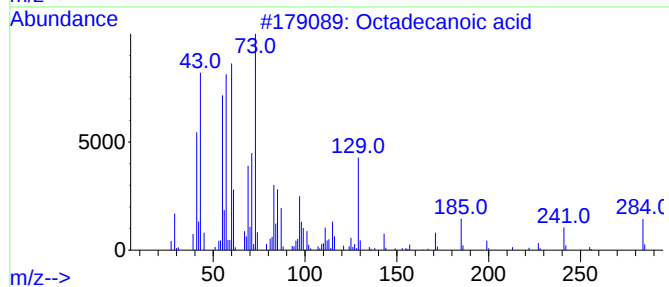
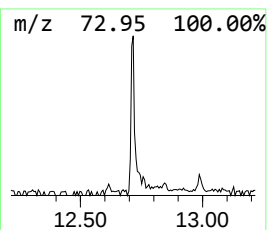
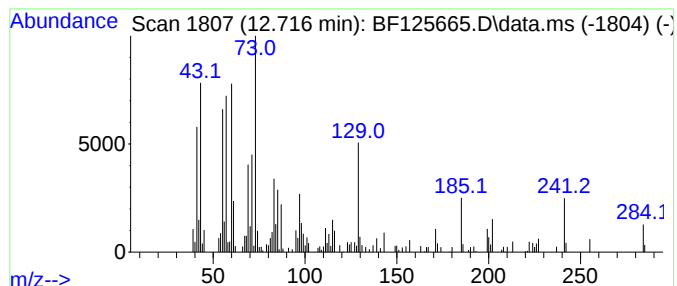
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	3.24 ng	188231	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125665.D
Acq On : 25 Sep 2021 19:39
Operator : JU/CG
Sample : M3941-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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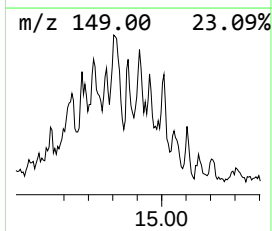
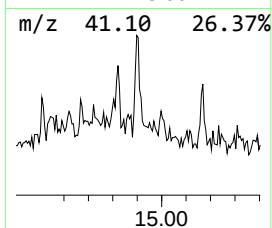
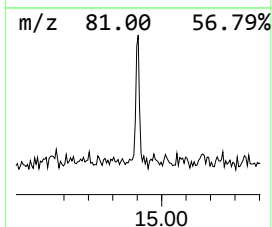
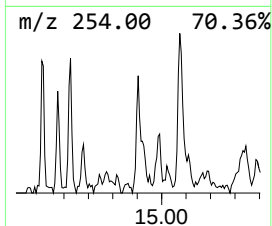
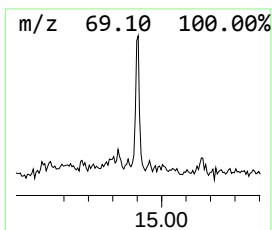
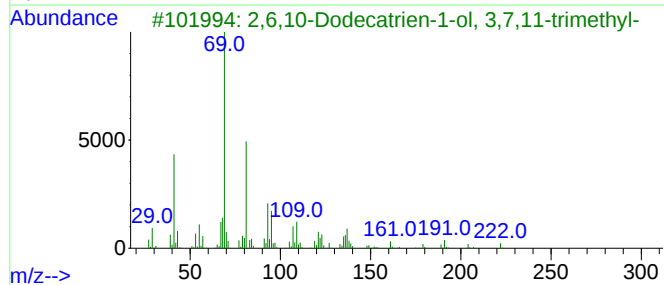
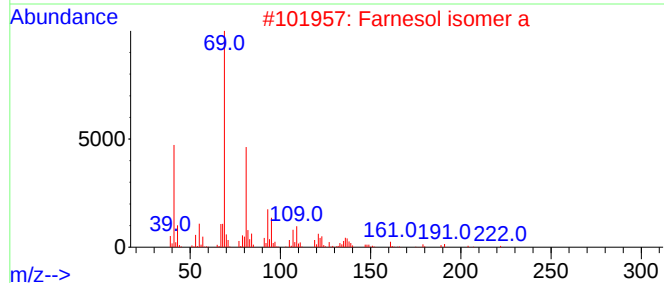
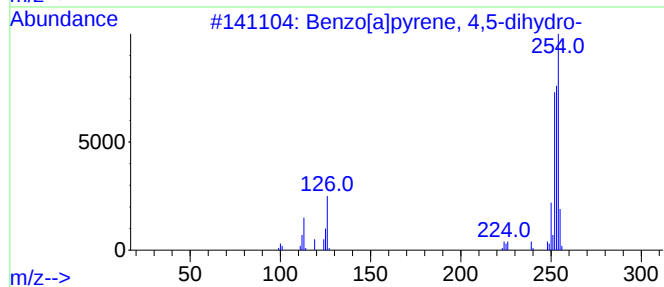
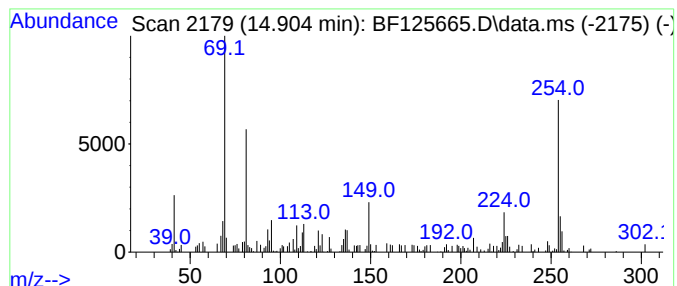
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.904 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	2.14 ng	124536	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene, 4,5-dihydro-	254	C20H14	057652-66-1	46
2			Farnesol isomer a	222	C15H26O	1000108-92-4	42
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	42
4			Squalene	410	C30H50	000111-02-4	41
5			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125665.D
Acq On : 25 Sep 2021 19:39
Operator : JU/CG
Sample : M3941-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

