

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060721\
 Data File : BF124166.D
 Acq On : 7 Jun 2021 20:20
 Operator : JU/CG
 Sample : M2589-19 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 18-B12(2-4)

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.434	396	399	403	rBB	30691	31890	7.92%	0.607%
2	5.063	501	506	509	rBV	276398	258927	64.34%	4.929%
3	5.487	575	578	582	rVB	59206	51040	12.68%	0.972%
4	6.498	747	750	756	rBV	190206	153927	38.25%	2.930%
5	6.692	779	783	786	rBB	6835	8454	2.10%	0.161%
6	6.857	808	811	815	rVB	352007	265571	65.99%	5.055%
7	7.416	903	906	909	rBV	217831	166614	41.40%	3.172%
8	7.457	911	913	915	rVB	12257	9056	2.25%	0.172%
9	8.139	1026	1029	1032	rVV	400158	314260	78.09%	5.982%
10	8.563	1098	1101	1103	rBV	10533	10229	2.54%	0.195%
11	8.733	1126	1130	1133	rBV	21717	18645	4.63%	0.355%
12	8.857	1148	1151	1154	rVB2	14745	13489	3.35%	0.257%
13	8.951	1164	1167	1171	rBV	9405	10455	2.60%	0.199%
14	9.163	1200	1203	1206	rBV3	9578	8409	2.09%	0.160%
15	9.216	1208	1212	1215	rBV	446218	327218	81.31%	6.229%
16	9.298	1221	1226	1229	rBV	28659	26963	6.70%	0.513%
17	9.486	1254	1258	1261	rBV4	9458	12159	3.02%	0.231%
18	9.551	1267	1269	1272	rBV2	19161	15372	3.82%	0.293%
19	9.616	1276	1280	1283	rVV4	16151	19997	4.97%	0.381%
20	9.757	1302	1304	1309	rBV3	6157	7862	1.95%	0.150%
21	9.827	1309	1316	1320	rVB	33169	31178	7.75%	0.594%
22	9.898	1324	1328	1331	rVB	491835	374981	93.18%	7.138%
23	9.927	1331	1333	1336	rBV2	17216	13229	3.29%	0.252%
24	9.998	1342	1345	1349	rVB2	6172	7781	1.93%	0.148%
25	10.063	1349	1356	1357	rBV4	5960	9415	2.34%	0.179%
26	10.098	1359	1362	1366	rVB3	16942	16474	4.09%	0.314%
27	10.139	1366	1369	1371	rBV3	8734	8791	2.18%	0.167%
28	10.210	1379	1381	1384	rBV3	9677	10454	2.60%	0.199%
29	10.304	1394	1397	1398	rBV2	10870	8422	2.09%	0.160%
30	10.327	1398	1401	1404	rVB	31833	27917	6.94%	0.531%
31	10.445	1414	1421	1424	rBV4	13527	21692	5.39%	0.413%
32	10.545	1434	1438	1441	rBV3	12705	15727	3.91%	0.299%
33	10.598	1445	1447	1451	rBV4	5729	8765	2.18%	0.167%
34	10.663	1455	1458	1460	rBV2	10584	11017	2.74%	0.210%
35	10.686	1460	1462	1467	rVB5	11450	12314	3.06%	0.234%
36	10.798	1478	1481	1487	rBV4	35334	53323	13.25%	1.015%

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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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37	10.986	1509	1513	1516	rBV5	28504	26431	6.57%	0.503%
38	11.021	1516	1519	1523	rVB6	8260	11236	2.79%	0.214%
39	11.127	1532	1537	1538	rBV4	7232	9678	2.40%	0.184%
40	11.145	1538	1540	1544	rVB5	8677	10328	2.57%	0.197%
41	11.192	1544	1548	1551	rBV5	10350	9795	2.43%	0.186%
42	11.245	1553	1557	1560	rBV	30038	32107	7.98%	0.611%
43	11.280	1560	1563	1568	rVB4	29075	31099	7.73%	0.592%
44	11.339	1568	1573	1576	rBV5	7306	12052	2.99%	0.229%
45	11.386	1577	1581	1583	rBV	401305	345647	85.89%	6.580%
46	11.410	1583	1585	1588	rVV	114047	87803	21.82%	1.671%
47	11.457	1591	1593	1596	rVV	24402	21289	5.29%	0.405%
48	11.616	1617	1620	1624	rVB5	12326	14094	3.50%	0.268%
49	11.674	1627	1630	1633	rBV3	22713	24679	6.13%	0.470%
50	11.716	1635	1637	1644	rVB7	10073	17899	4.45%	0.341%
51	11.768	1644	1646	1651	rBV6	7748	15050	3.74%	0.286%
52	11.845	1655	1659	1660	rBV3	7846	10106	2.51%	0.192%
53	11.886	1663	1666	1668	rBV	11467	10003	2.49%	0.190%
54	11.916	1668	1671	1676	rVB	27605	28862	7.17%	0.549%
55	11.968	1676	1680	1682	rBV3	7033	9283	2.31%	0.177%
56	11.998	1682	1685	1688	rBV3	29432	27324	6.79%	0.520%
57	12.086	1697	1700	1703	rVB2	20481	18228	4.53%	0.347%
58	12.180	1714	1716	1719	rBV2	12235	13693	3.40%	0.261%
59	12.210	1719	1721	1724	rVB4	13095	11249	2.80%	0.214%
60	12.257	1724	1729	1730	rBV4	6817	9058	2.25%	0.172%
61	12.363	1745	1747	1749	rBV3	10144	8088	2.01%	0.154%
62	12.439	1757	1760	1762	rBV4	18111	15859	3.94%	0.302%
63	12.474	1762	1766	1768	rVB3	28309	28669	7.12%	0.546%
64	12.521	1772	1774	1778	rVB5	15824	18663	4.64%	0.355%
65	12.557	1778	1780	1782	rBV3	9679	12542	3.12%	0.239%
66	12.598	1784	1787	1792	rVB	145167	117550	29.21%	2.238%
67	12.639	1792	1794	1796	rBV2	13802	12714	3.16%	0.242%
68	12.827	1821	1826	1831	rBV	123933	141045	35.05%	2.685%
69	12.968	1846	1850	1853	rBV	362795	293169	72.85%	5.581%
70	13.051	1860	1864	1867	rBV6	15427	22979	5.71%	0.437%
71	13.157	1879	1882	1884	rVV3	25680	23992	5.96%	0.457%
72	13.204	1888	1890	1892	rVV2	14692	13233	3.29%	0.252%
73	13.221	1892	1893	1895	rVB2	16984	9789	2.43%	0.186%
74	13.257	1897	1899	1903	rVV5	15536	19159	4.76%	0.365%
75	13.351	1914	1915	1917	rVB2	17379	9461	2.35%	0.180%
76	13.386	1919	1921	1924	rVV4	11098	13308	3.31%	0.253%

