

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
 Data File : BF133856.D
 Acq On : 20 Jun 2023 15:02
 Operator : CG\JU
 Sample : 03223-01 2X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSIT-SB-04

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133856.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	13	rVB	229053	285461	22.68%	1.807%
2	2.240	22	26	33	rVB3	12121	18079	1.44%	0.114%
3	5.081	506	509	516	rVB	79300	78226	6.21%	0.495%
4	5.487	574	578	593	rBV	1164524	1050124	83.41%	6.649%
5	6.492	745	749	759	rBV	1096631	1044979	83.01%	6.616%
6	6.692	777	783	787	rBV5	13849	17586	1.40%	0.111%
7	6.857	807	811	815	rBV	822000	637465	50.64%	4.036%
8	7.416	902	906	909	rBV	833265	679858	54.00%	4.304%
9	8.133	1025	1028	1037	rVB	878582	757434	60.17%	4.796%
10	8.851	1147	1150	1156	rBV	18823	17957	1.43%	0.114%
11	9.210	1208	1211	1215	rBV	1417328	1165843	92.61%	7.381%
12	9.292	1222	1225	1227	rBV	20272	15983	1.27%	0.101%
13	9.316	1227	1229	1234	rVB3	9057	14283	1.13%	0.090%
14	9.551	1266	1269	1271	rBV	16212	13755	1.09%	0.087%
15	9.751	1300	1303	1307	rBV	39218	35235	2.80%	0.223%
16	9.892	1324	1327	1331	rBV	866412	699412	55.56%	4.428%
17	9.928	1331	1333	1338	rVB	46671	37827	3.00%	0.239%
18	10.098	1358	1362	1366	rVB	26557	22887	1.82%	0.145%
19	10.445	1417	1421	1427	rBV	34177	36151	2.87%	0.229%
20	10.610	1445	1449	1455	rVB	231182	194277	15.43%	1.230%
21	10.686	1458	1462	1473	rVB	603521	568574	45.16%	3.600%
22	10.810	1479	1483	1487	rVB4	23175	29907	2.38%	0.189%
23	10.922	1499	1502	1505	rVB	34995	27424	2.18%	0.174%