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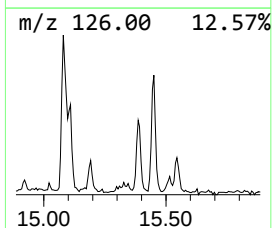
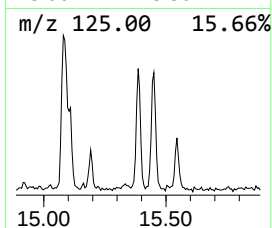
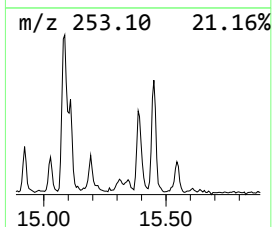
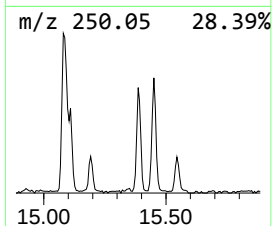
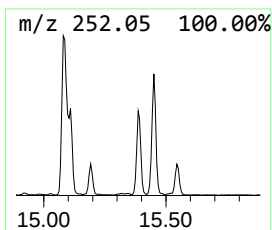
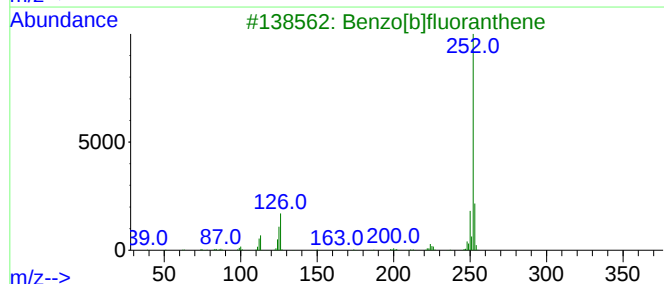
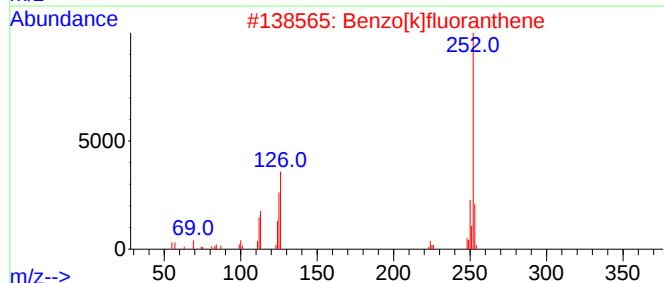
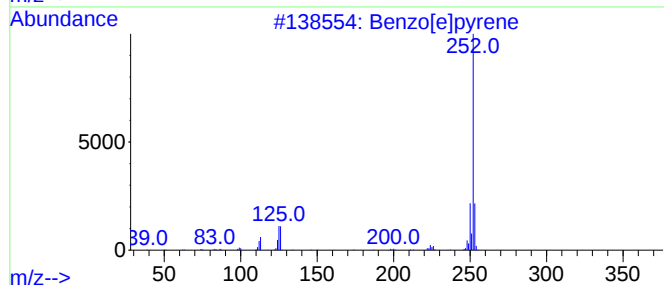
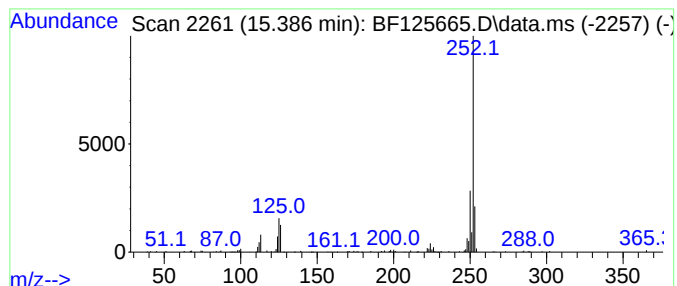
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	4.58 ng	266936	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[k]fluoranthene	252	C20H12	000207-08-9	96
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5			Benzo[a]pyrene	252	C20H12	000050-32-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125665.D
Acq On : 25 Sep 2021 19:39
Operator : JU/CG
Sample : M3941-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	30.6	ng	1382650	1	6.886	902737	20.0
Ethanol, 2-(2-b...	8.063	6.5	ng	405641	2	8.169	1245090	20.0
n-Hexadecanoic ...	11.927	6.0	ng	346389	4	11.404	1160480	20.0
4H-Cyclopenta[d...	12.016	3.4	ng	199679	4	11.404	1160480	20.0
Cyclopenta(def)...	12.539	2.5	ng	146475	4	11.404	1160480	20.0
Octadecanoic acid	12.716	3.2	ng	188231	4	11.404	1160480	20.0
unknown14.904	14.904	2.1	ng	124536	6	15.515	1164650	20.0
Benzo[e]pyrene	15.386	4.6	ng	266936	6	15.515	1164650	20.0