

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101624\
 Data File : BF139829.D
 Acq On : 16 Oct 2024 14:07
 Operator : RC/JU
 Sample : P4401-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-03-101424

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-BF101524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139829.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	496	504	515	rVB	68410	102586	6.60%	0.618%
2	5.469	568	574	596	rVB	1124697	1453617	93.58%	8.758%
3	6.487	741	747	761	rBV	1086207	1477960	95.15%	8.905%
4	6.851	804	809	814	rVB	441100	529585	34.09%	3.191%
5	7.416	894	905	914	rBV	715741	966404	62.22%	5.823%
6	7.669	942	948	954	rVB3	30107	50171	3.23%	0.302%
7	8.134	1014	1027	1034	rBV	541319	733441	47.22%	4.419%
8	8.422	1071	1076	1080	rBV6	10770	16190	1.04%	0.098%
9	8.634	1108	1112	1116	rBV2	19401	23669	1.52%	0.143%
10	8.716	1122	1126	1130	rBV	29768	39277	2.53%	0.237%
11	8.786	1135	1138	1146	rVB6	11684	23972	1.54%	0.144%
12	8.951	1162	1166	1171	rBV3	20273	29333	1.89%	0.177%
13	9.081	1184	1188	1193	rVB4	11784	18170	1.17%	0.109%
14	9.145	1196	1199	1204	rVV3	14984	20186	1.30%	0.122%
15	9.204	1204	1209	1214	rVV	1245663	1553288	100.00%	9.359%
16	9.281	1218	1222	1226	rBV	49404	64731	4.17%	0.390%
17	9.357	1231	1235	1238	rVB	14152	17983	1.16%	0.108%
18	9.539	1260	1266	1268	rVV5	17650	33301	2.14%	0.201%
19	9.598	1272	1276	1280	rVV4	32194	58842	3.79%	0.355%
20	9.663	1284	1287	1292	rVB5	15861	20502	1.32%	0.124%
21	9.751	1297	1302	1306	rBV	33342	49516	3.19%	0.298%
22	9.810	1308	1312	1317	rVB	55915	69401	4.47%	0.418%
23	9.886	1320	1325	1329	rBV	517278	632022	40.69%	3.808%
24	10.133	1363	1367	1371	rBV5	15585	20039	1.29%	0.121%
