

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
 Data File : BF136077.D
 Acq On : 01 Nov 2023 15:27
 Operator : CG\JU
 Sample : 05138-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 348

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-BF103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136077.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	10	rVB	509649	500396	16.59%	1.851%
2	3.916	307	311	318	rVB	40284	54318	1.80%	0.201%
3	5.057	497	505	511	rVB	85121	101557	3.37%	0.376%
4	5.422	564	567	568	rBV	63240	50411	1.67%	0.186%
5	5.457	568	573	576	rVB	2700051	2643847	87.66%	9.777%
6	5.675	603	610	614	rBV2	68717	83399	2.77%	0.308%
7	6.457	735	743	746	rBV	2615069	2627682	87.13%	9.718%
8	6.651	772	776	782	rBV2	107549	121392	4.02%	0.449%
9	6.822	801	805	808	rBV	1104865	855325	28.36%	3.163%
10	7.081	845	849	855	rVB2	55353	60604	2.01%	0.224%
11	7.386	896	901	904	rVB	1967856	1704896	56.53%	6.305%
12	8.104	1019	1023	1025	rBV	1417072	1214358	40.26%	4.491%
13	8.122	1025	1026	1030	rVB	747845	479307	15.89%	1.773%
14	8.692	1120	1123	1126	rVB2	34229	33287	1.10%	0.123%
15	8.816	1141	1144	1147	rVB	222754	161603	5.36%	0.598%
16	8.916	1157	1161	1165	rVB	111261	89449	2.97%	0.331%