24	10.992	1509	1514	1517	rBV6	12316	18061	1.43%	0.114%
25	11.127	1531	1537	1538	rBV6	11304	16503	1.31%	0.104%
26	11.192	1545	1548	1551	rVV2	18981	18018	1.43%	0.114%
27	11.251	1552	1558	1561	rVV7	14394	24166	1.92%	0.153%
28	11.280	1561	1563	1569	rVB	22225	21601	1.72%	0.137%
29	11.386	1577	1581	1583	rBV	655275	563857	44.79%	3.570%
30	11.410	1583	1585	1589	rVV	351156	281798	22.38%	1.784%
31	11.463	1591	1594	1598	rVB	90969	73905	5.87%	0.468%
32	11.622	1618	1621	1627	rVB	29935	31595	2.51%	0.200%
33	11.680	1629	1631	1635	rBV3	16734	15774	1.25%	0.100%
34	11.892	1664	1667	1669	rBV	54255	49460	3.93%	0.313%
35	11.922	1669	1672	1678	rVV2	140864	193041	15.33%	1.222%
36	12.004	1682	1686	1688	rVV	89578	100154	7.96%	0.634%

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37	12.027	1688	1690	1694	rVB	35983	36189	2.87%	0.229%
38	12.192	1715	1718	1720	rBV	33630	35232	2.80%	0.223%
39	12.216	1720	1722	1725	rVB	39302	34841	2.77%	0.221%
40	12.369	1746	1748	1750	rBV3	18033	17202	1.37%	0.109%
41	12.445	1758	1761	1764	rBV2	46725	58177	4.62%	0.368%
42	12.480	1764	1767	1770	rVV4	33605	41672	3.31%	0.264%
43	12.527	1773	1775	1780	rVV2	39048	45609	3.62%	0.289%
44	12.610	1785	1789	1792	rBV	757570	687637	54.62%	4.354%
45	12.663	1794	1798	1802	rVV4	45667	89175	7.08%	0.565%
46	12.710	1803	1806	1810	rVB3	41184	59027	4.69%	0.374%
47	12.839	1822	1828	1831	rBV	716667	713134	56.65%	4.515%
48	12.886	1834	1836	1841	rVB2	40842	44503	3.54%	0.282%
49	12.957	1845	1848	1849	rBV	37080	35432	2.81%	0.224%
50	12.980	1849	1852	1856	rVB	1211424	1042668	82.82%	6.602%