25	10.204	1375	1379	1385	rBV7	13482	28028	1.80%	0.169%
26	10.310	1391	1397	1401	rBV	65855	87516	5.63%	0.527%
27	10.433	1414	1418	1424	rBV2	15172	25103	1.62%	0.151%
28	10.528	1430	1434	1441	rVB	22766	41340	2.66%	0.249%
29	10.598	1441	1446	1452	rVV	83364	116397	7.49%	0.701%
30	10.675	1453	1459	1470	rVB	552568	723217	46.56%	4.357%
31	10.786	1473	1478	1486	rVB	65698	114084	7.34%	0.687%
32	11.233	1549	1554	1556	rBV	36948	52461	3.38%	0.316%
33	11.263	1556	1559	1565	rVB2	28848	43329	2.79%	0.261%
34	11.369	1572	1577	1586	rBV2	432379	757932	48.80%	4.567%
35	11.445	1586	1590	1594	rVB	44755	56551	3.64%	0.341%
36	11.604	1613	1617	1622	rVB	21007	28233	1.82%	0.170%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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

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37	11.657	1623	1626	1631	rVB2	25948	31752	2.04%	0.191%
38	11.898	1659	1667	1672	rBV2	136865	237669	15.30%	1.432%
39	11.986	1678	1682	1690	rVB	71759	127689	8.22%	0.769%
40	12.063	1691	1695	1700	rBV2	27379	41803	2.69%	0.252%
41	12.169	1710	1713	1715	rBV	16177	18594	1.20%	0.112%
42	12.422	1752	1756	1759	rBV	30866	48524	3.12%	0.292%
43	12.457	1759	1762	1767	rVV2	32267	49192	3.17%	0.296%
44	12.510	1768	1771	1776	rVV	29168	37025	2.38%	0.223%
45	12.586	1779	1784	1789	rBV	545779	678404	43.68%	4.087%
46	12.680	1796	1800	1805	rBV2	38834	56241	3.62%	0.339%
47	12.816	1816	1823	1828	rBV	507029	741022	47.71%	4.465%
48	12.863	1829	1831	1836	rVB2	24048	32351	2.08%	0.195%
49	12.957	1840	1847	1854	rVB	956953	1284767	82.71%	7.741%
50	13.033	1855	1860	1864	rBV3	37541	69693	4.49%	0.420%
51	13.139	1871	1878	1882	rVB	77114	133209	8.58%	0.803%