17	9.180	1202	1206	1210	rBV	3330620	3015982	100.00%	11.154%
18	9.298	1224	1226	1229	rVB	43141	35404	1.17%	0.131%
19	9.445	1248	1251	1255	rVB2	33159	40091	1.33%	0.148%
20	9.516	1261	1263	1266	rBV	37346	41763	1.38%	0.154%
21	9.551	1266	1269	1273	rVV2	140888	149695	4.96%	0.554%
22	9.722	1293	1298	1302	rVB4	49941	59639	1.98%	0.221%
23	9.863	1318	1322	1325	rVB	1529727	1186108	39.33%	4.386%
24	10.069	1353	1357	1360	rBV3	89988	88869	2.95%	0.329%
25	10.104	1360	1363	1366	rVB	45406	34237	1.14%	0.127%
26	10.398	1408	1413	1416	rBV3	54176	61434	2.04%	0.227%
27	10.651	1452	1456	1460	rBV	2093796	1799729	59.67%	6.656%
28	10.780	1474	1478	1485	rBV5	35830	47961	1.59%	0.177%
29	10.880	1492	1495	1499	rBV	28303	32207	1.07%	0.119%
30	10.945	1503	1506	1507	rBV	41737	38788	1.29%	0.143%
31	10.980	1510	1512	1516	rVB3	28192	33398	1.11%	0.124%
32	11.251	1556	1558	1565	rVB3	20089	34522	1.14%	0.128%
33	11.351	1572	1575	1578	rBV	1178419	1112035	36.87%	4.112%
34	11.374	1578	1579	1583	rVV	243823	163829	5.43%	0.606%
35	11.427	1586	1588	1591	rVB	49705	37534	1.24%	0.139%
36	11.857	1658	1661	1663	rBV	85843	72879	2.42%	0.270%

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37	11.892	1663	1667	1671	rVV2	509294	543500	18.02%	2.010%
38	11.969	1676	1680	1682	rVV	135147	150970	5.01%	0.558%