51	13.063	1862	1866	1869	rBV2	36567	48158	3.83%	0.305%
52	13.145	1877	1880	1881	rBV3	43008	45709	3.63%	0.289%
53	13.168	1881	1884	1887	rVB	104651	95809	7.61%	0.607%
54	13.216	1890	1892	1893	rBV2	23467	17955	1.43%	0.114%
55	13.233	1893	1895	1898	rVB	66733	58045	4.61%	0.368%
56	13.274	1898	1902	1905	rBV2	75537	91708	7.28%	0.581%
57	13.368	1915	1918	1920	rVB	44391	43165	3.43%	0.273%
58	13.398	1920	1923	1927	rBV	52730	60619	4.82%	0.384%
59	13.680	1968	1971	1976	rVB	66522	65786	5.23%	0.417%
60	13.792	1987	1990	1992	rBV2	56779	54501	4.33%	0.345%
61	13.821	1993	1995	1997	rBV	48017	35751	2.84%	0.226%
62	13.845	1997	1999	2000	rVV	52367	39381	3.13%	0.249%
63	13.892	2004	2007	2010	rVB2	76640	74284	5.90%	0.470%
64	14.045	2026	2033	2036	rBV2	887645	1258917	100.00%	7.971%
65	14.074	2036	2038	2043	rVB	382797	340707	27.06%	2.157%
66	14.151	2048	2051	2054	rVB2	98455	100892	8.01%	0.639%
67	14.468	2103	2105	2109	rBV2	49427	45900	3.65%	0.291%
68	15.110	2210	2214	2217	rBV	281219	451943	35.90%	2.861%
69	15.421	2264	2267	2274	rVB	149696	211074	16.77%	1.336%
70	15.486	2274	2278	2284	rBV	210061	294174	23.37%	1.863%
71	15.551	2285	2289	2293	rBV	287875	390647	31.03%	2.473%
72	17.098	2549	2552	2560	rVB2	89268	171900	13.65%	1.088%

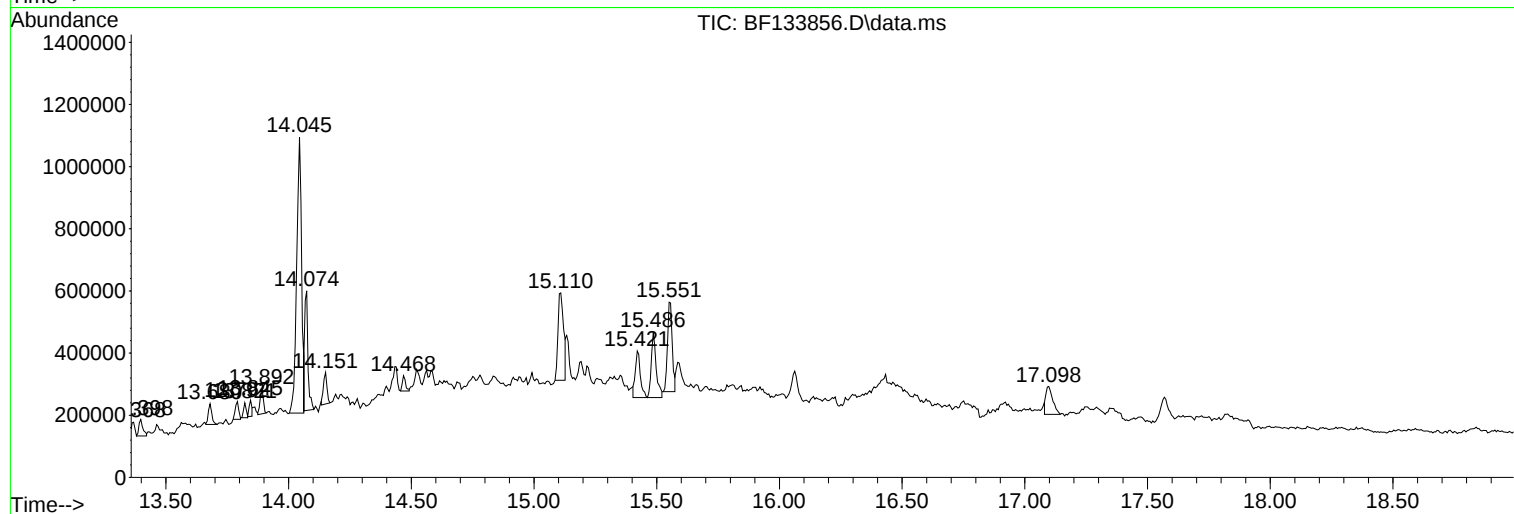
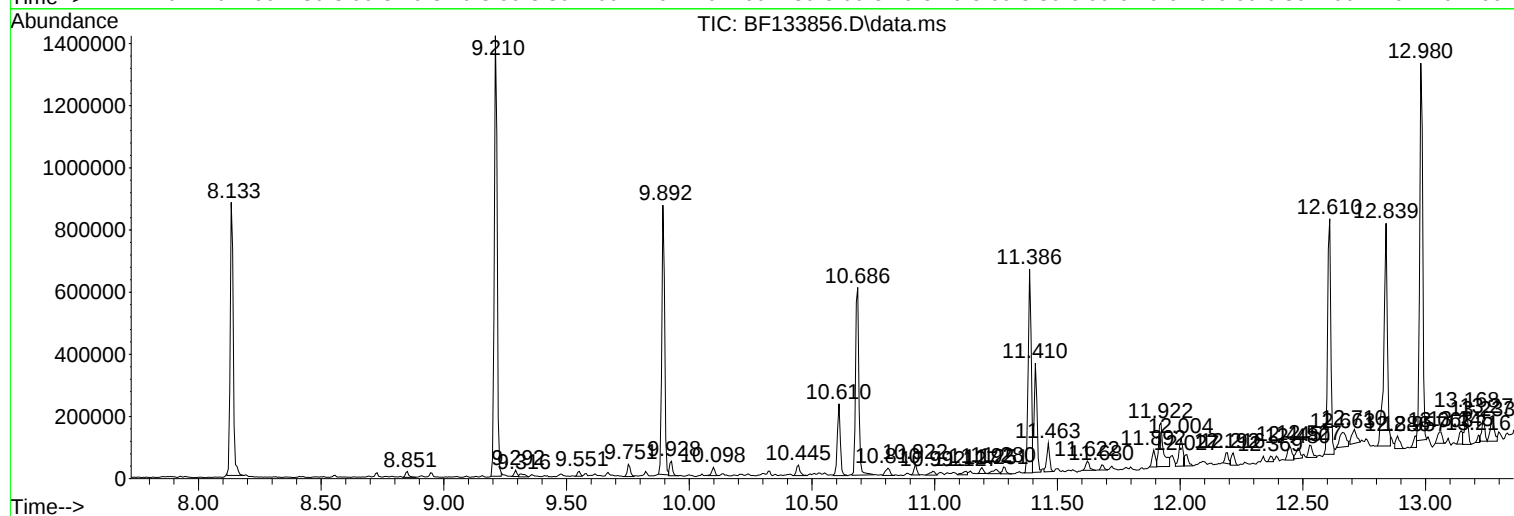
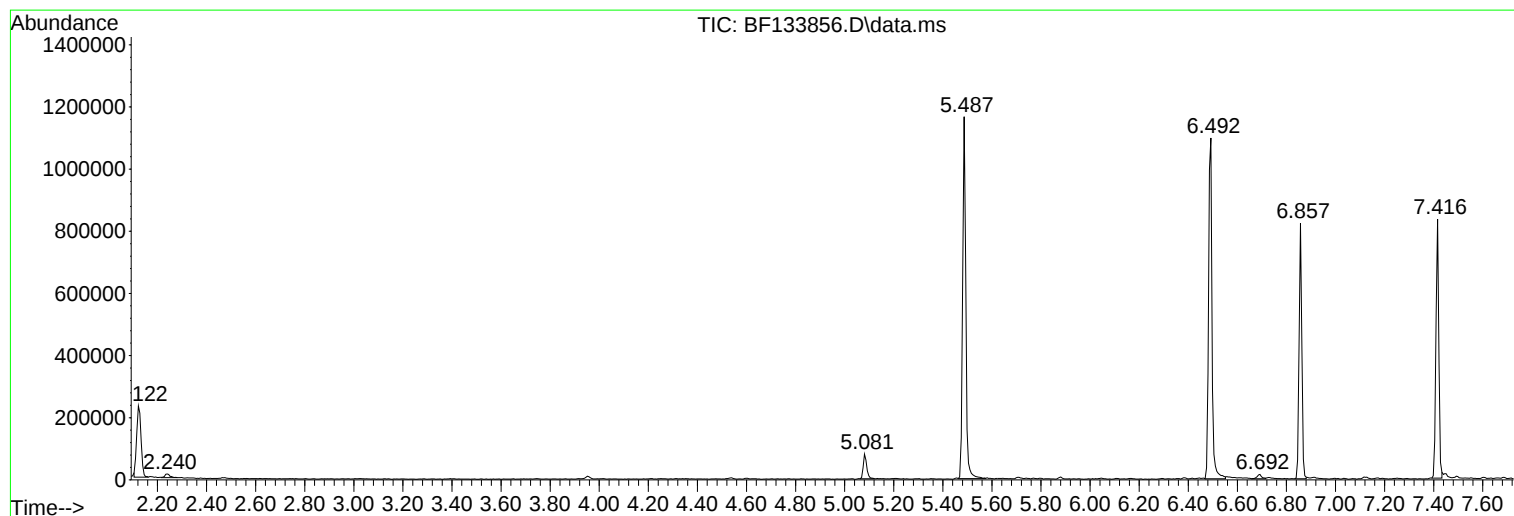
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : 03223-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-04

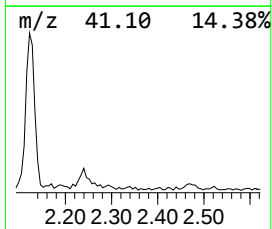
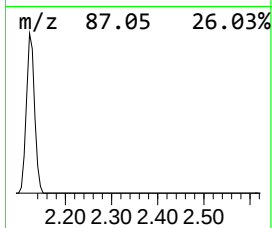