52	13.210	1887	1890	1892	rVV	41663	51211	3.30%	0.309%
53	13.245	1893	1896	1903	rVB2	46112	65478	4.22%	0.395%
54	13.757	1981	1983	1986	rBV3	29984	36614	2.36%	0.221%
55	13.857	1997	2000	2009	rVB4	66063	109869	7.07%	0.662%
56	14.010	2020	2026	2029	rBV2	544453	929693	59.85%	5.601%
57	15.051	2198	2203	2211	rBV	238896	517950	33.35%	3.121%
58	15.351	2251	2254	2260	rVB	121661	189154	12.18%	1.140%
59	15.415	2261	2265	2271	rVV	191595	293654	18.91%	1.769%
60	15.480	2271	2276	2288	rVB2	209507	423815	27.29%	2.554%
61	16.939	2520	2524	2533	rVB2	87944	178312	11.48%	1.074%
62	17.386	2596	2600	2608	rVB	70326	135311	8.71%	0.815%

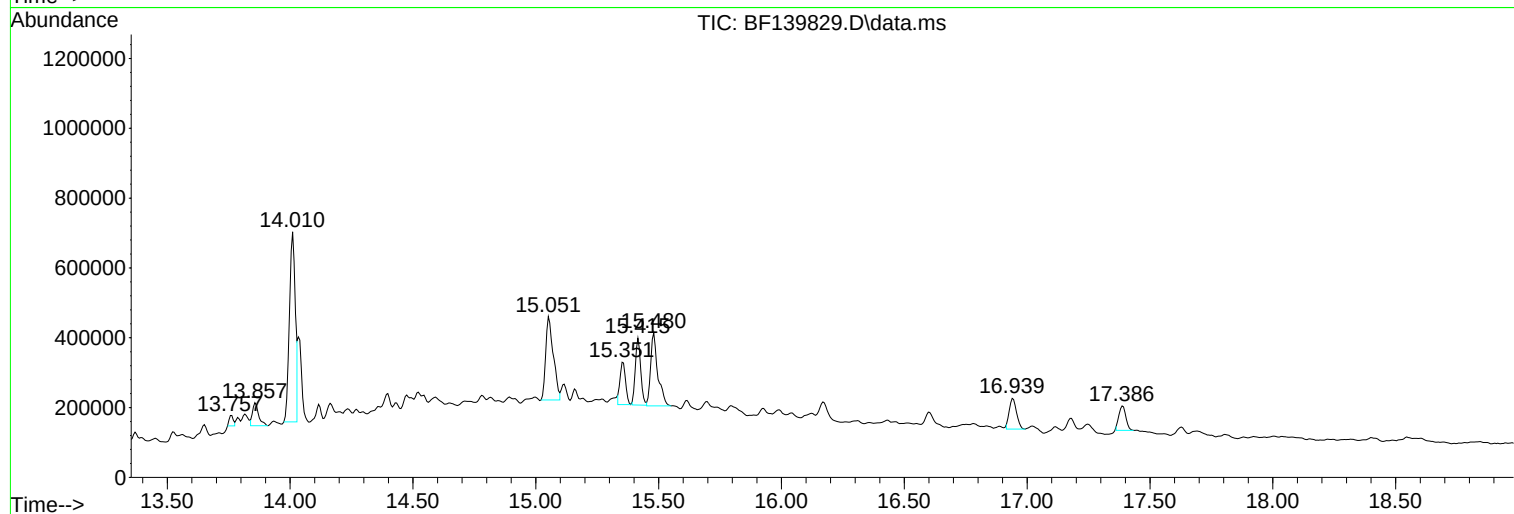
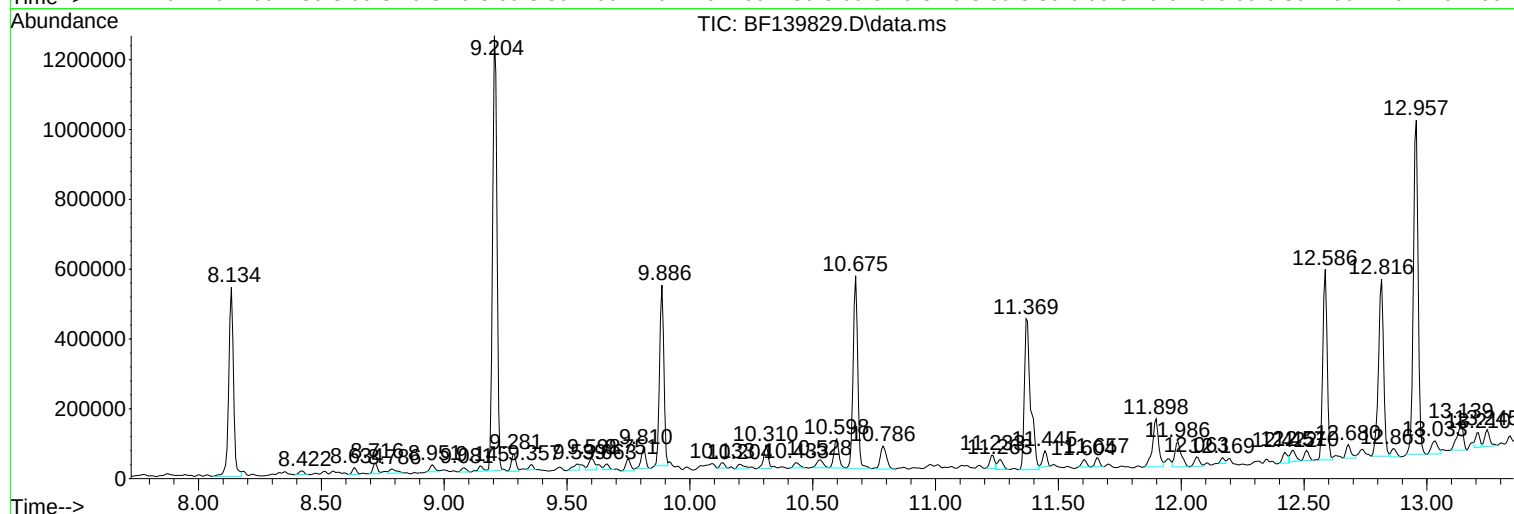
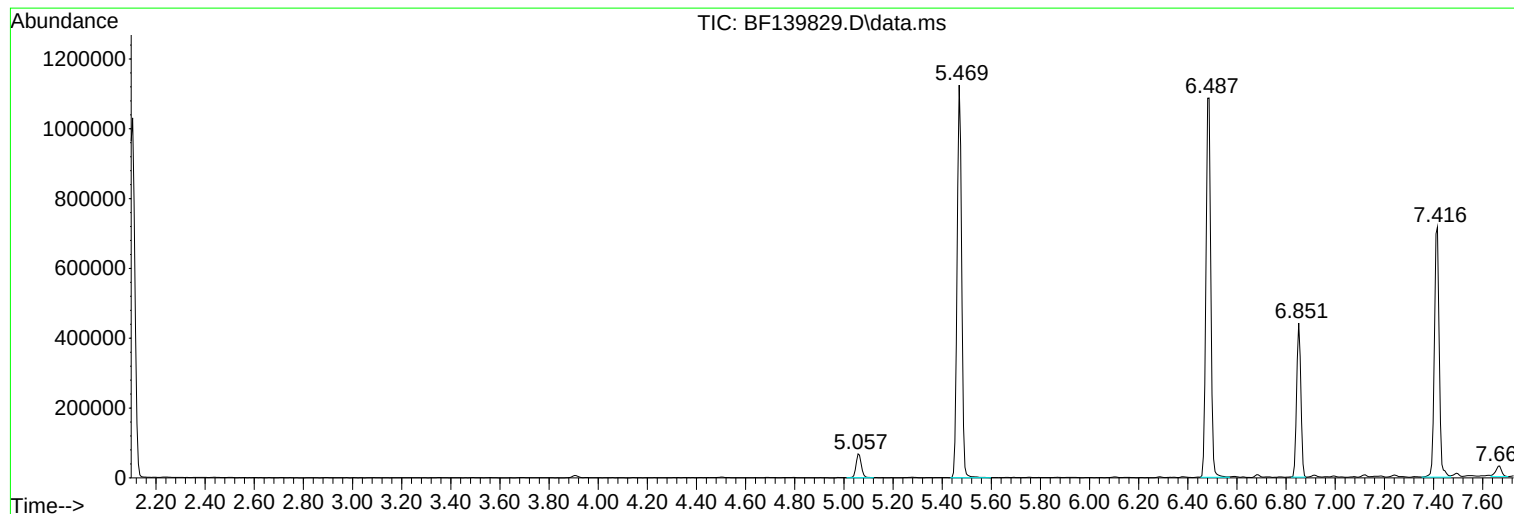
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
BNA_F
ClientSampleId :
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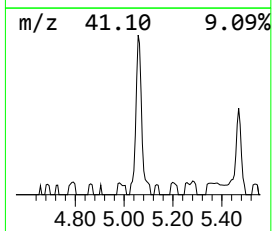
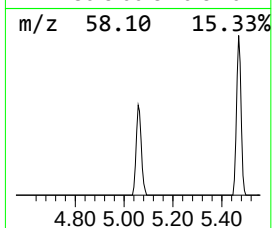
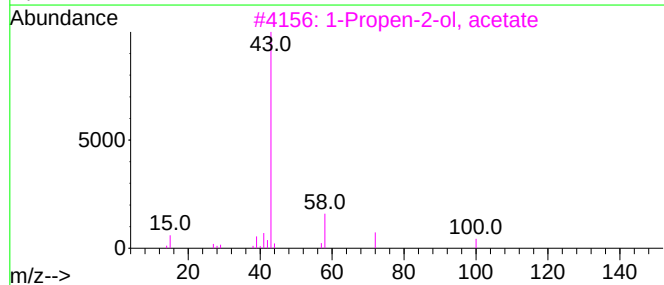
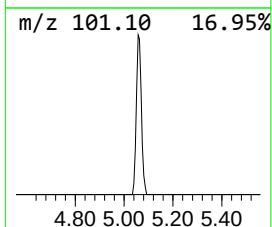
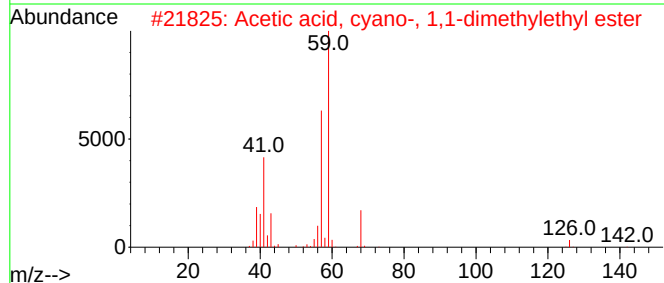
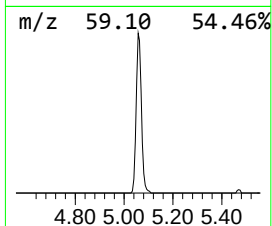
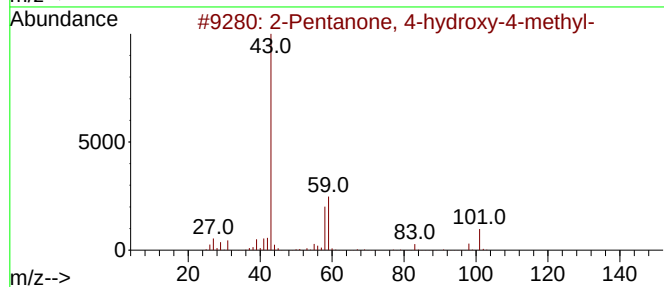
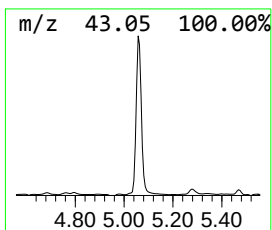
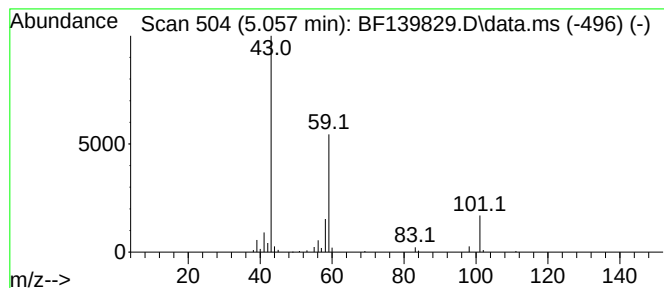
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	3.87 ng	102586	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9		



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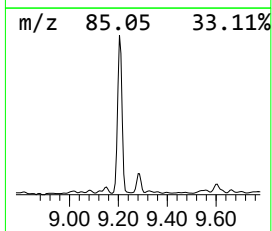
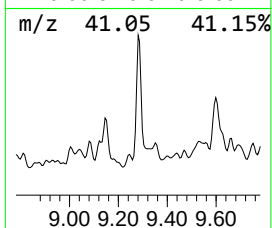
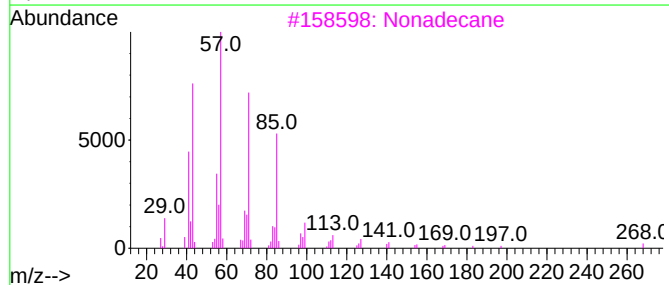
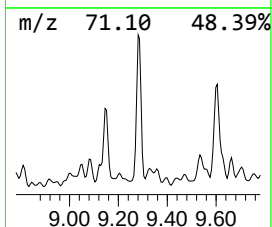
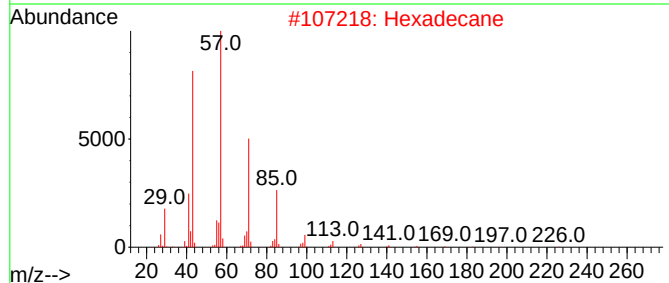
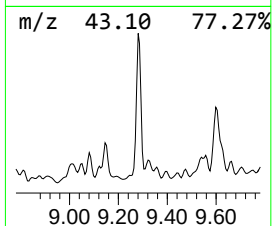
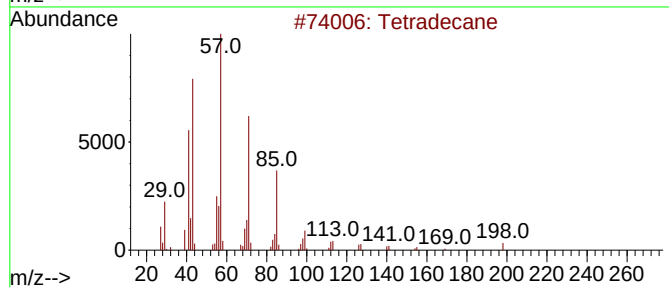