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77	13.415	1924	1926	1928	rVV3	13021	12875	3.20%	0.245%
78	13.451	1929	1932	1937	rVB4	49209	53445	13.28%	1.017%
79	13.545	1946	1948	1951	rVB4	13835	12702	3.16%	0.242%
80	13.639	1961	1964	1965	rBV3	9511	11613	2.89%	0.221%
81	13.662	1965	1968	1973	rVB7	20907	33012	8.20%	0.628%
82	13.733	1978	1980	1982	rBV3	11094	9498	2.36%	0.181%
83	13.833	1994	1997	1998	rBV3	17871	20892	5.19%	0.398%
84	13.874	2001	2004	2008	rVB6	40293	52802	13.12%	1.005%
85	14.027	2023	2030	2033	rBV2	365726	402431	100.00%	7.661%
86	14.051	2033	2034	2040	rVB	53707	56340	14.00%	1.072%
87	14.139	2046	2049	2050	rVB3	18340	15982	3.97%	0.304%
88	14.498	2108	2110	2111	rBV2	24514	14447	3.59%	0.275%
89	15.080	2205	2209	2211	rBV3	58674	76890	19.11%	1.464%
90	15.145	2218	2220	2225	rVB5	37065	36470	9.06%	0.694%
91	15.451	2268	2272	2277	rVV2	32075	46229	11.49%	0.880%
92	15.509	2278	2282	2292	rVB2	190902	275512	68.46%	5.245%
93	15.833	2333	2337	2339	rBV5	25490	36119	8.98%	0.688%
94	15.980	2358	2362	2365	rBV6	28879	44438	11.04%	0.846%
95	16.415	2434	2436	2437	rBV2	14560	12928	3.21%	0.246%
96	16.662	2476	2478	2484	rVB7	34987	51303	12.75%	0.977%
97	16.903	2517	2519	2521	rVB3	17640	13391	3.33%	0.255%
98	17.309	2586	2588	2589	rBV2	11210	8613	2.14%	0.164%
99	18.497	2788	2790	2792	rBV3	11362	13255	3.29%	0.252%
100	18.562	2799	2801	2803	rBV3	13835	12813	3.18%	0.244%