39	11.992	1682	1684	1689	rVB	92715	76268	2.53%	0.282%
40	12.157	1709	1712	1714	rBV	52652	48865	1.62%	0.181%
41	12.410	1752	1755	1758	rBV	92598	89391	2.96%	0.331%
42	12.445	1758	1761	1763	rVV2	47886	53675	1.78%	0.198%
43	12.492	1767	1769	1774	rBV3	60340	71360	2.37%	0.264%
44	12.574	1779	1783	1786	rBV	338446	309125	10.25%	1.143%
45	12.686	1798	1802	1807	rBV3	201339	223554	7.41%	0.827%
46	12.804	1816	1822	1824	rBV	411402	404292	13.40%	1.495%
47	12.957	1843	1848	1851	rBV	2527218	2316121	76.79%	8.565%
48	13.021	1856	1859	1862	rBV	62922	82851	2.75%	0.306%
49	13.115	1872	1875	1876	rBV3	30868	36867	1.22%	0.136%
50	13.198	1886	1889	1892	rVB2	55494	56512	1.87%	0.209%
51	13.239	1892	1896	1899	rBV2	90604	85179	2.82%	0.315%
52	13.333	1909	1912	1914	rVB	67160	58222	1.93%	0.215%
53	13.363	1914	1917	1921	rVB	72516	58760	1.95%	0.217%
54	13.539	1945	1947	1950	rVB3	51039	47938	1.59%	0.177%
55	13.639	1962	1964	1973	rVB	52245	58938	1.95%	0.218%
56	13.751	1980	1983	1987	rBV2	57385	92163	3.06%	0.341%
57	13.786	1987	1989	1991	rVV	61576	56664	1.88%	0.210%
58	13.810	1991	1993	1997	rVV3	55898	61251	2.03%	0.227%
59	13.874	2001	2004	2011	rVB2	134260	187735	6.22%	0.694%
60	14.010	2022	2027	2030	rBV3	1079082	1176793	39.02%	4.352%