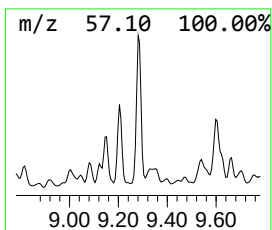
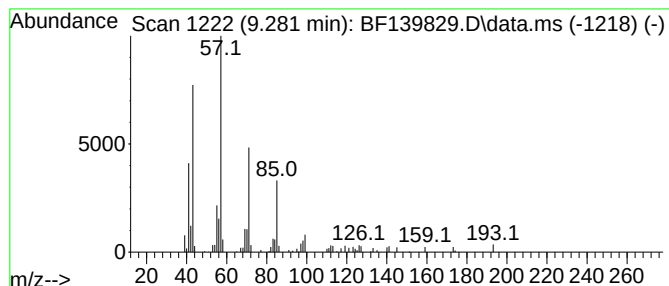
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Tetradecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.281	2.05 ng	64731	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	87
2			Hexadecane	226	C16H34	000544-76-3	86
3			Nonadecane	268	C19H40	000629-92-5	80
4			Tridecane	184	C13H28	000629-50-5	80
5			10-Methylnonadecane	282	C20H42	056862-62-5	80



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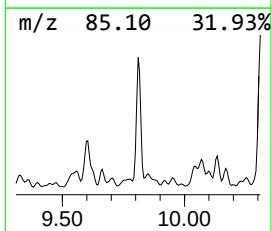
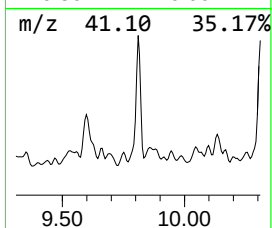
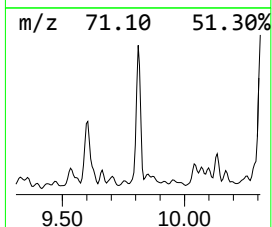
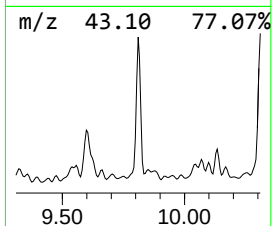
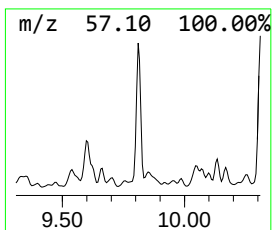
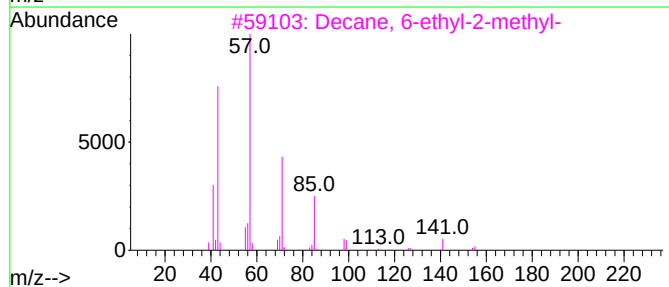
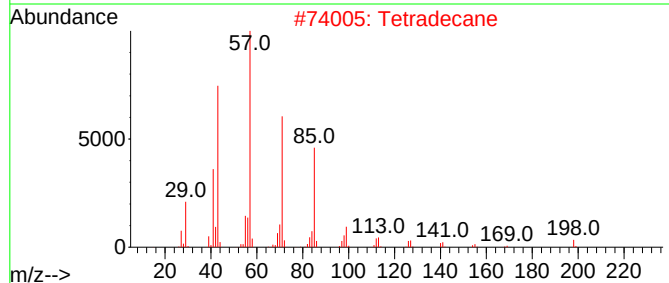
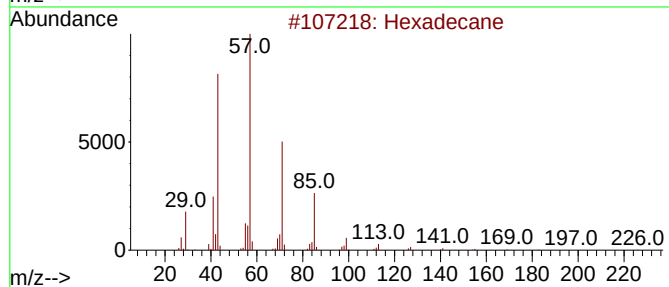
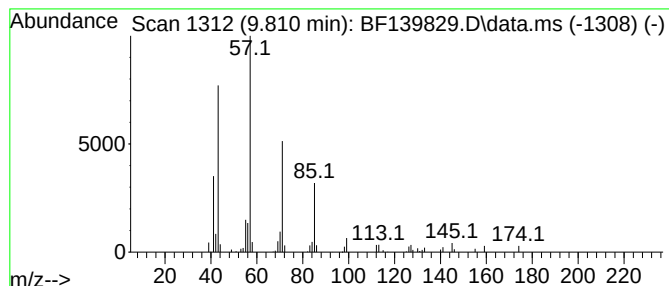
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.810	2.20 ng	69401	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			Tetradecane	198	C14H30	000629-59-4	83
3			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	83
4			Pentadecane	212	C15H32	000629-62-9	72
5			Tridecane	184	C13H28	000629-50-5	64



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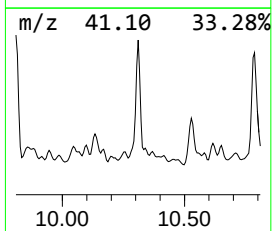
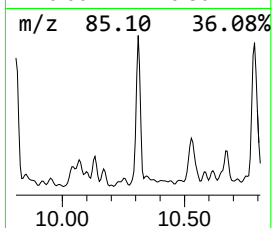
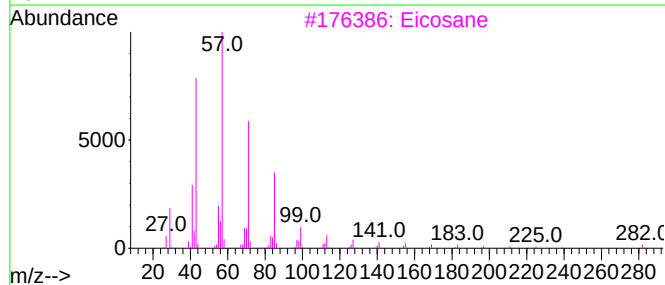
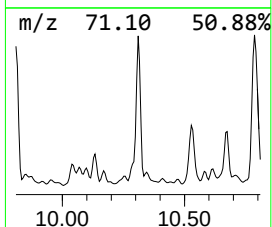
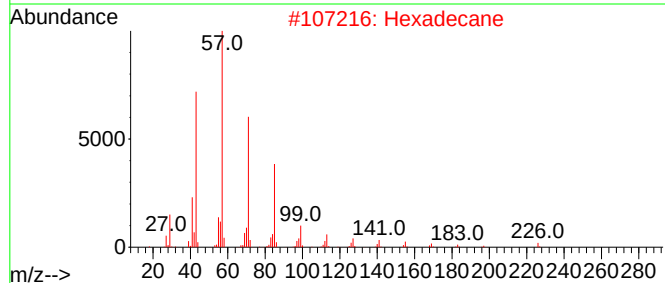
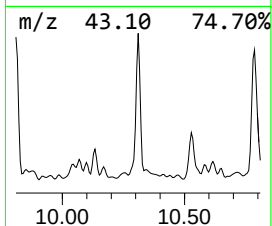
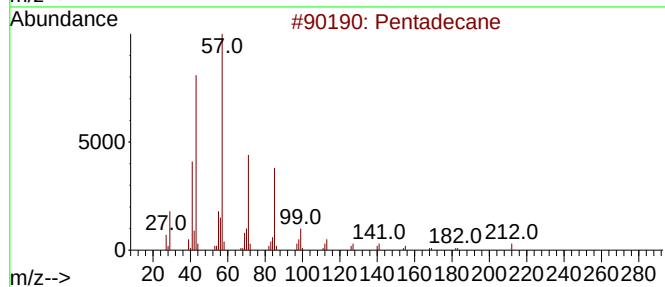
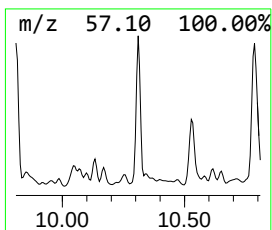
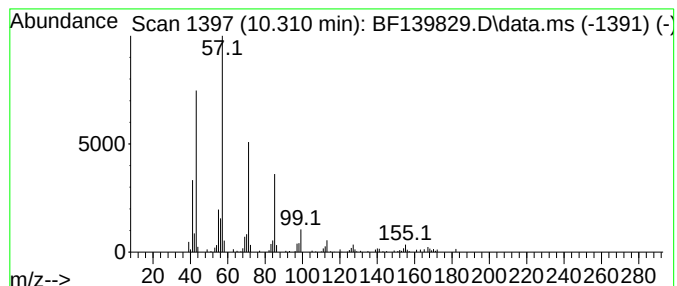