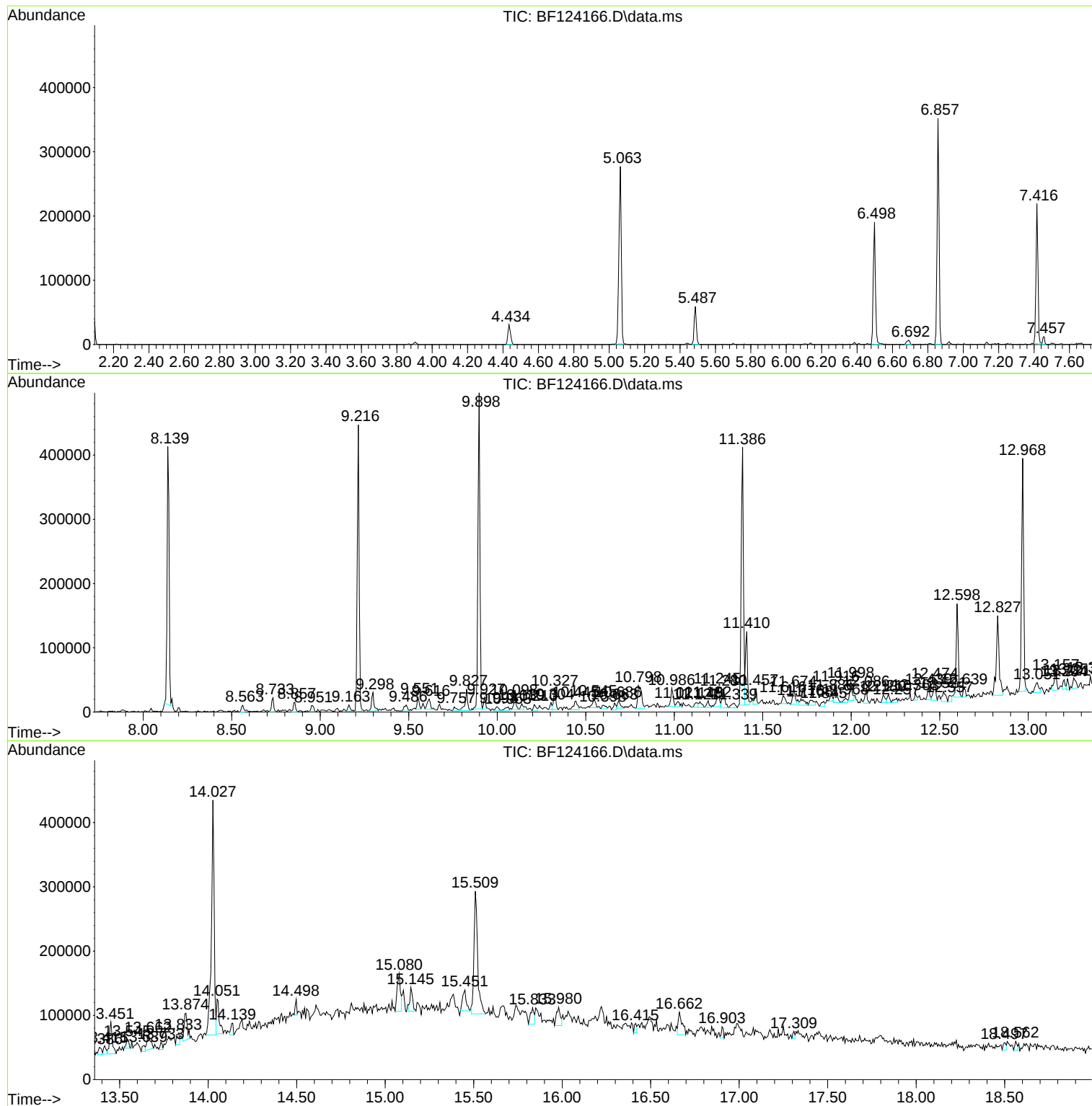
Sum of corrected areas: 5253230

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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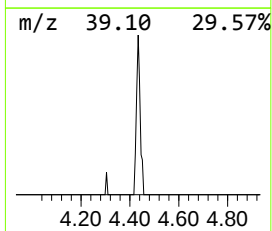
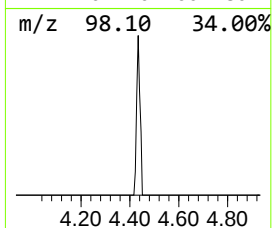
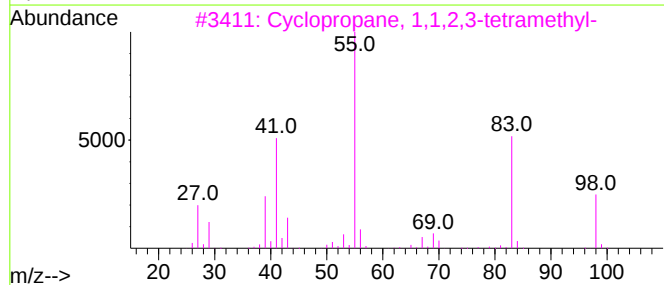
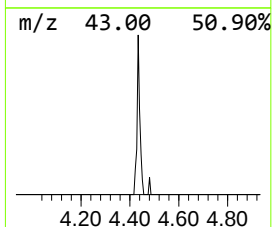
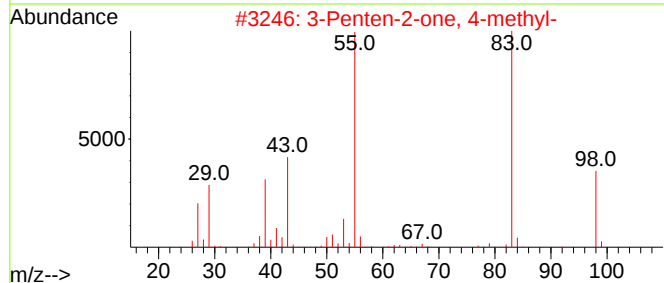
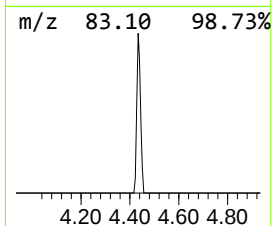
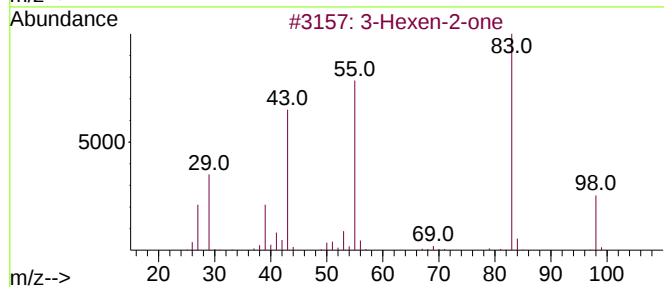
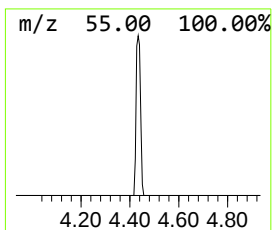
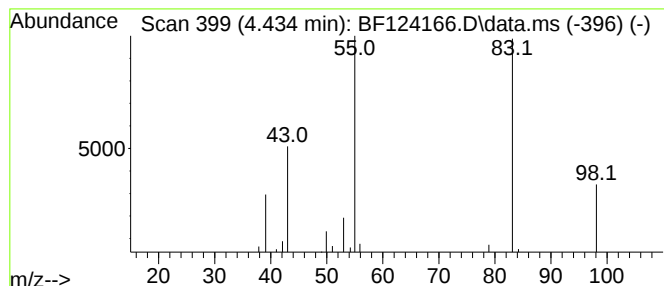
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.434	2.40 ng	31890	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one			98	C6H10O	000763-93-9	72
2	3-Penten-2-one, 4-methyl-			98	C6H10O	000141-79-7	72
3	Cyclopropane, 1,1,2,3-tetramethyl-			98	C7H14	074752-93-5	64
4	2-Pentene, 4,4-dimethyl-, (E)-			98	C7H14	000690-08-4	59
5	2-Pentene, 3,4-dimethyl-, (E)-			98	C7H14	004914-92-5	59