61	14.033	2030	2031	2037	rVB	216628	196257	6.51%	0.726%
62	14.192	2056	2058	2061	rVB2	48559	39335	1.30%	0.145%
63	14.398	2091	2093	2097	rVB	65209	62575	2.07%	0.231%
64	14.433	2097	2099	2103	rVB	56355	48360	1.60%	0.179%
65	14.498	2108	2110	2112	rBV2	42047	34185	1.13%	0.126%
66	14.657	2135	2137	2142	rVB2	45479	52471	1.74%	0.194%
67	14.815	2162	2164	2171	rVB2	45247	62358	2.07%	0.231%
68	15.062	2202	2206	2209	rBV2	141245	209373	6.94%	0.774%
69	15.168	2222	2224	2228	rVB	63796	73041	2.42%	0.270%
70	15.374	2255	2259	2265	rVB	102883	119550	3.96%	0.442%
71	15.433	2266	2269	2276	rBV	114109	144629	4.80%	0.535%
72	15.504	2276	2281	2285	rBV	688343	783540	25.98%	2.898%

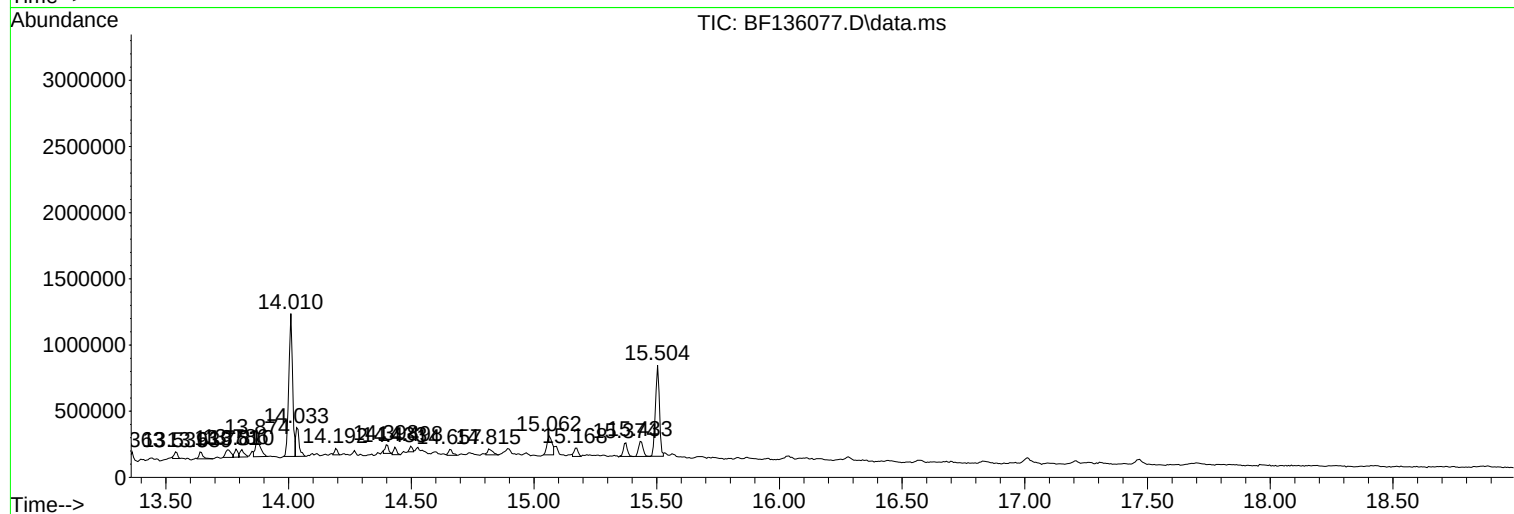
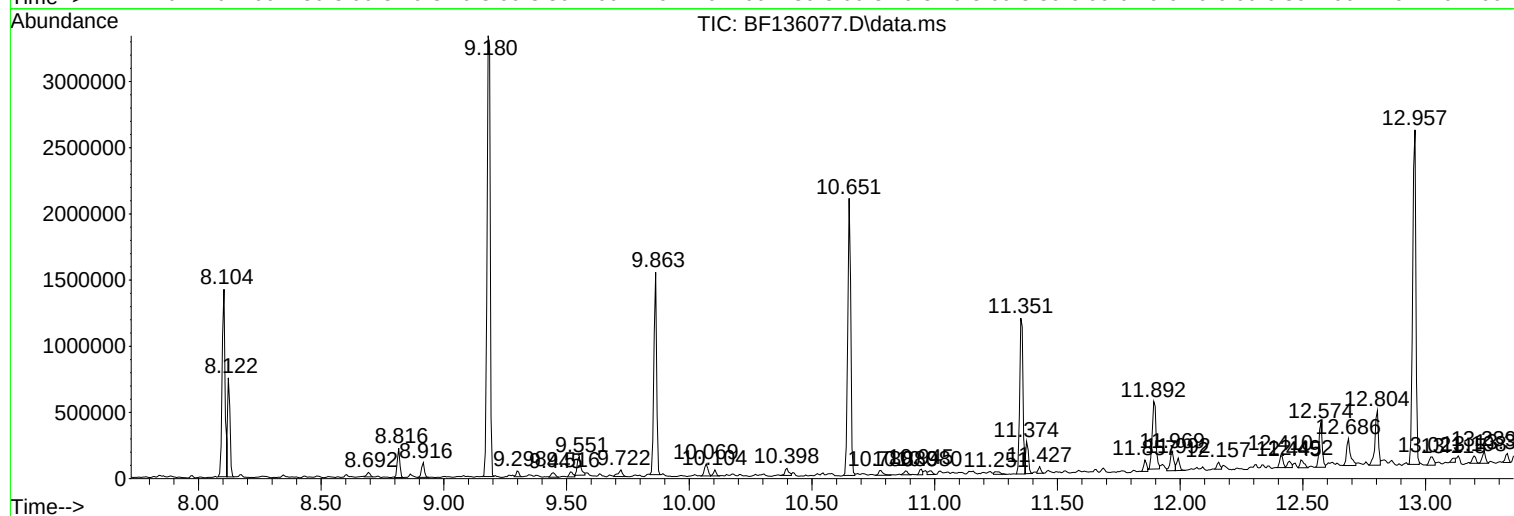
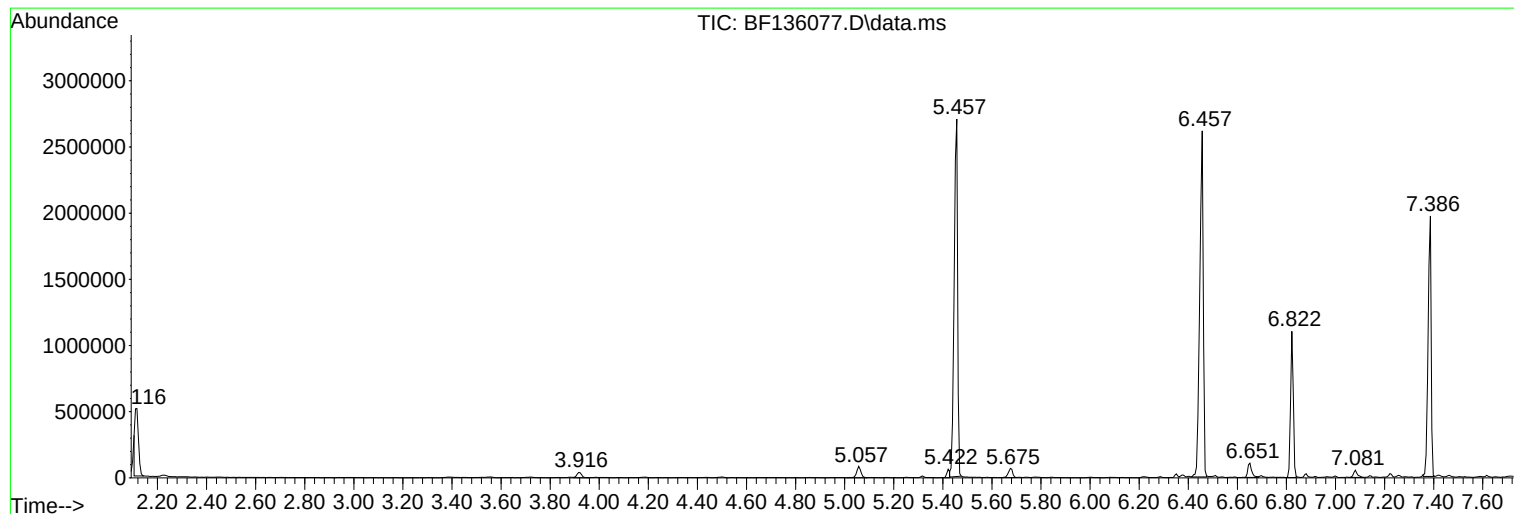
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
Data File : BF136077.D
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Operator : CG\JU
Sample : 05138-01
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Instrument :
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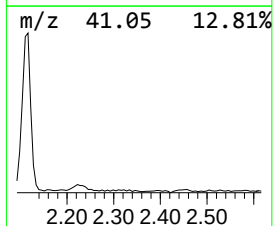
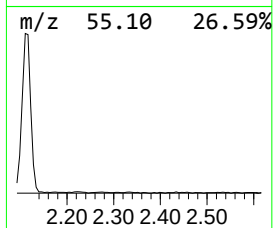
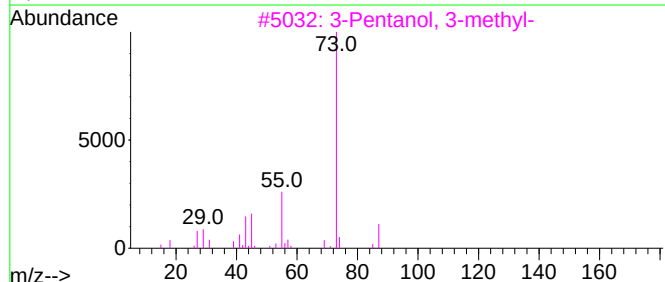