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.310	2.77 ng	87516	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	87
2			Hexadecane	226	C16H34	000544-76-3	86
3			Eicosane	282	C20H42	000112-95-8	86
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5			Undecane, 2-methyl-	170	C12H26	007045-71-8	83



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SU-03-101424

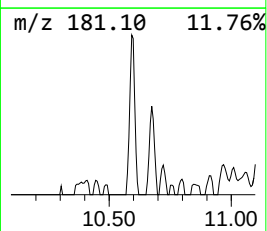
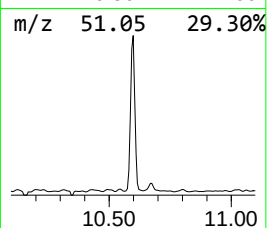
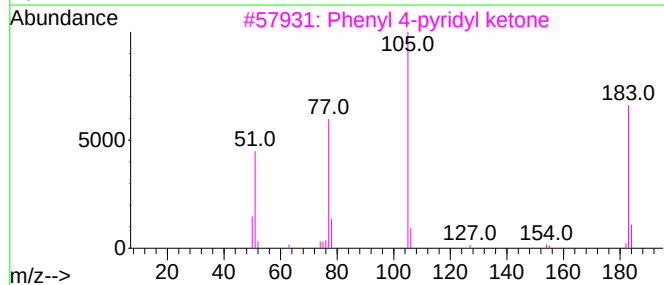
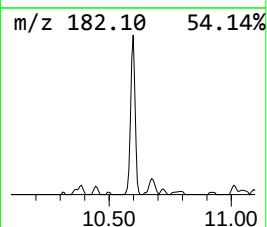
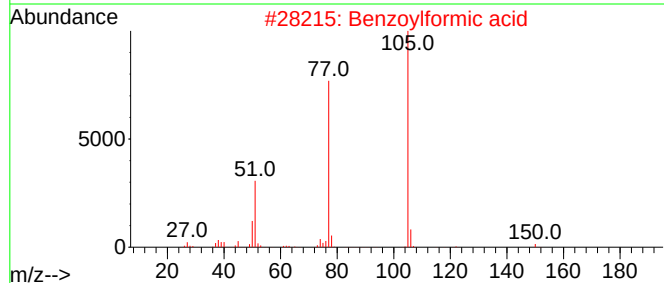
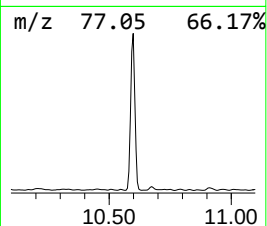
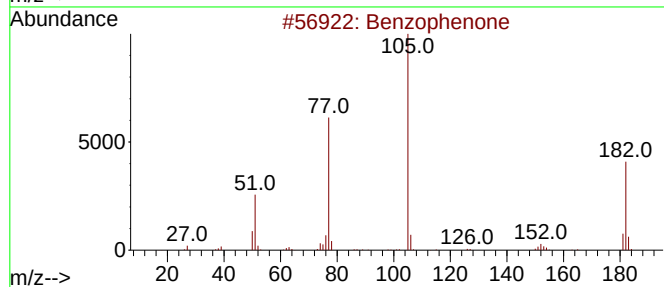
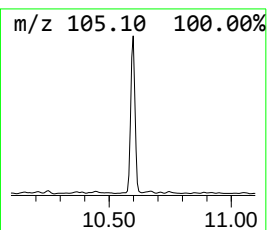
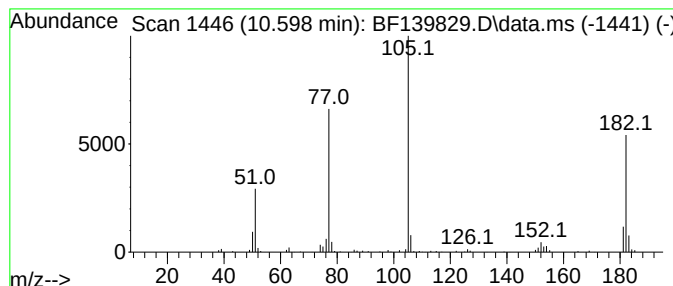
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	3.68 ng	116397	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzoylformic acid	150	C8H6O3	000611-73-4	55
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	53
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101624\
Data File : BF139829.D
Acq On : 16 Oct 2024 14:07
Operator : RC/JU
Sample : P4401-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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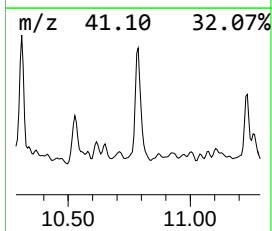
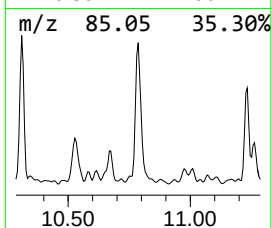
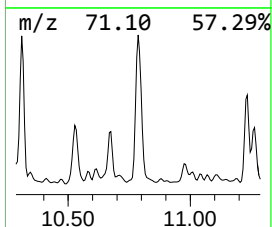
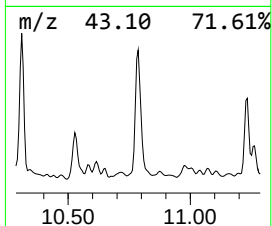
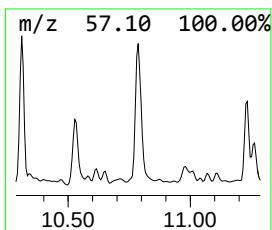
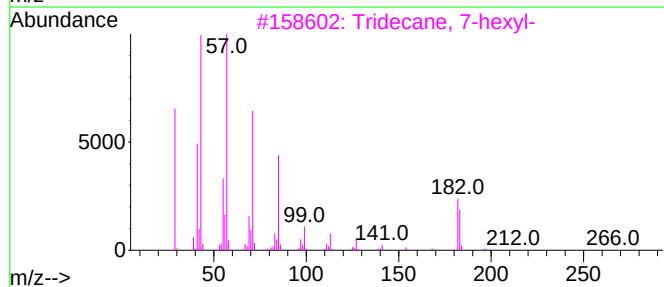
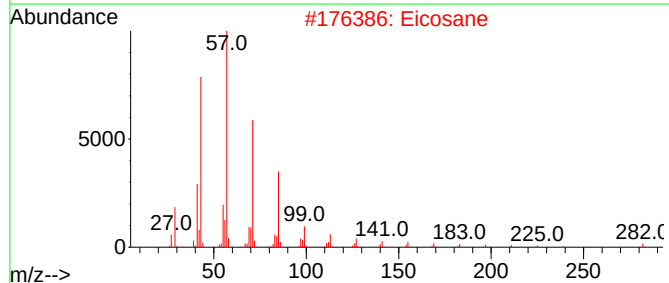
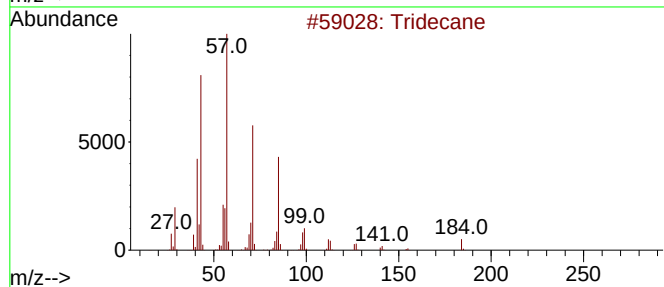
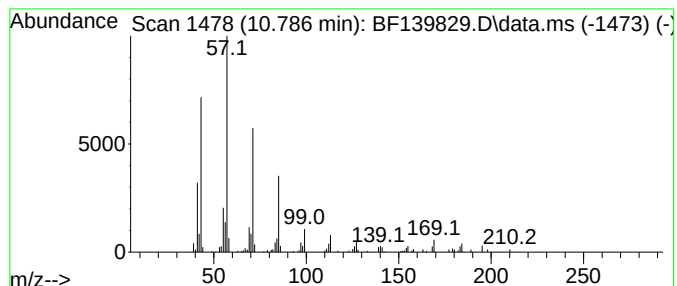
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.786	3.01 ng	114084	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	91