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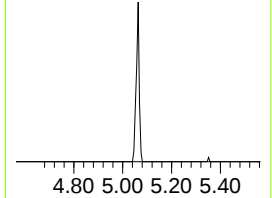
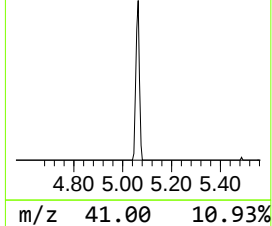
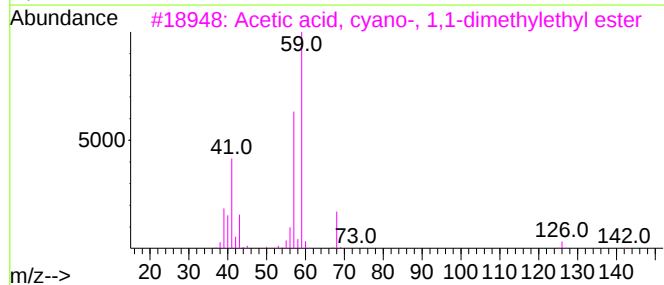
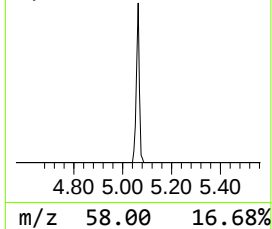
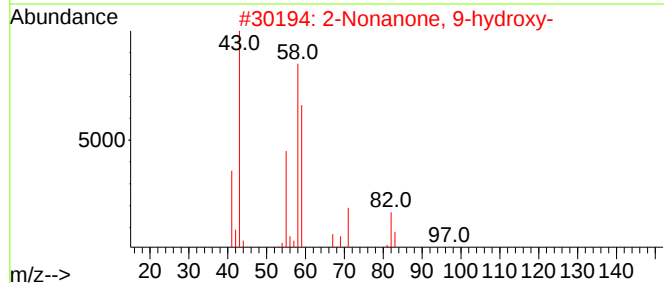
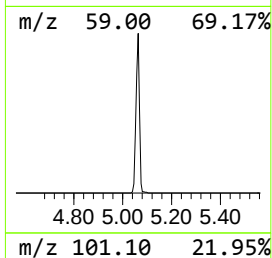
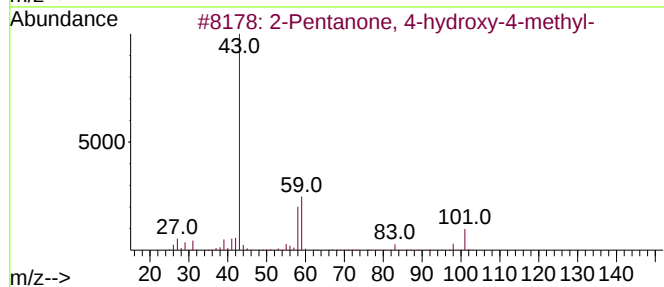
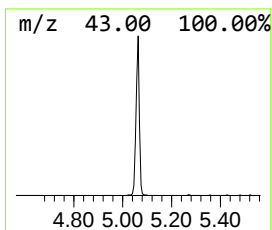
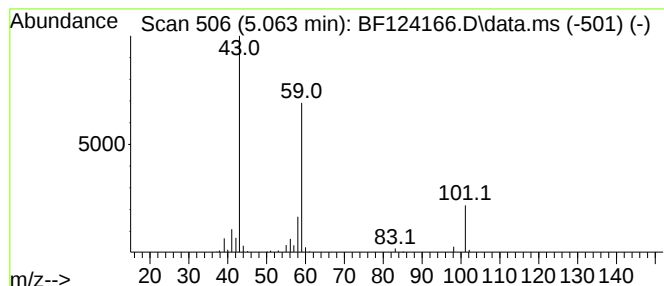
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	19.50 ng	258927	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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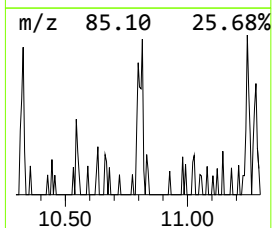
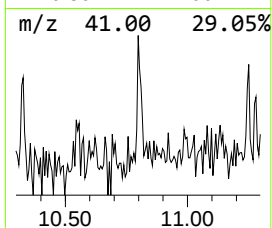
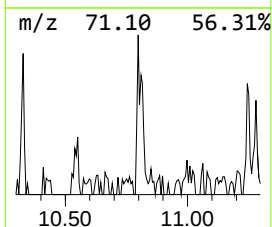
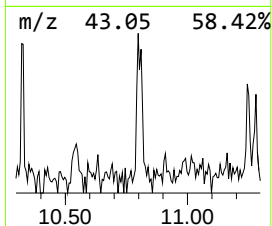
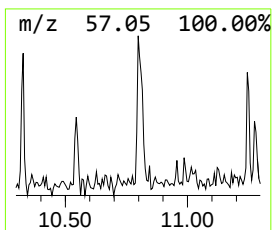
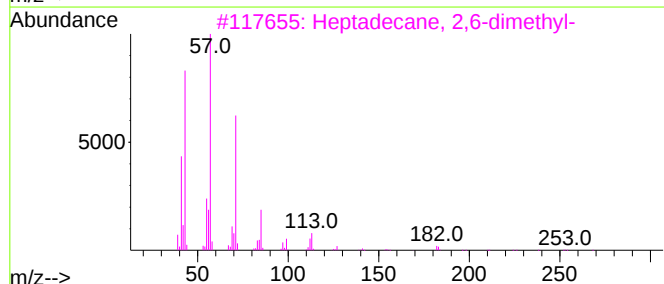
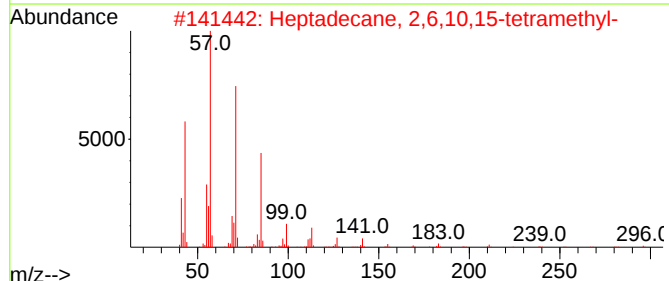
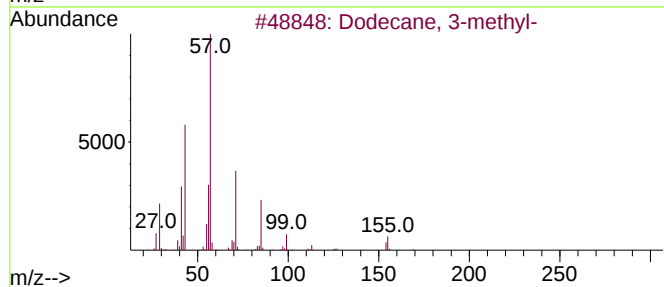
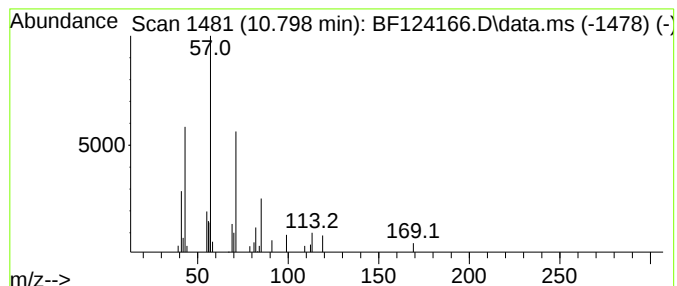
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Dodecane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	3.09 ng	53323	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 3-methyl-	184	C13H28	017312-57-1	64
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	59
3			Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	59
4			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	53
5			Tetracosane	338	C24H50	000646-31-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060721\
Data File : BF124166.D
Acq On : 7 Jun 2021 20:20
Operator : JU/CG
Sample : M2589-19 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
18-B12(2-4)