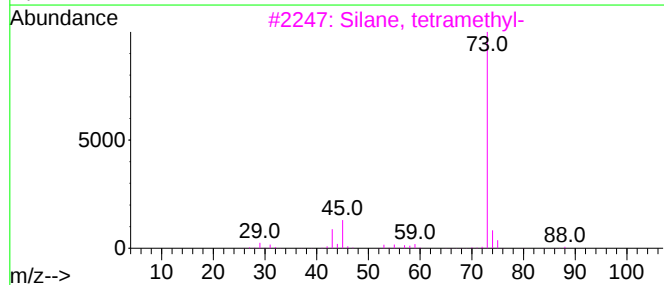
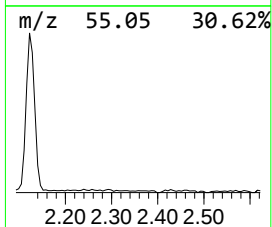
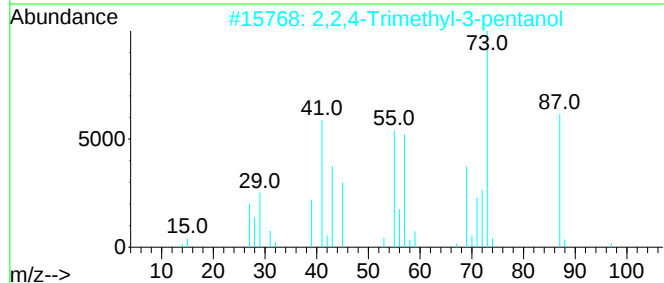
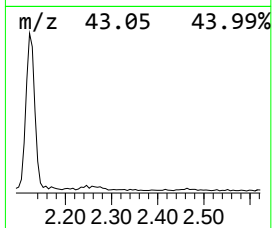
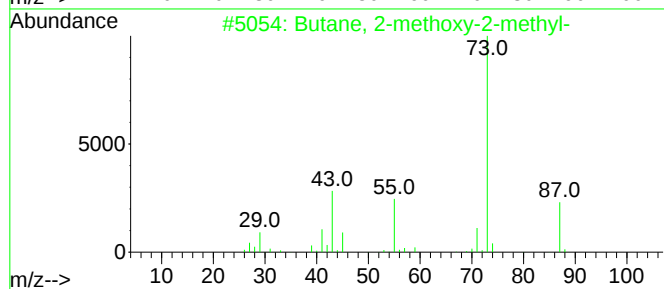
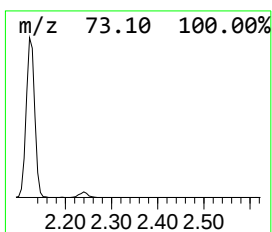
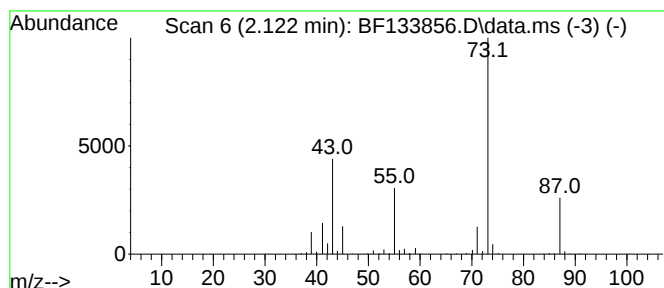
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	8.96 ng	285461	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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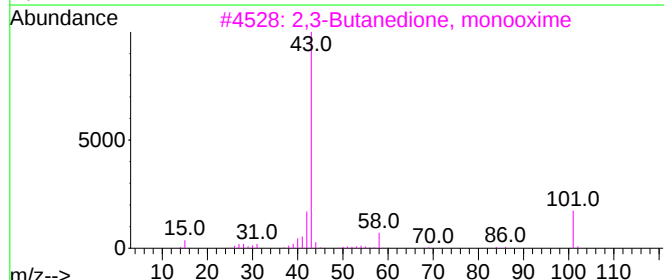
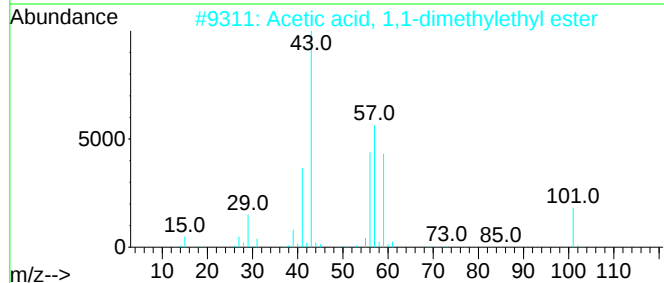
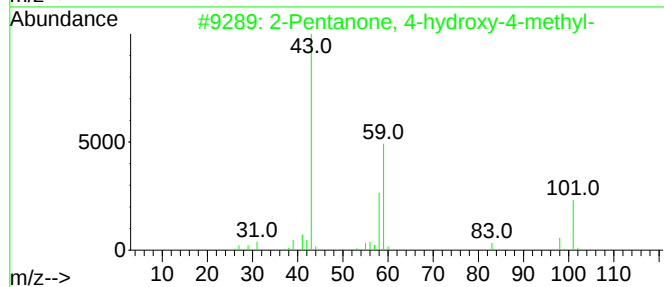
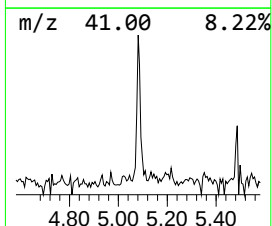
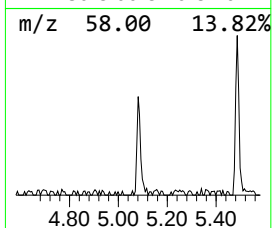
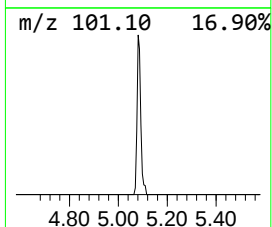
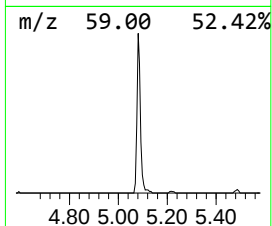
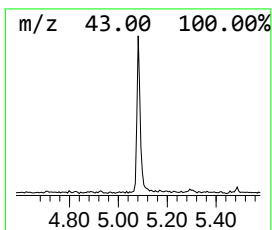
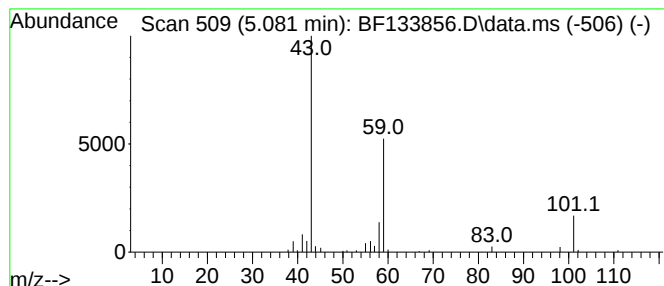
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	2.45 ng	78226	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	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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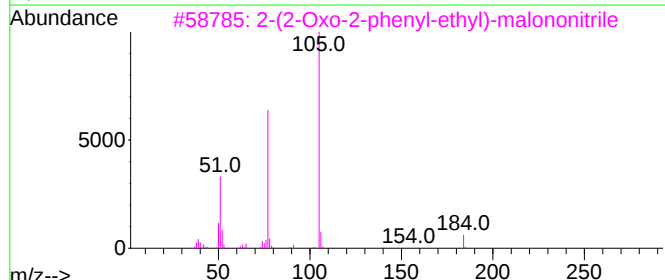
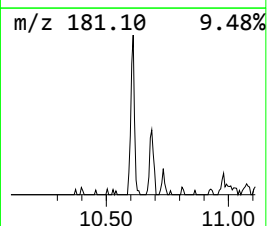
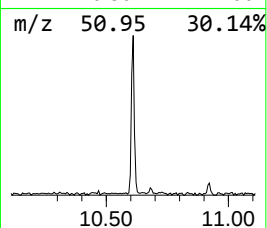
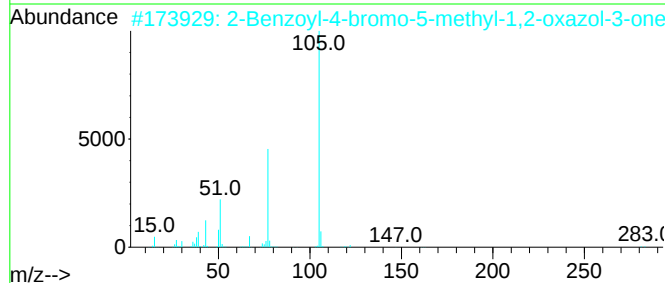
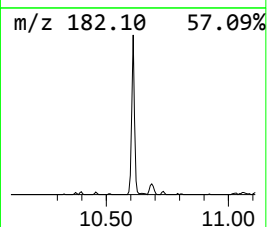
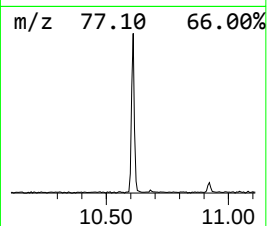
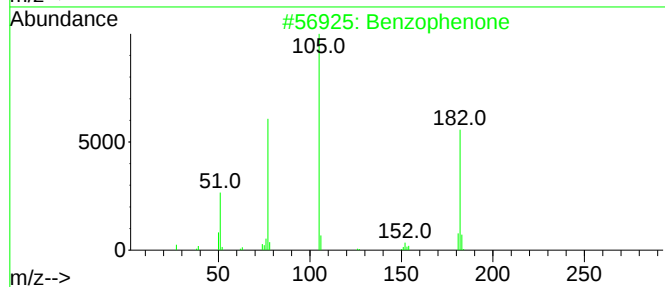
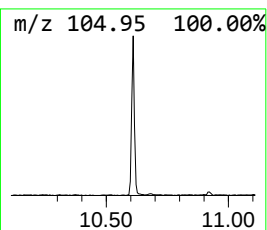
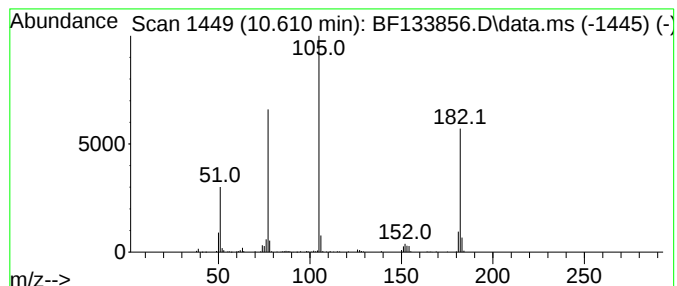
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	5.56 ng	194277	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