2			Eicosane	282	C20H42	000112-95-8	87
3			Tridecane, 7-hexyl-	268	C19H40	007225-66-3	87
4			Heptacosane	380	C27H56	000593-49-7	86
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101624\
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ClientSampleId :
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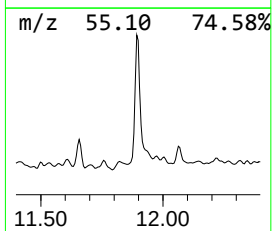
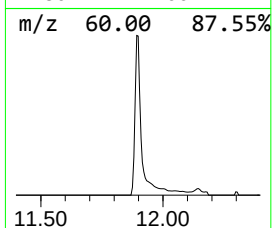
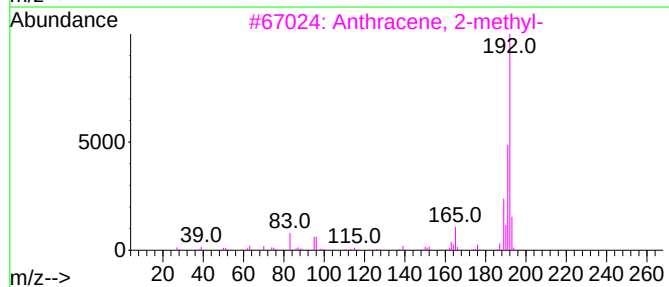
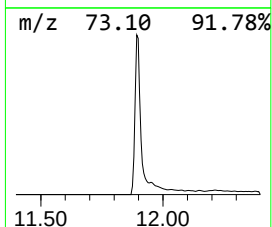
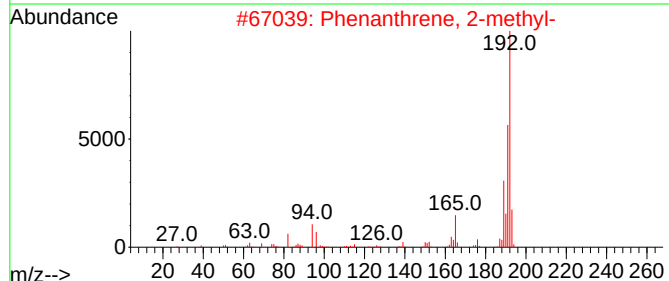
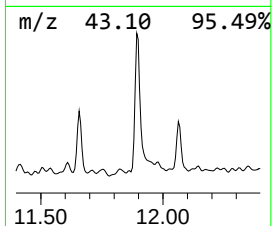
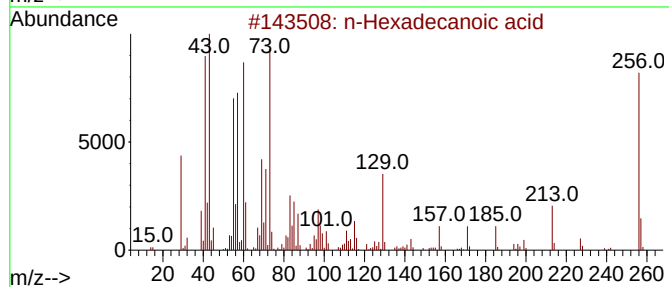
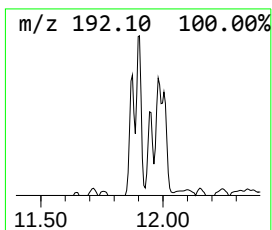
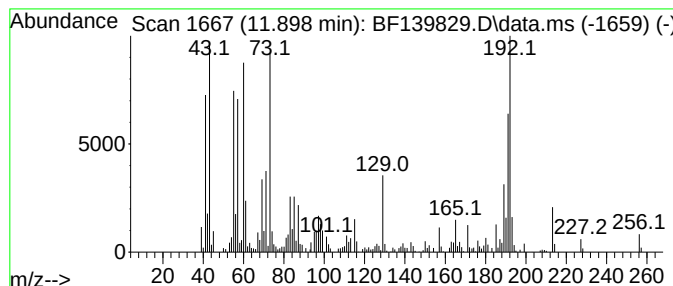
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	6.27 ng	237669	Phenanthrene-d10	11.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
5			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101624\
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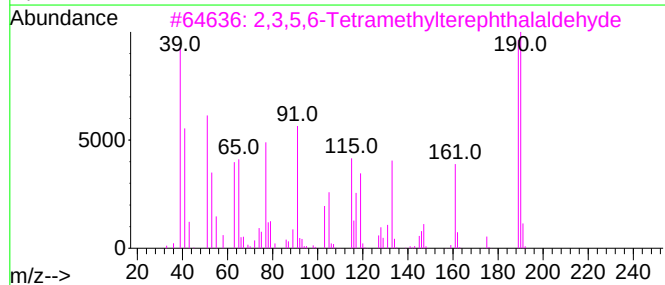
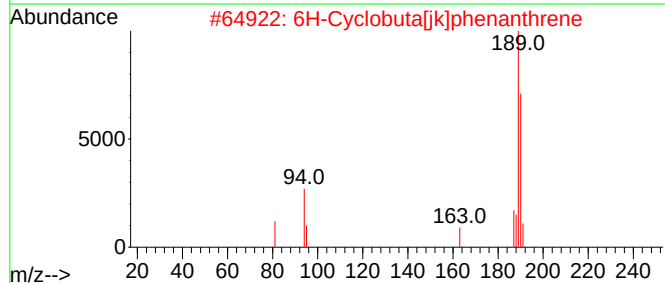
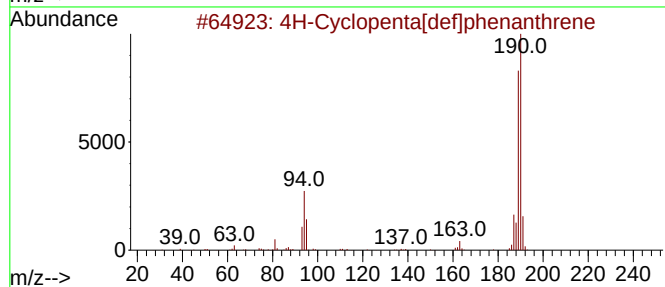
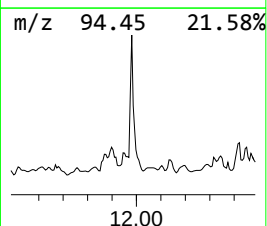
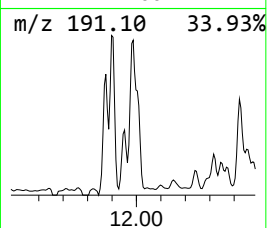
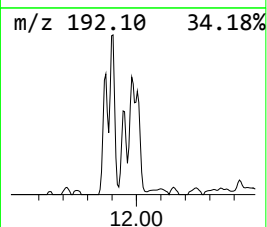
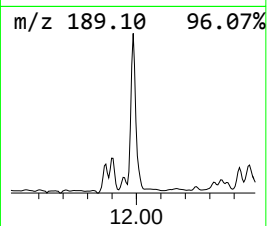
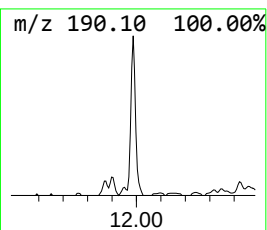
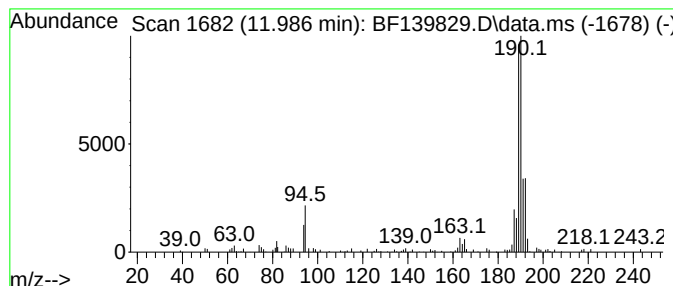
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.986	3.37 ng	127689	Phenanthrene-d10	11.369	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	49
4	Megastigmatrienone	190	C13H18O	038818-55-2	25
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101624\
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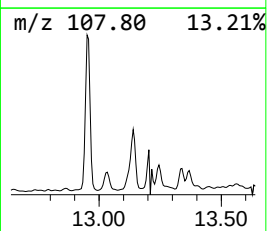