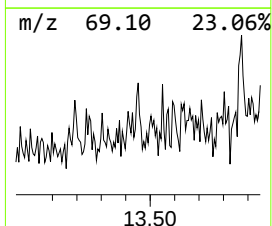
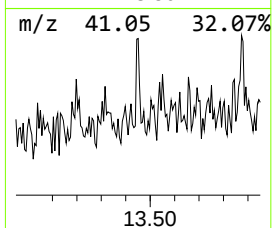
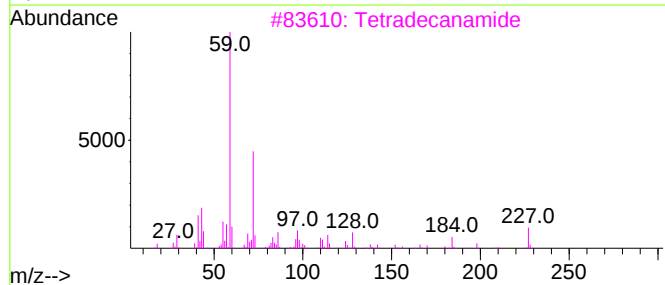
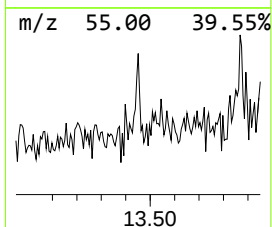
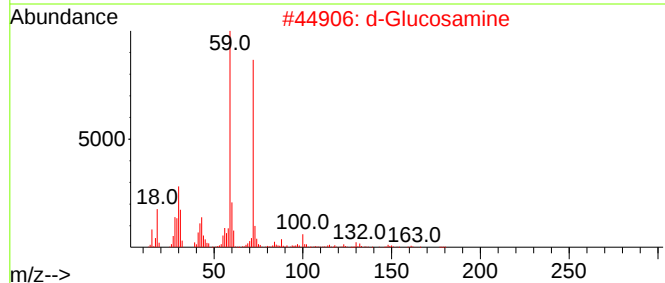
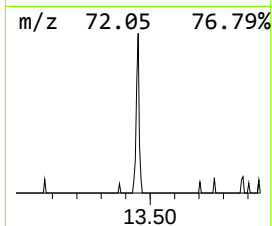
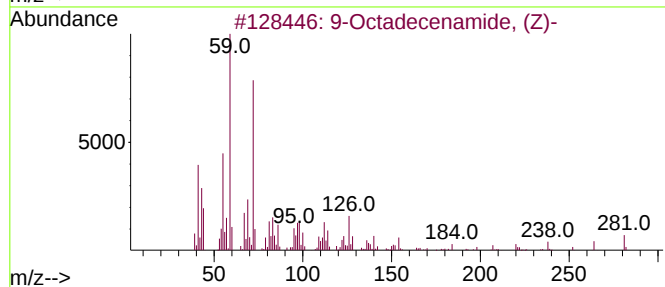
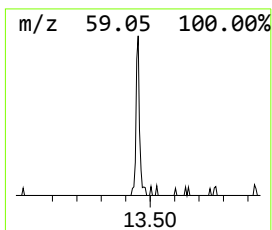
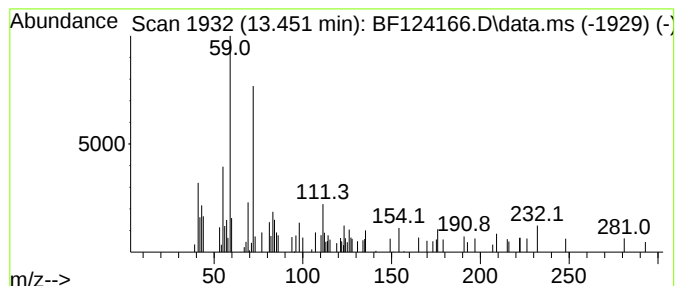
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	2.66 ng	53445	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	70
2			d-Glucosamine	179	C6H13NO5	000090-77-7	53
3			Tetradecanamide	227	C14H29NO	000638-58-4	35
4			Octadecanamide	283	C18H37NO	000124-26-5	35
5			Dodecanamide	199	C12H25NO	001120-16-7	35



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Operator : JU/CG
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ClientSampleId :
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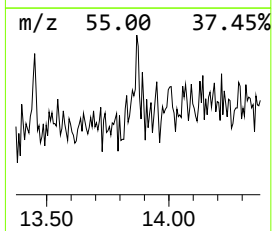
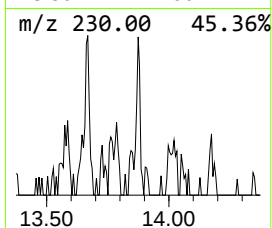
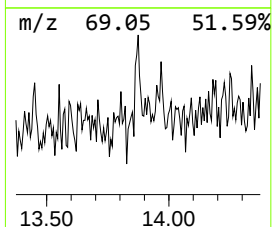
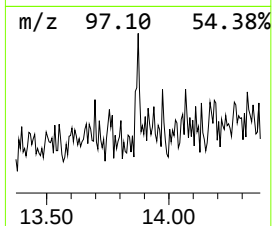
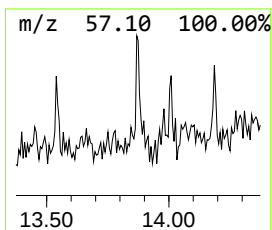
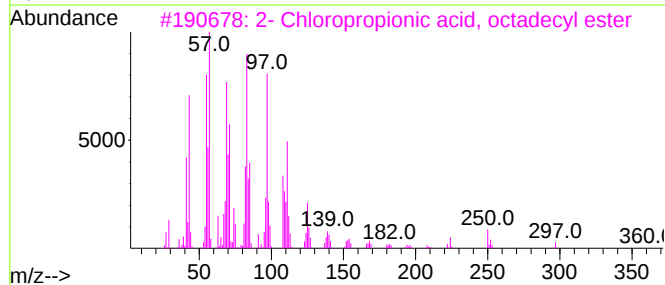
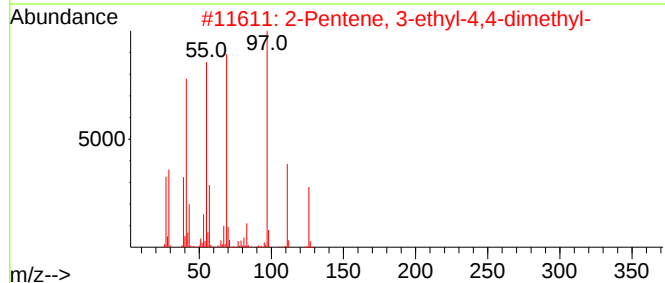
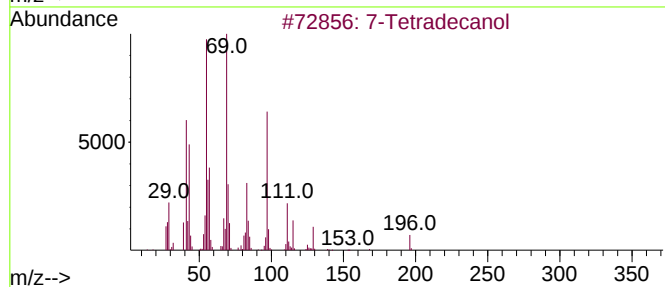
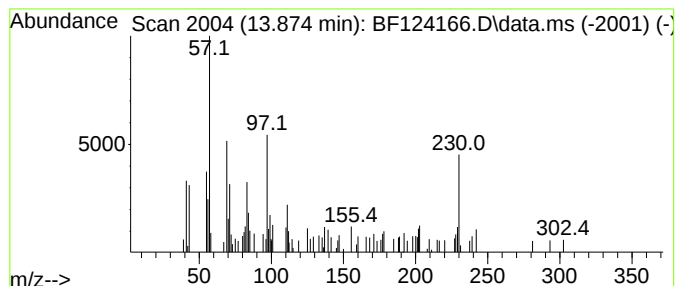
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown13.874 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.62 ng	52802	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Tetradecanol		214	C14H30O	003981-79-1	27	
2	2-Pentene, 3-ethyl-4,4-dimethyl-		126	C9H18	053907-59-8	27	
3	2-Chloropropionic acid, octadec...		360	C21H41ClO2	088104-31-8	16	
4	1,3-Dioxolane, 4-ethyl-5-octyl-2...		350	C15H24F6O2	038274-72-5	14	
5	4-(3-Oxocyclohexyl)butyric acid,...		198	C11H18O3	147895-12-3	10	