3			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
4			Methyl benzilate	242	C15H14O3	000076-89-1	47
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47



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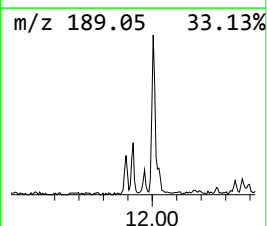
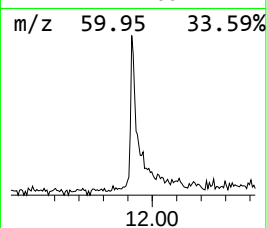
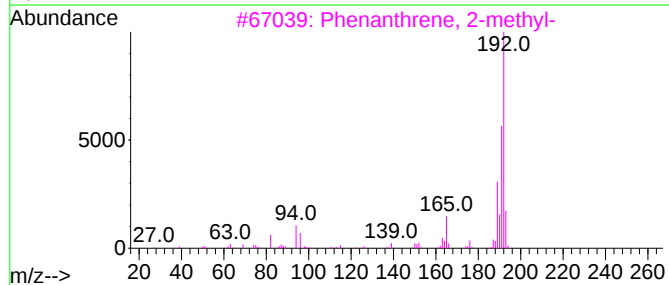
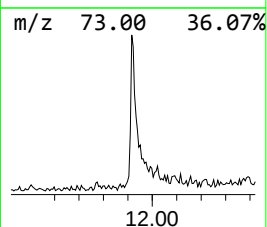
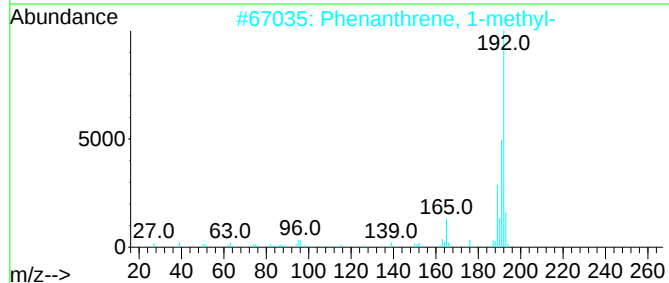
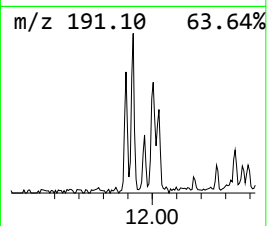
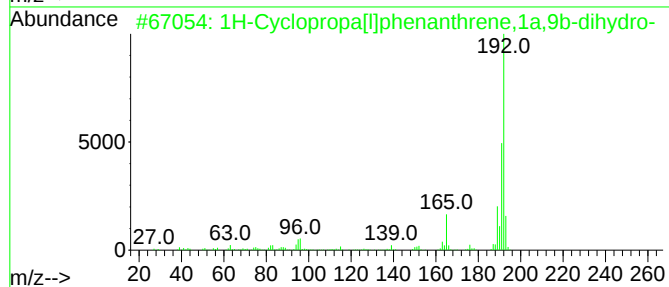
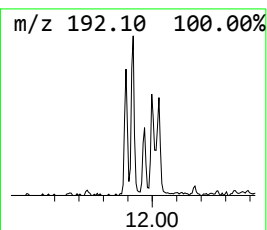
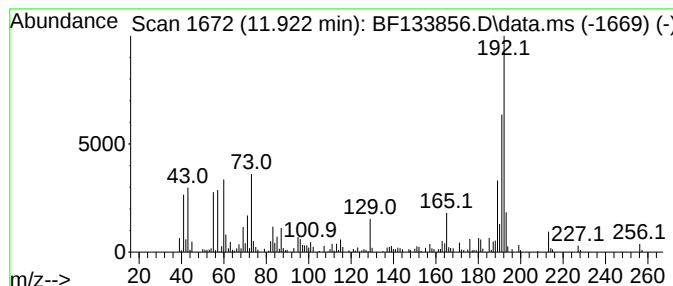
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1H-Cyclopropa[l]phenanthren... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	6.85 ng	193041	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	97
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
4			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	92



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133856.D
Acq On : 20 Jun 2023 15:02
Operator : CG\JU
Sample : 03223-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-SB-04

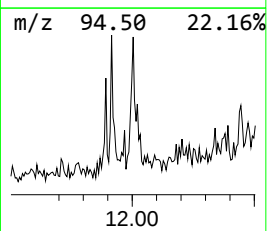
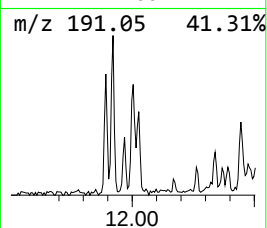
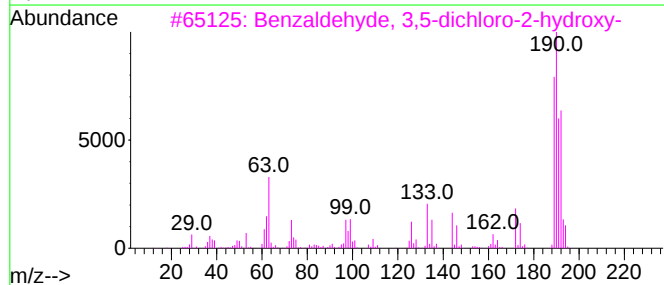
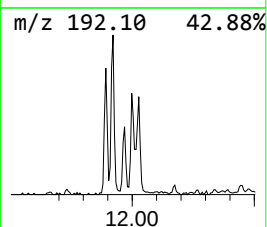
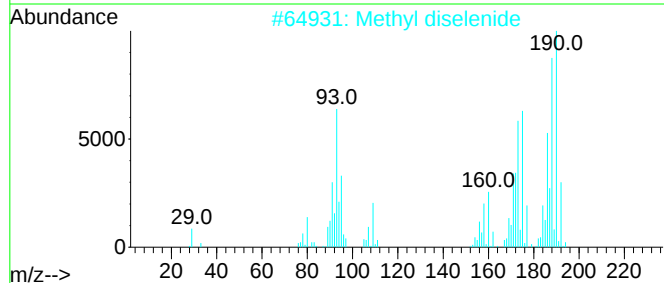
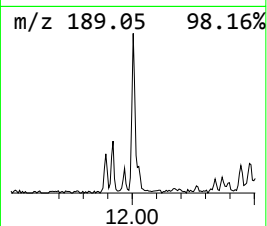
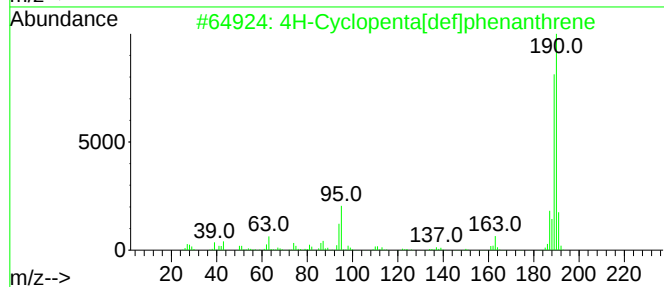
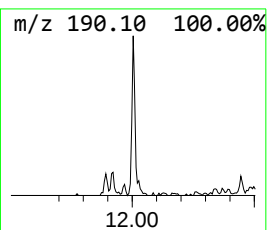
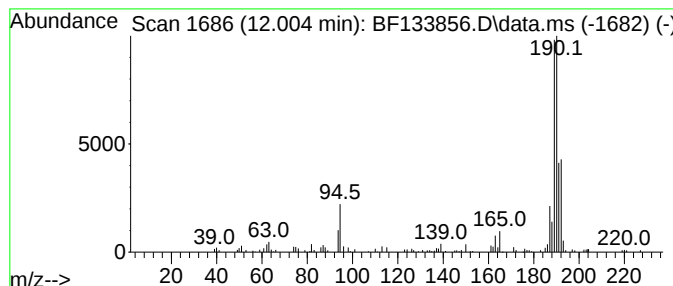