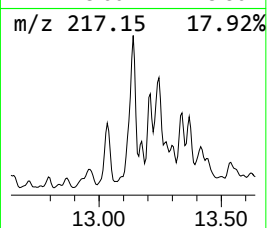
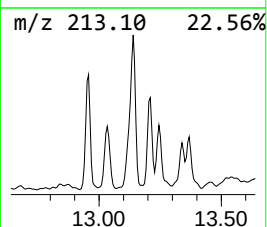
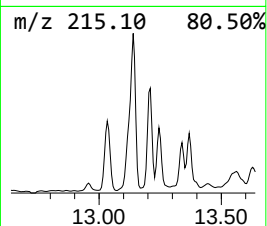
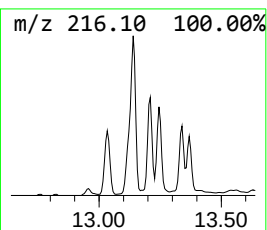
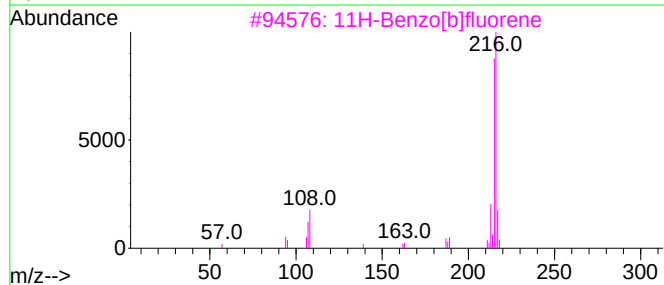
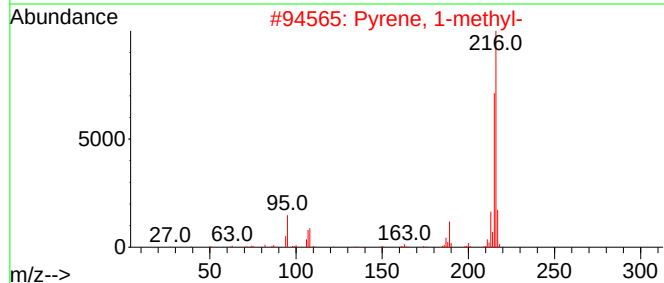
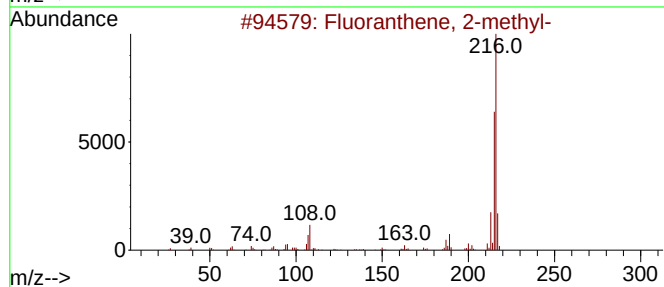
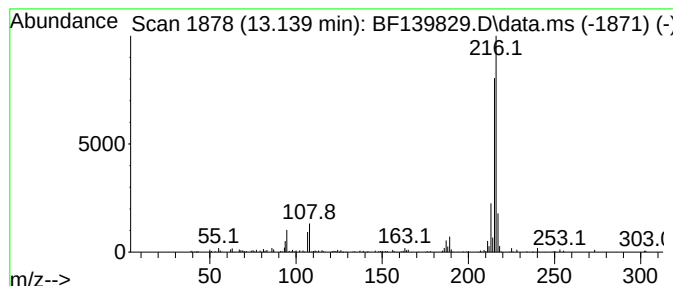
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Fluoranthene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	2.87 ng	133209	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	94
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4			Pyrene, 2-methyl-	216	C17H12	003442-78-2	91
5			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101624\
Data File : BF139829.D
Acq On : 16 Oct 2024 14:07
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Sample : P4401-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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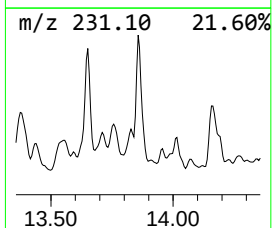
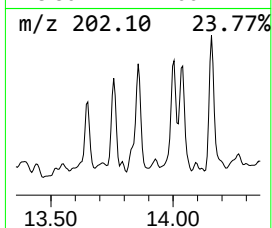
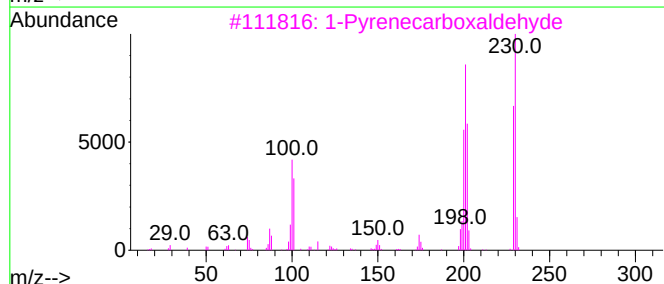
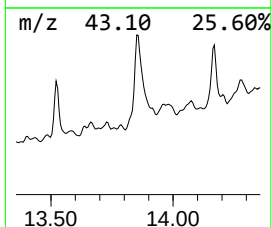
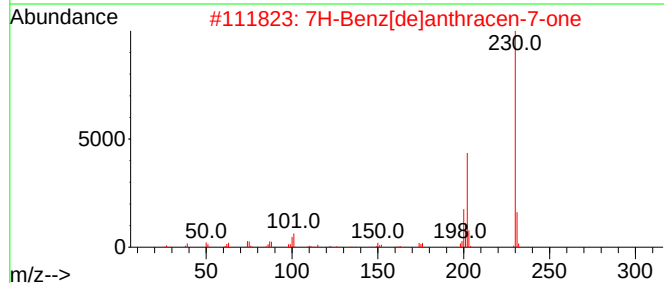
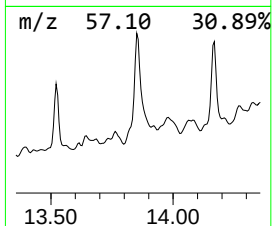
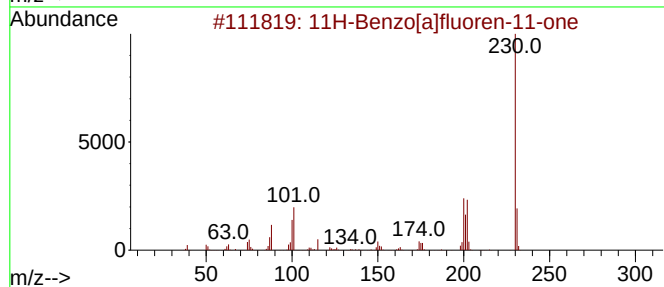
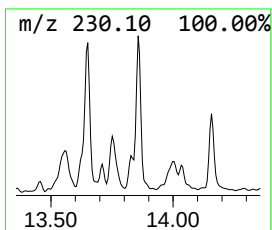
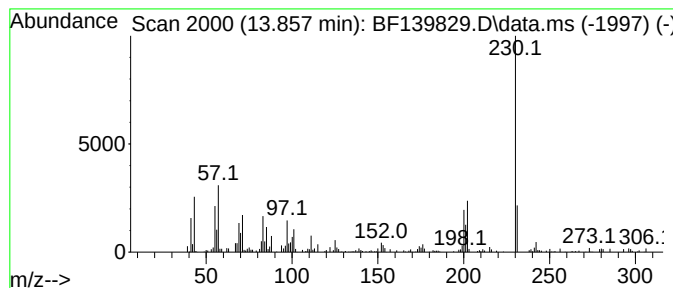
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 11H-Benzo[a]fluoren-11-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.36 ng	109869	Chrysene-d12	14.010

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	87
2		7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	76
3		1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	64
4		m-Terphenyl	230	C18H14	000092-06-8	50