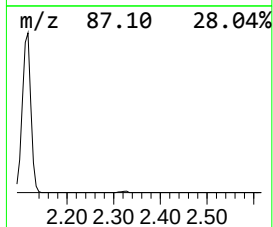
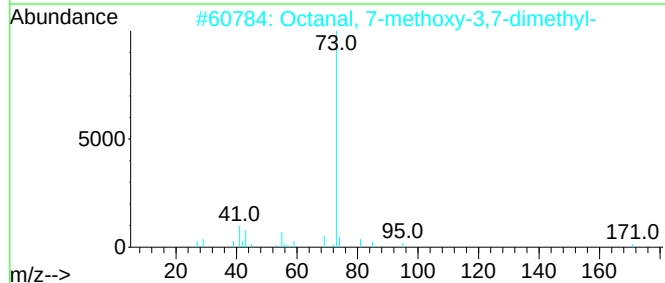
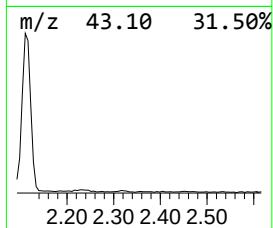
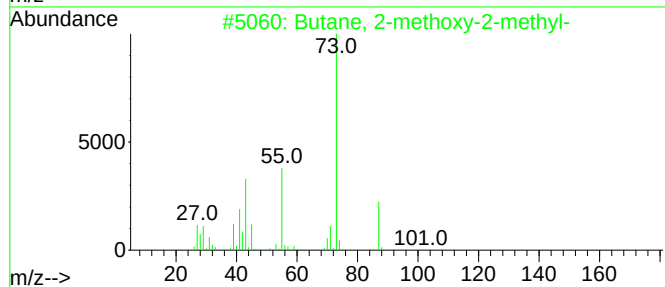
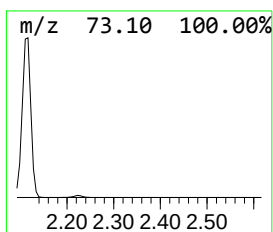
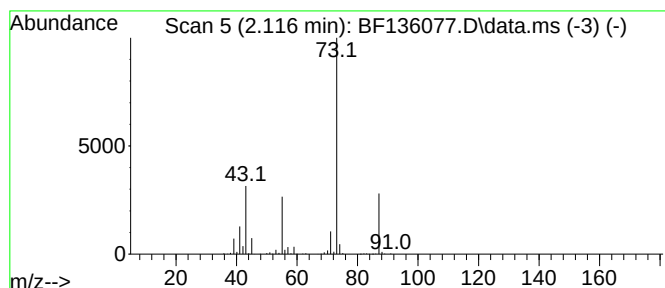
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.116	11.70 ng	500396	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	25
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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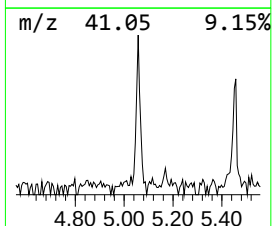
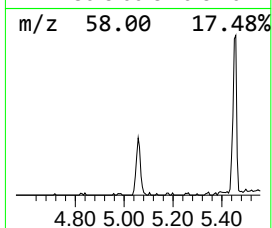
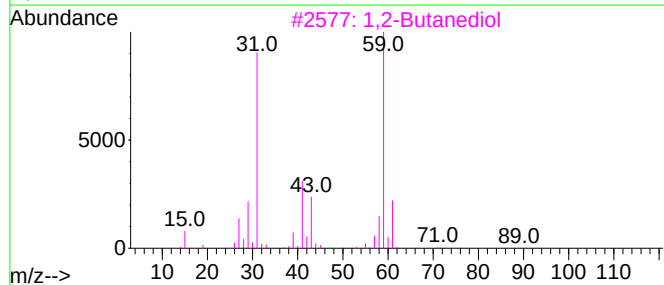
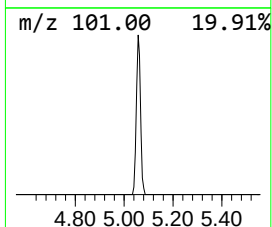
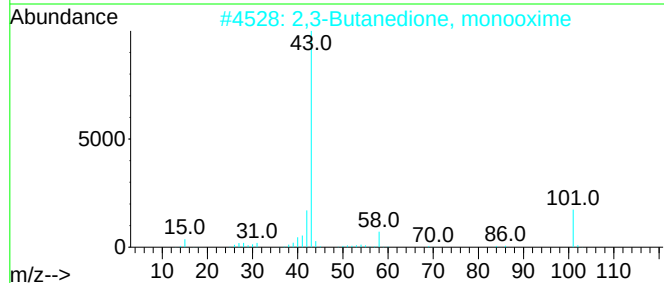
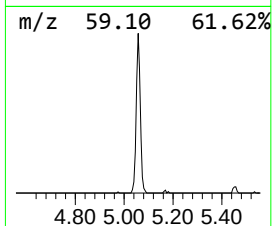
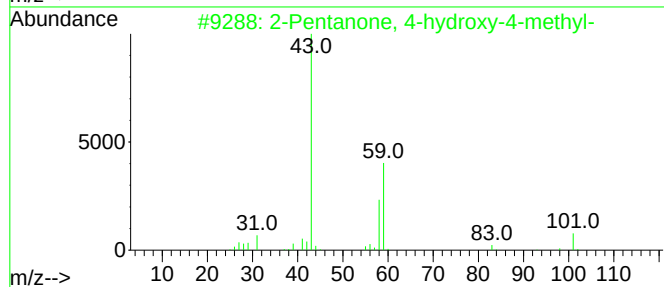
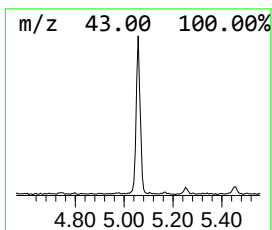
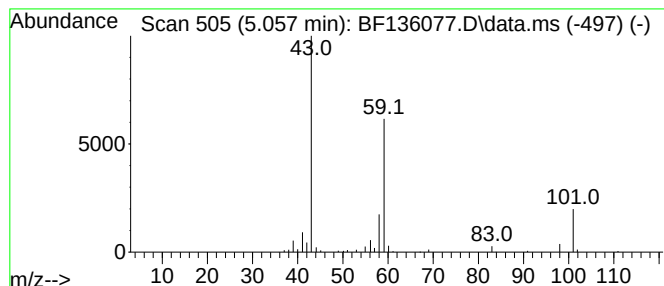
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	2.37 ng	101557	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	1,2-Butanediol	90	C4H10O2	000584-03-2	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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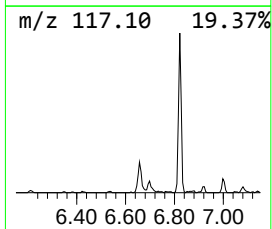
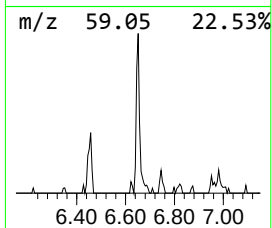
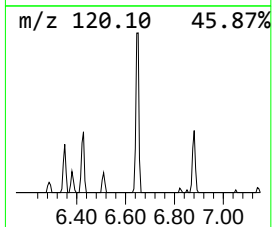