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	3.55 ng	100154	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2			Methyl diselenide	190	C2H6Se2	007101-31-7	43
3			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	33
4			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	27
5			1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133856.D
Acq On : 20 Jun 2023 15:02
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ClientSampleId :
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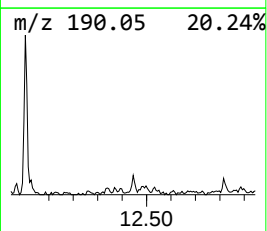
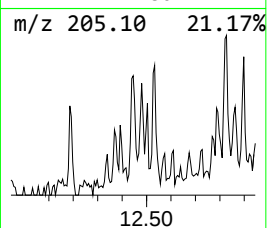
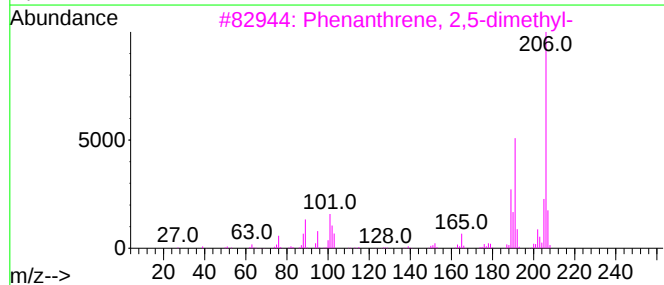
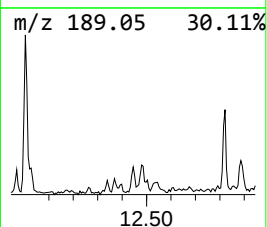
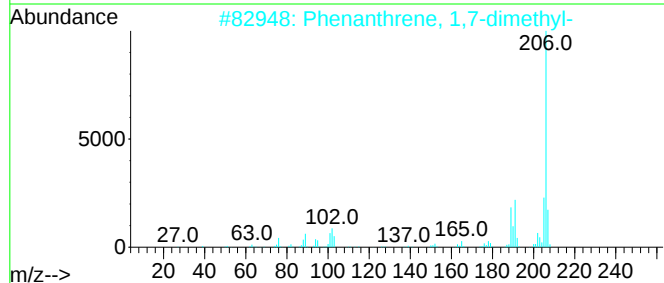
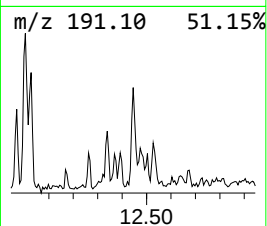
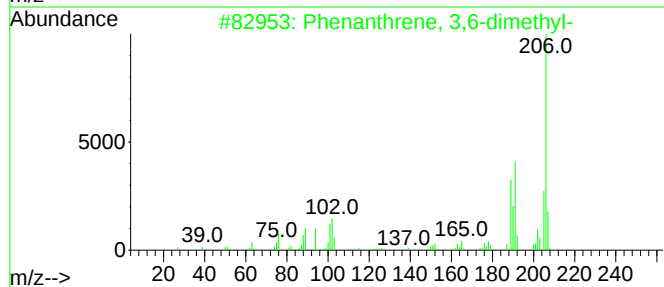
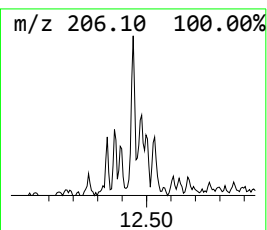
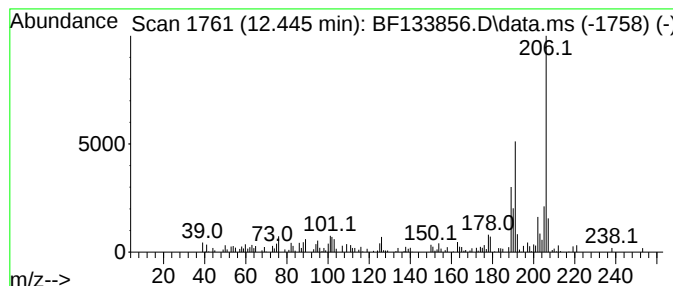
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenanthrene, 3,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	2.06 ng	58177	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
2			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
3			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
4			di-p-Tolylacetylene	206	C16H14	002789-88-0	90
5			9,10-Dimethylanthracene	206	C16H14	000781-43-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133856.D
Acq On : 20 Jun 2023 15:02
Operator : CG\JU
Sample : 03223-01 2X
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ALS Vial : 14 Sample Multiplier: 1

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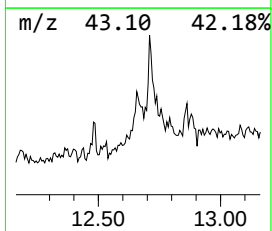