5		2-Chloro-9-xanthenone	230	C13H7ClO2	013210-15-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101624\
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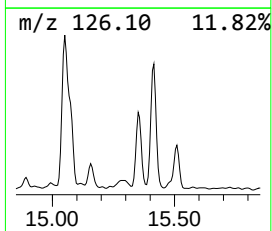
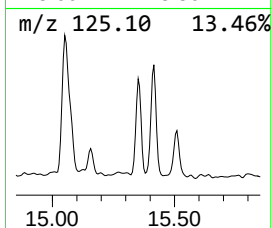
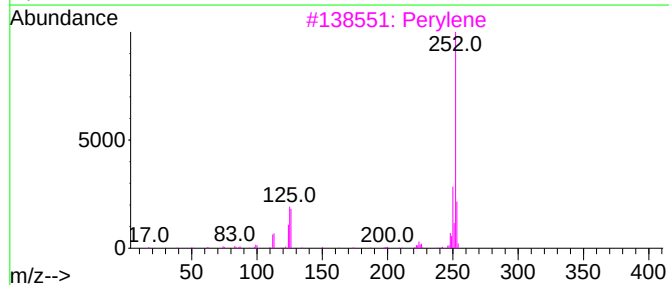
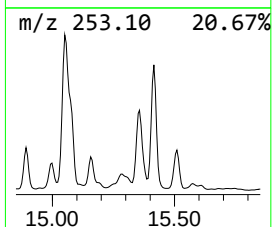
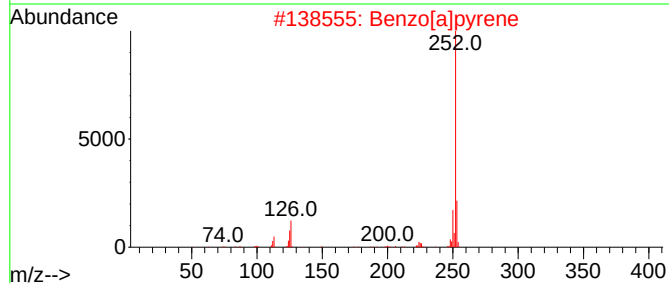
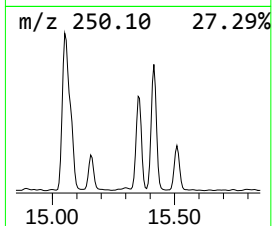
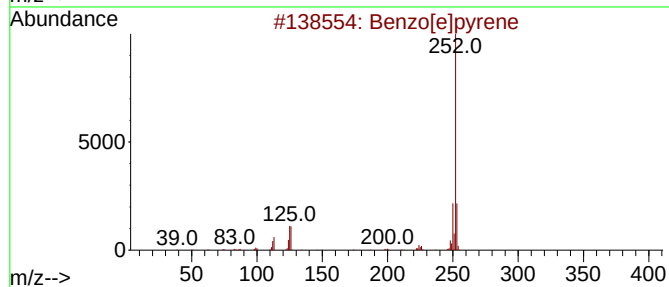
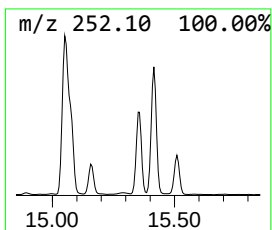
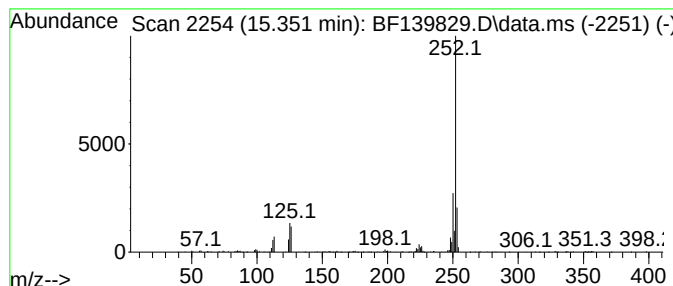
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	8.93 ng	189154	Perylene-d12	15.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[a]pyrene	252	C20H12	000050-32-8	97
3			Perylene	252	C20H12	000198-55-0	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101624\
Data File : BF139829.D
Acq On : 16 Oct 2024 14:07
Operator : RC/JU
Sample : P4401-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-101424

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101524.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
2-Pentanone, 4-...	5.057	3.9	ng	102586	1	6.851	529585	20.0
Tetradecane	9.281	2.0	ng	64731	3	9.886	632022	20.0
Hexadecane	9.810	2.2	ng	69401	3	9.886	632022	20.0
Pentadecane	10.310	2.8	ng	87516	3	9.886	632022	20.0
Benzophenone	10.598	3.7	ng	116397	3	9.886	632022	20.0
Tridecane	10.786	3.0	ng	114084	4	11.369	757932	20.0
n-Hexadecanoic ...	11.898	6.3	ng	237669	4	11.369	757932	20.0
4H-Cyclopenta[d]...	11.986	3.4	ng	127689	4	11.369	757932	20.0
Fluoranthene, 2...	13.139	2.9	ng	133209	5	14.010	929693	20.0
11H-Benzo[a]flu...	13.857	2.4	ng	109869	5	14.010	929693	20.0
Benzo[e]pyrene	15.351	8.9	ng	189154	6	15.480	423815	20.0