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Sample : M2589-19 2X
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ALS Vial : 17 Sample Multiplier: 1

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18-B12(2-4)

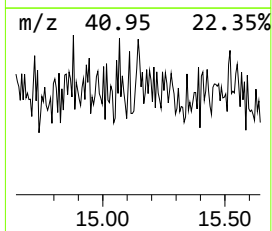
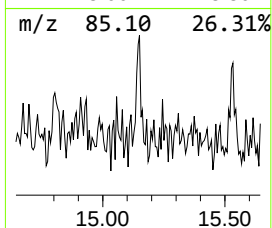
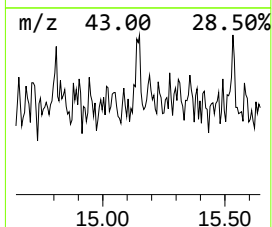
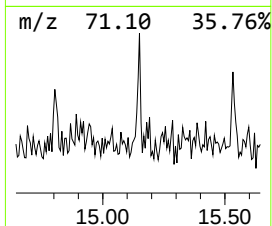
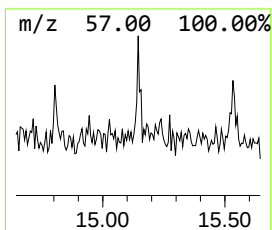
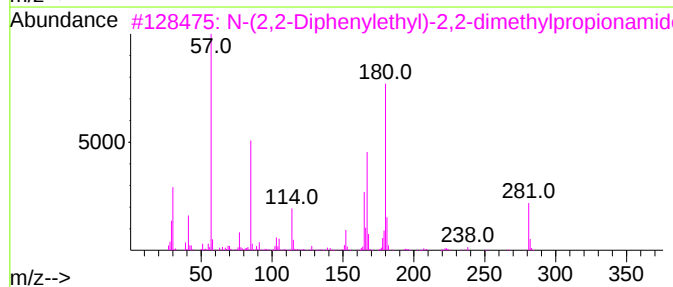
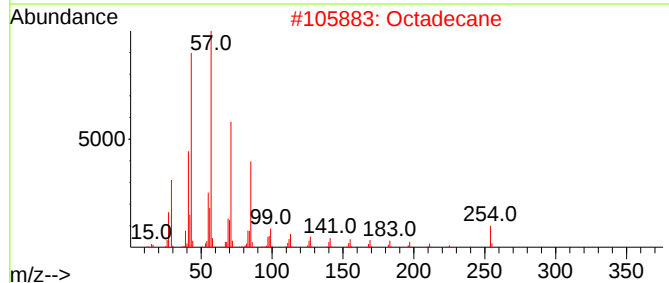
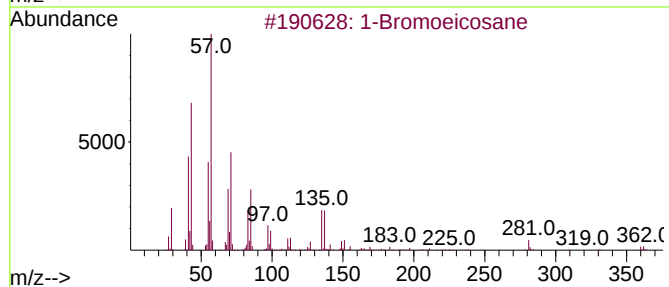
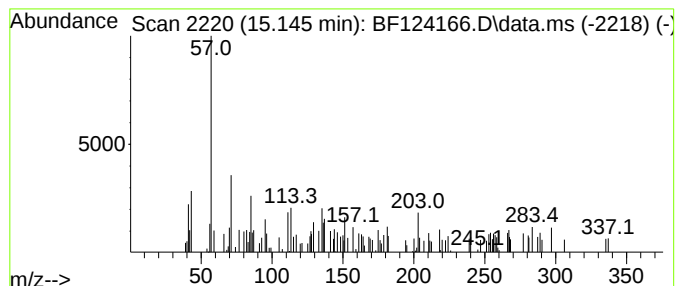
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.145 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.65 ng	36470	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Bromoeicosane	360	C20H41Br	004276-49-7	16
2			Octadecane	254	C18H38	000593-45-3	11
3			N-(2,2-Diphenylethyl)-2,2-dimeth...	281	C19H23NO	1000211-18-7	10
4			Caprolactam	113	C6H11NO	000105-60-2	10
5			Hentriacontane	437	C31H64	000630-04-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060721\
Data File : BF124166.D
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Misc :
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ClientSampleId :
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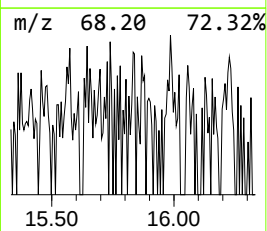
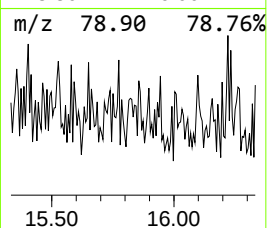
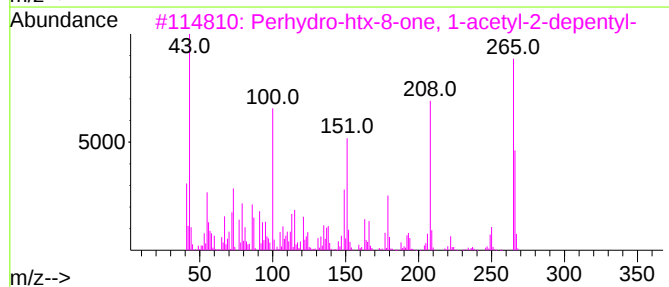
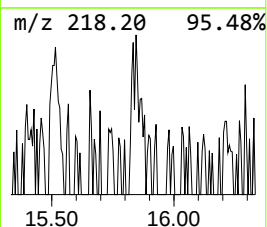
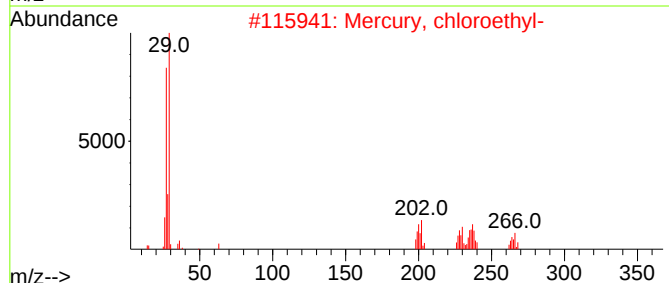
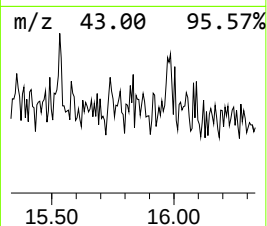
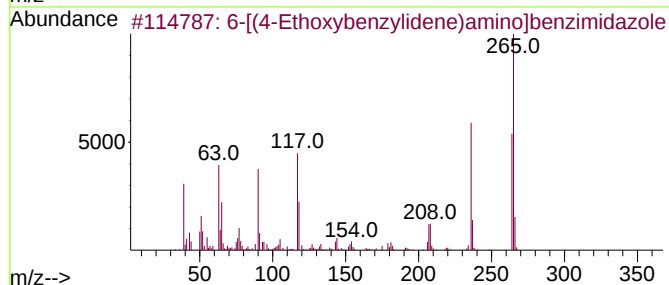
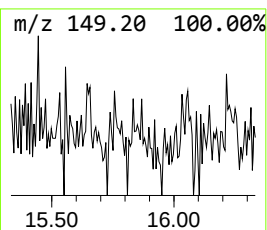
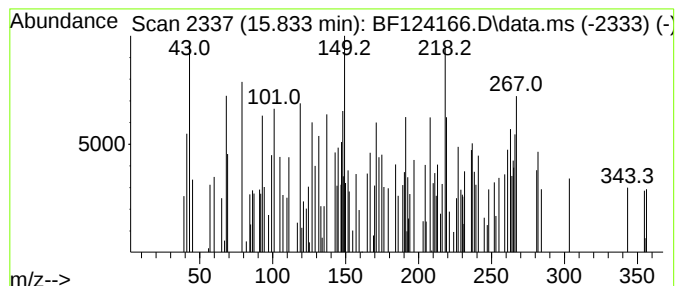
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.833 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.833	2.62 ng	36119	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-[(4-Ethoxybenzylidene)amino]be...	265	C16H15N3O	349572-21-0	14		
2	Mercury, chloroethyl-	266	C2H5ClHg	000107-27-7	14		
3	Perhydro-htx-8-one, 1-acetyl-2-d...	265	C16H27NO2	082267-11-6	14		
4	Methanone, (2-amino-5-chlorophen...	265	C13H9Cl2NO	002958-36-3	14		
5	2,6-Dibromo-4-methylaniline	263	C7H7Br2N	006968-24-7	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060721\
Data File : BF124166.D
Acq On : 7 Jun 2021 20:20
Operator : JU/CG
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
18-B12(2-4)