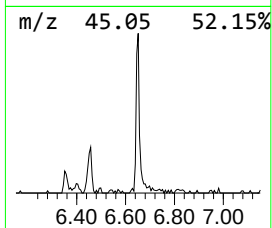
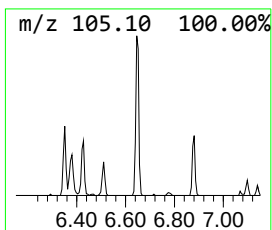
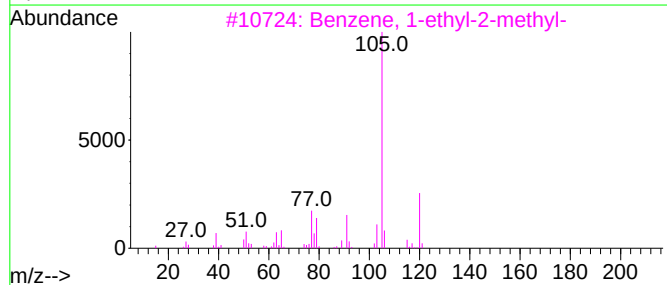
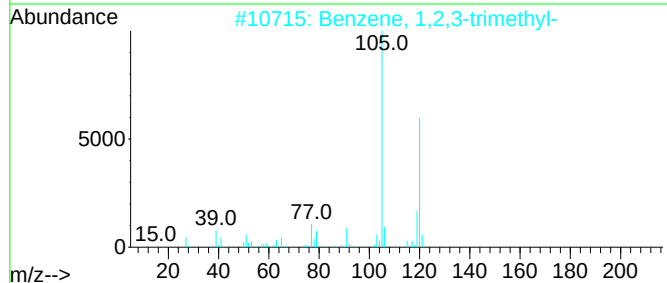
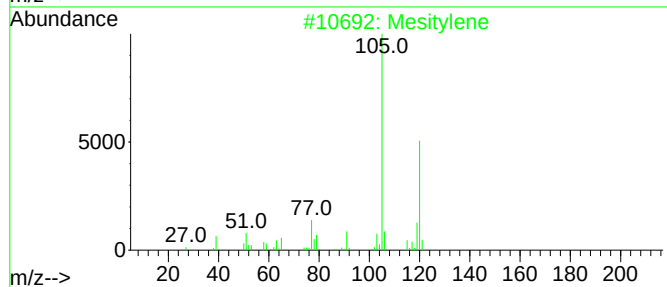
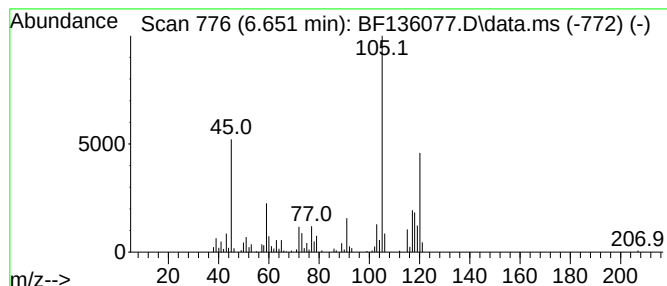
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.651 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.651	2.84 ng	121392	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	46
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	46
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	42
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	42
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	41



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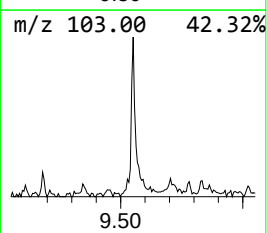
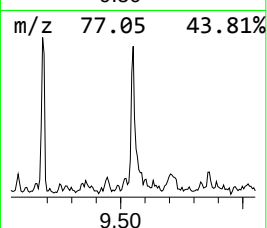
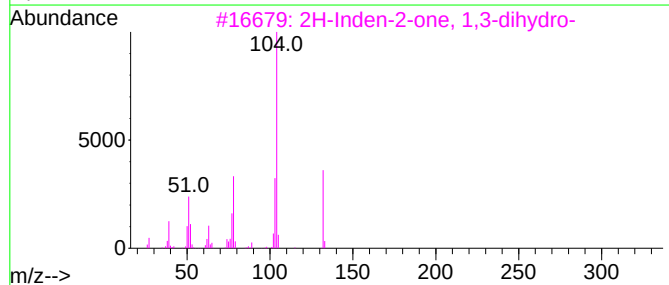
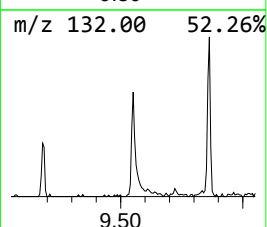
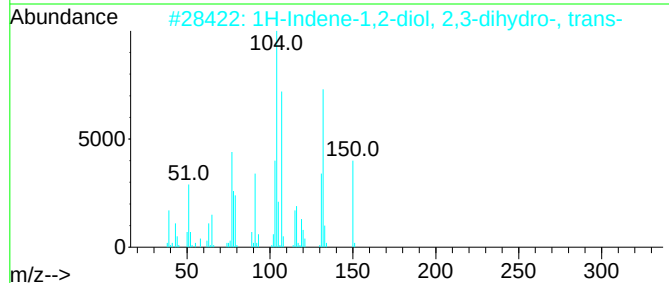
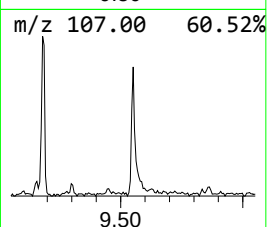
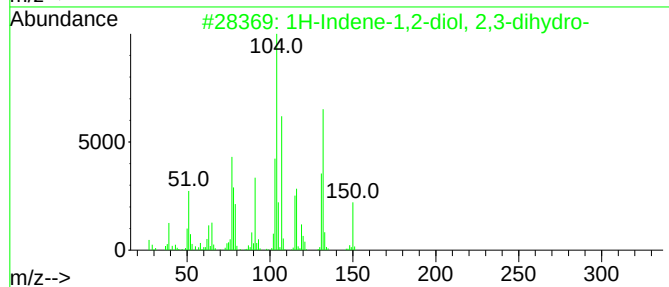
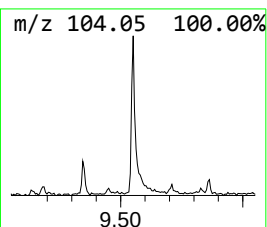
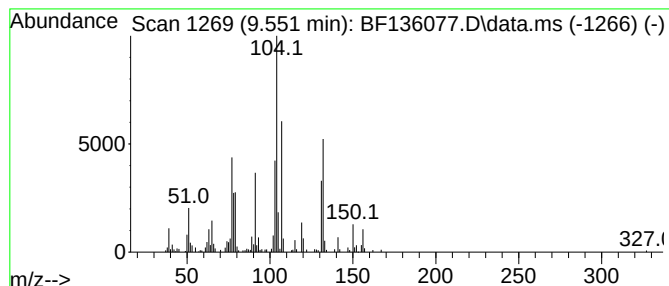
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1H-Indene-1,2-diol, 2,3-dih... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.551	2.52 ng	149695	Acenaphthene-d10	9.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene-1,2-diol, 2,3-dihydro-	150	C9H10O2	004370-02-9	93