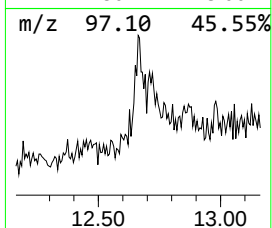
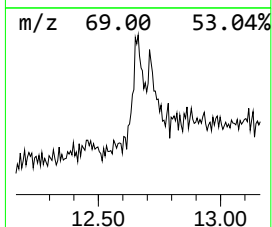
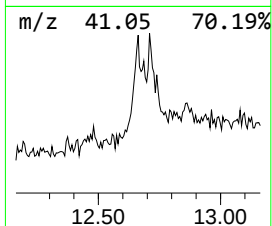
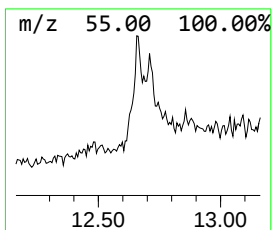
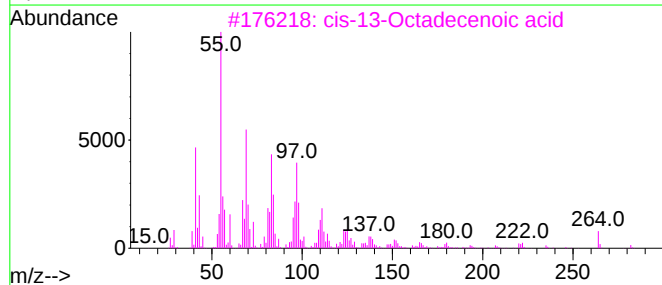
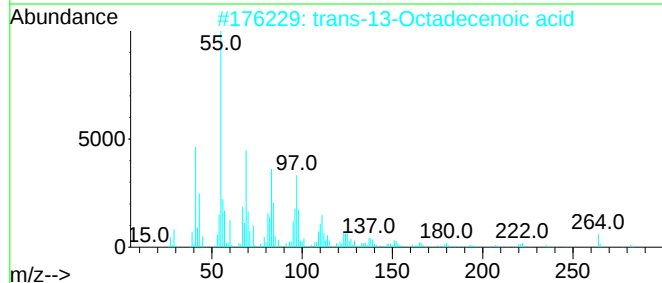
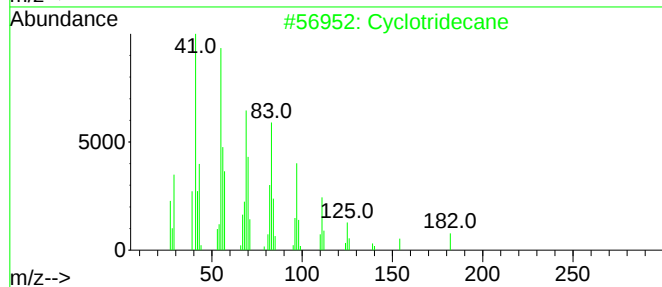
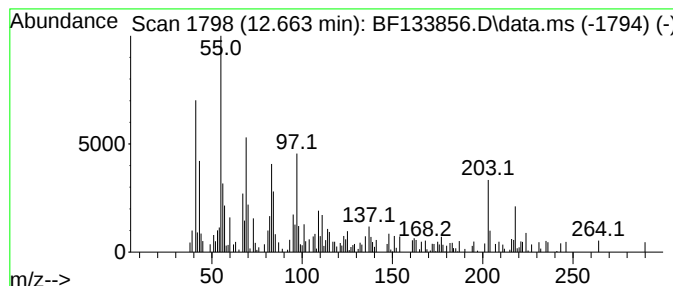
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclotridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	3.16 ng	89175	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotridecane	182	C13H26	000295-02-3	52
2			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	49
3			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	47
4			Z-8-Hexadecene	224	C16H32	1000130-87-5	38
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133856.D
Acq On : 20 Jun 2023 15:02
Operator : CG\JU
Sample : 03223-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSIT-SB-04

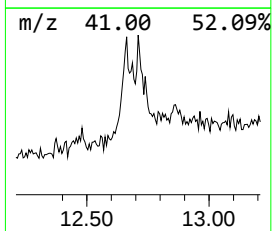
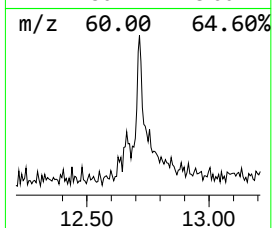
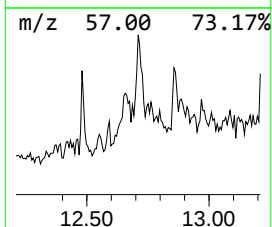
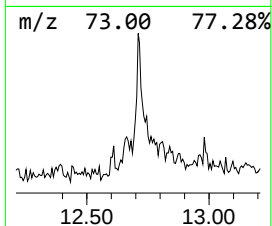
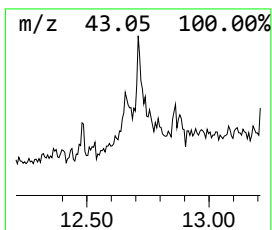
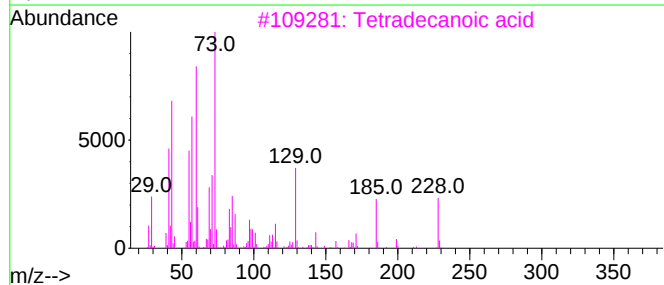
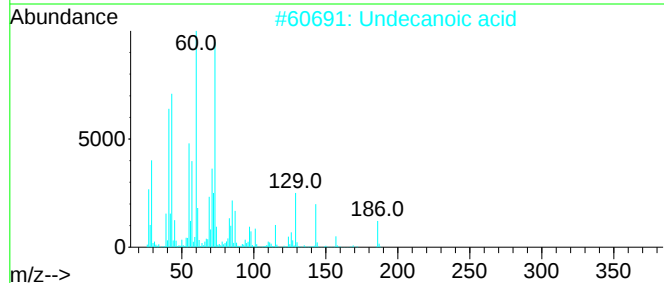
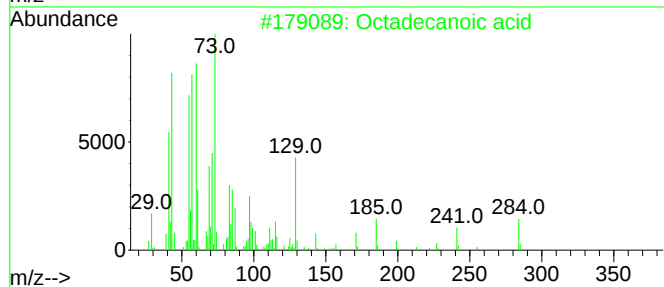
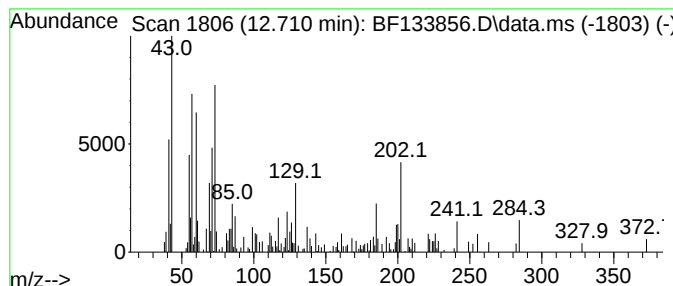
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	2.09 ng	59027	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	86
2			Undecanoic acid	186	C11H22O2	000112-37-8	49
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4			Dodecanoic acid	200	C12H24O2	000143-07-7	46