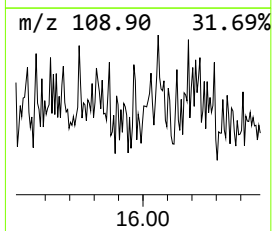
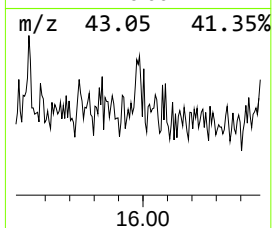
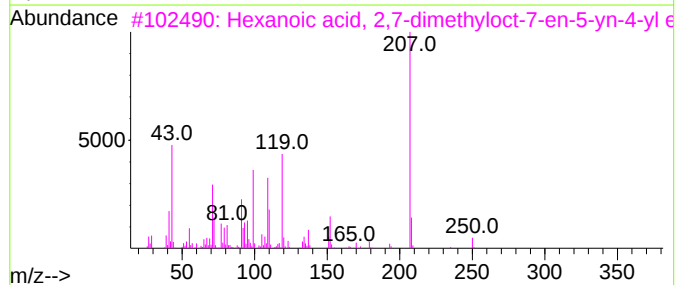
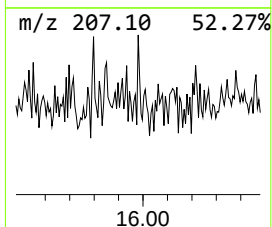
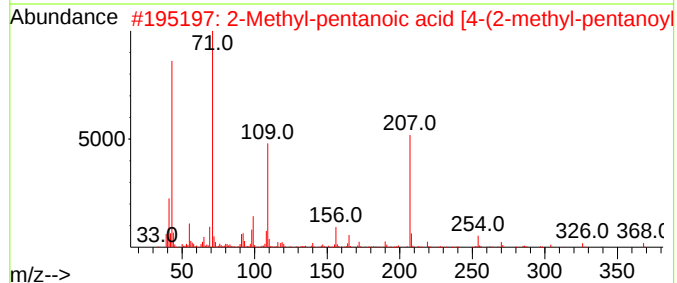
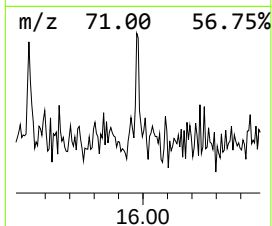
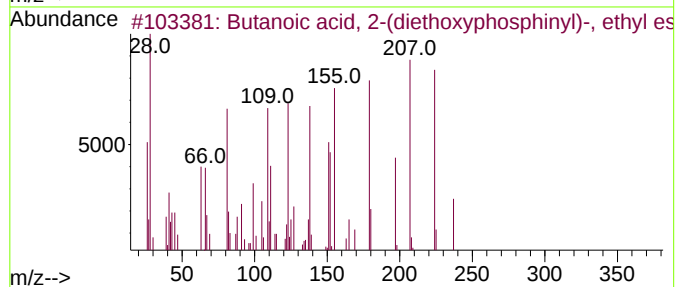
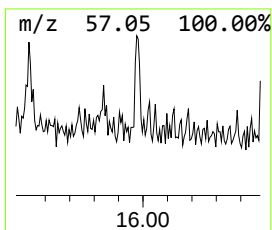
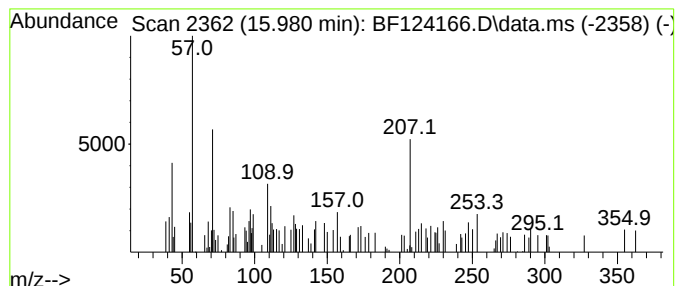
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.980 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	3.23 ng	44438	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-(diethoxyphosph...	252	C10H21O5P	017145-91-4	23
2			2-Methyl-pentanoic acid [4-(2-me...	368	C18H28N2O4S	1000296-31-0	16
3			Hexanoic acid, 2,7-dimethyloct-7...	250	C16H26O2	1000299-35-7	10
4			1-Methyl-3-phenylindole	207	C15H13N	030020-98-5	9
5			3-Methyl-2-phenylindole	207	C15H13N	010257-92-8	9