2		1H-Indene-1,2-diol, 2,3-dihydro-...	150	C9H10O2	004647-43-2	90
3		2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	55
4		1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	53
5		Indan, epoxide	132	C9H8O	000768-22-9	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
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Acq On : 01 Nov 2023 15:27
Operator : CG\JU
Sample : 05138-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

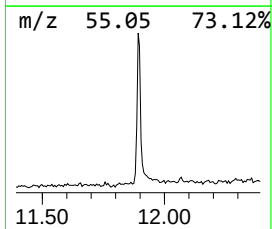
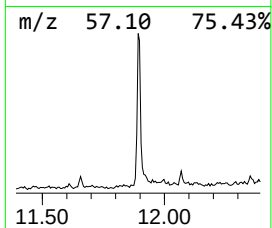
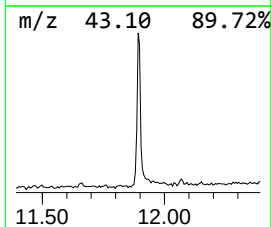
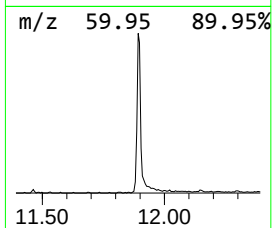
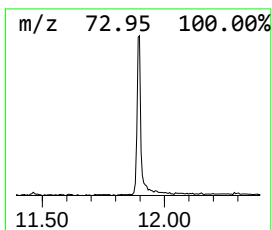
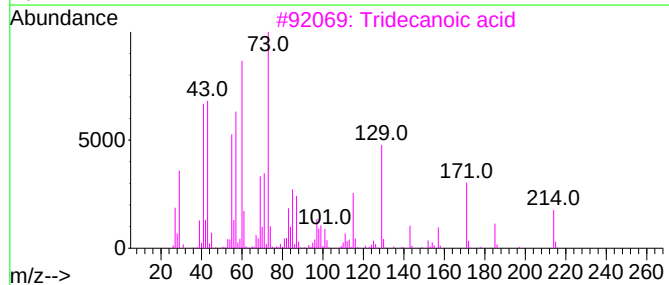
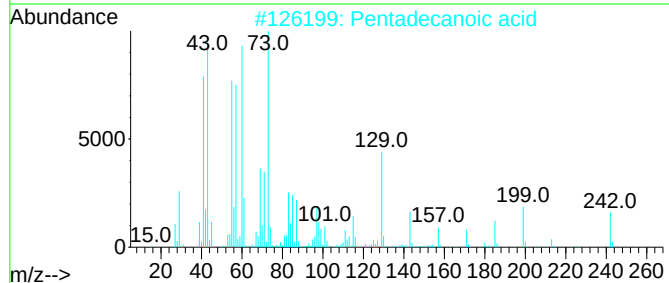
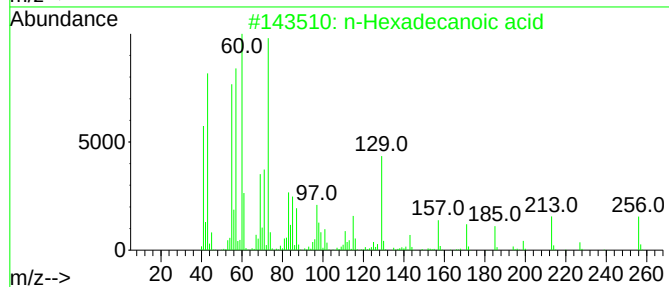
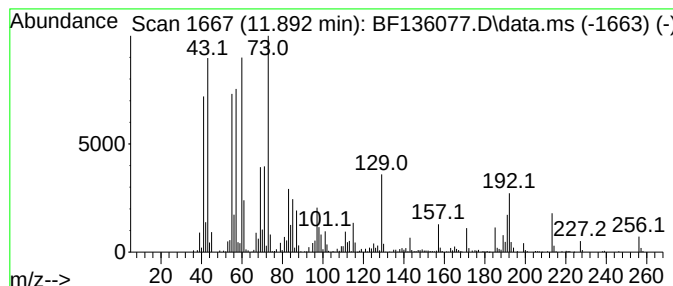
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.892	9.77 ng	543500	Phenanthrene-d10	11.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
Data File : BF136077.D
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Sample : 05138-01