5			.alpha.-D-Galactopyranoside, met...	306	C15H30O6	1010157-05-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133856.D
Acq On : 20 Jun 2023 15:02
Operator : CG\JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

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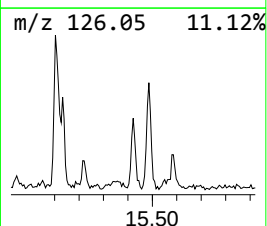
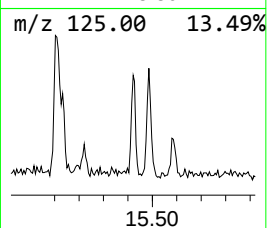
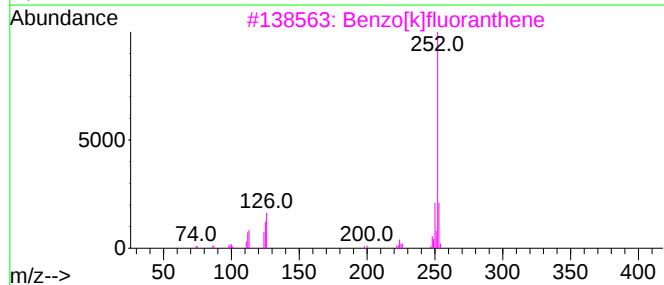
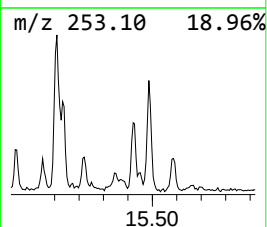
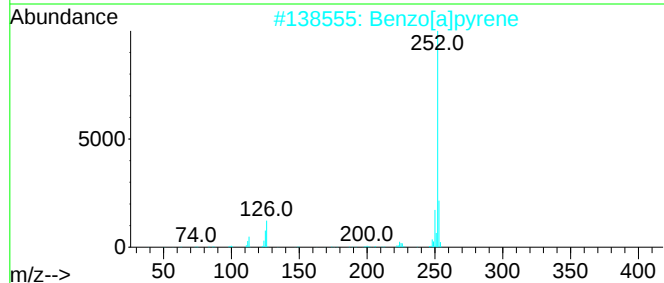
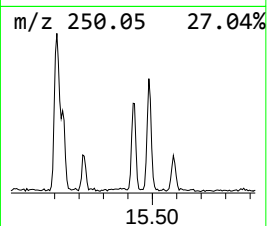
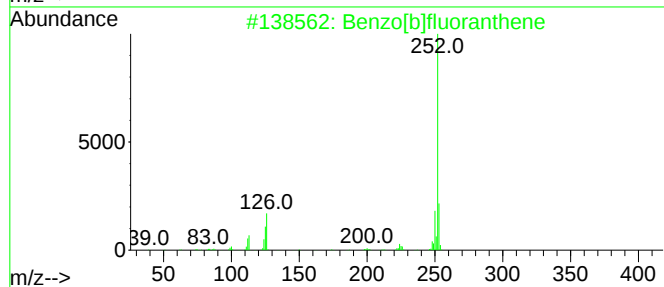
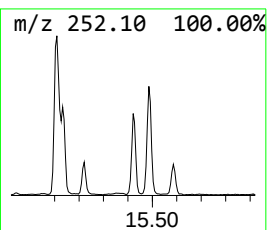
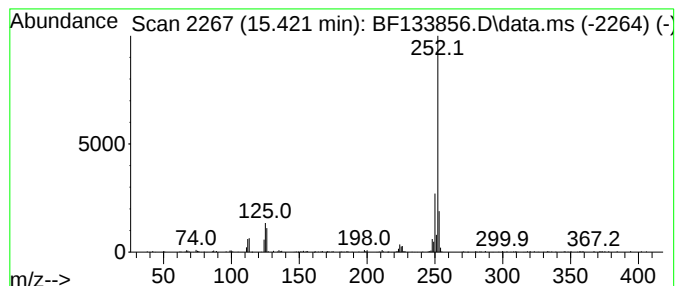
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.421	10.81 ng	211074	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
2			Benzo[a]pyrene	252	C20H12	000050-32-8	96
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4			Benzo[e]pyrene	252	C20H12	000192-97-2	93
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133856.D
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSIT-SB-04

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-...	5.081	2.5	ng	78226	1	6.857	637465	20.0
Benzophenone	10.610	5.6	ng	194277	3	9.892	699412	20.0
1H-Cyclopropa[1...	11.922	6.8	ng	193041	4	11.386	563857	20.0
4H-Cyclopenta[d...	12.004	3.5	ng	100154	4	11.386	563857	20.0
Phenanthrene, 3...	12.445	2.1	ng	58177	4	11.386	563857	20.0
Cyclotridecane	12.663	3.2	ng	89175	4	11.386	563857	20.0
Octadecanoic acid	12.710	2.1	ng	59027	4	11.386	563857	20.0
Benzo[e]pyrene	15.421	10.8	ng	211074	6	15.557	390647	20.0