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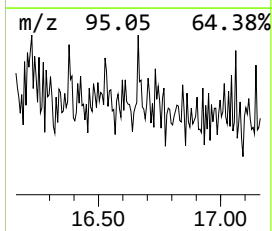
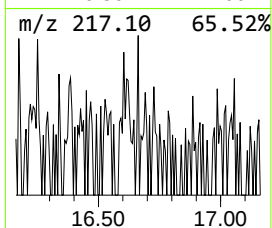
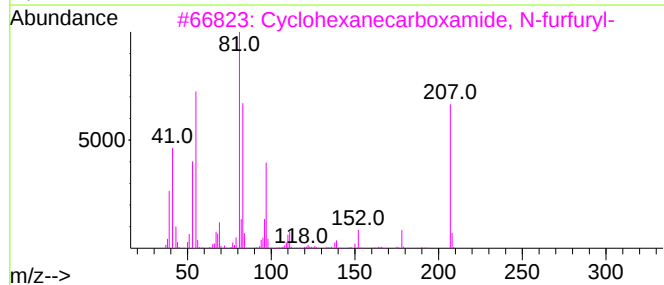
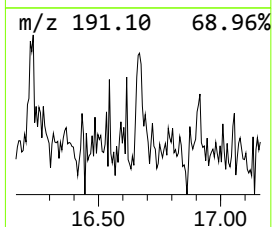
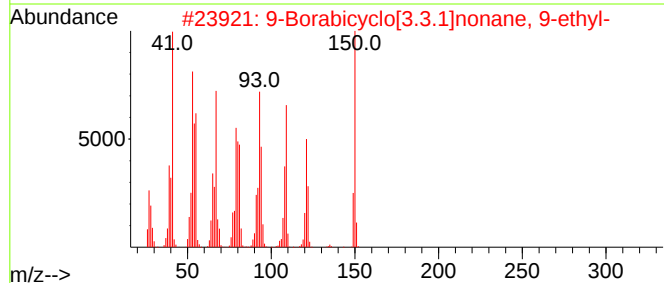
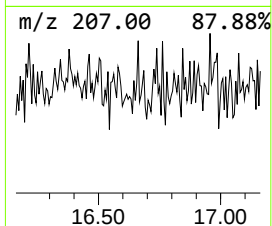
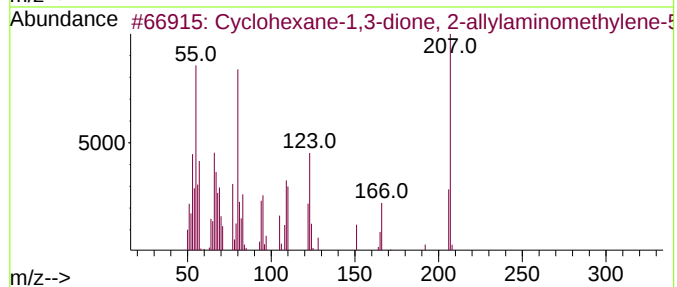
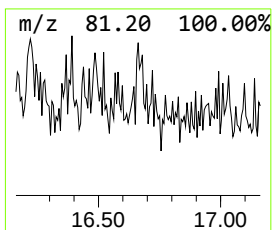
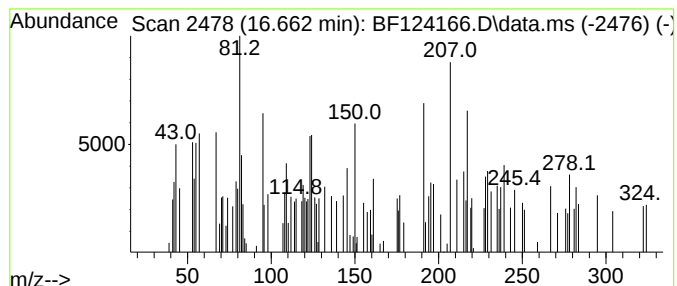
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexane-1,3-dione, 2-al... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.662	3.72 ng	51303	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	60
2			9-Borabicyclo[3.3.1]nonane, 9-et...	150	C10H19B	052102-17-7	56
3			Cyclohexanecarboxamide, N-furfuryl-	207	C12H17NO2	006341-32-8	47
4			N-(4-Chlorophenyl)-2-pyrrolidino...	276	C14H13ClN2O2	1000224-05-1	35
5			2-Furfurylthiol	114	C5H6OS	000098-02-2	30



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Instrument :
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ClientSampleId :
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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
3-Hexen-2-one	4.434	2.4	ng	31890	1	6.857	265571	20.0
2-Pentanone, 4-...	5.063	19.5	ng	258927	1	6.857	265571	20.0
Dodecane, 3-met...	10.798	3.1	ng	53323	4	11.386	345647	20.0
9-Octadecenamid...	13.451	2.7	ng	53445	5	14.027	402431	20.0
unknown13.874	13.874	2.6	ng	52802	5	14.027	402431	20.0
unknown15.145	15.145	2.6	ng	36470	6	15.509	275512	20.0
unknown15.833	15.833	2.6	ng	36119	6	15.509	275512	20.0
unknown15.980	15.980	3.2	ng	44438	6	15.509	275512	20.0
Cyclohexane-1,3...	16.662	3.7	ng	51303	6	15.509	275512	20.0