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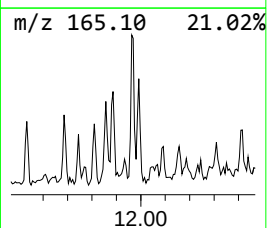
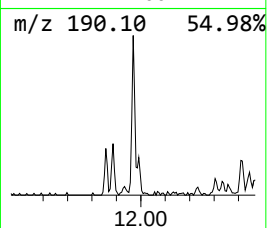
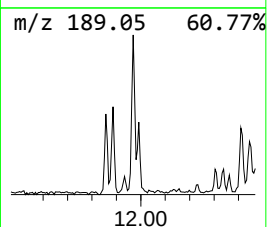
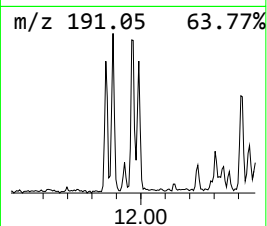
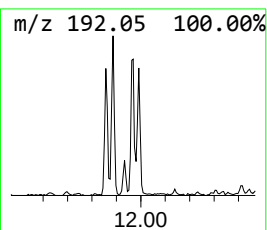
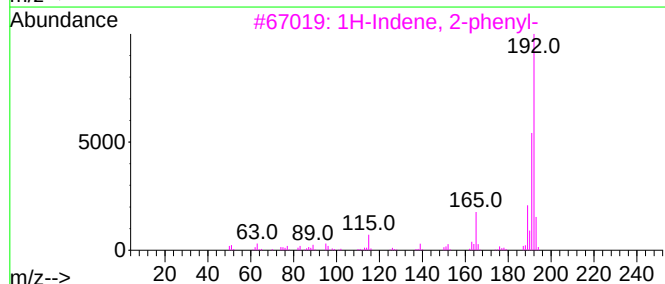
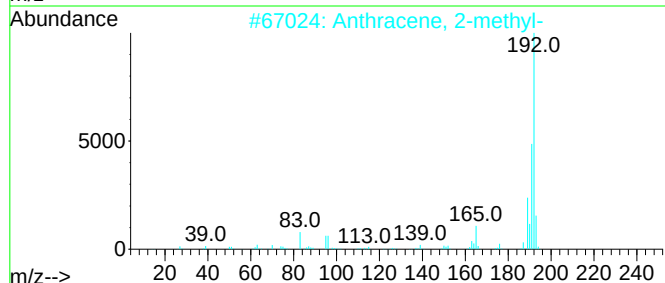
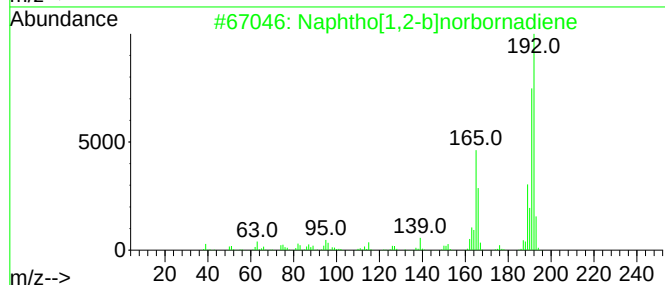
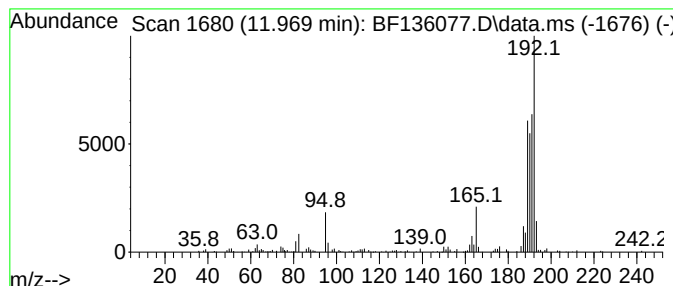
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Naphtho[1,2-b]norbornadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.969	2.72 ng	150970	Phenanthrene-d10	11.351	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	64
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	60
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	60
5	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
Data File : BF136077.D
Acq On : 01 Nov 2023 15:27
Operator : CG\JU
Sample : 05138-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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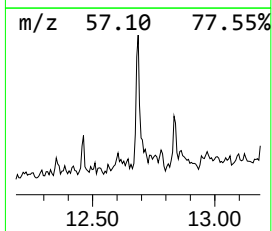
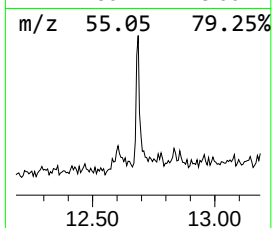
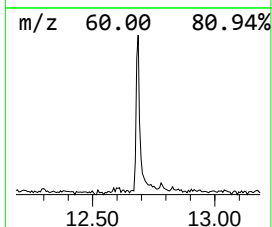
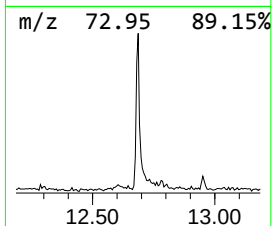
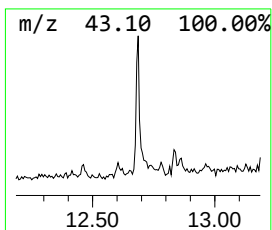
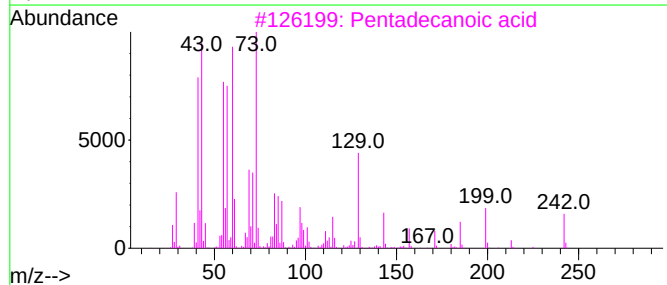
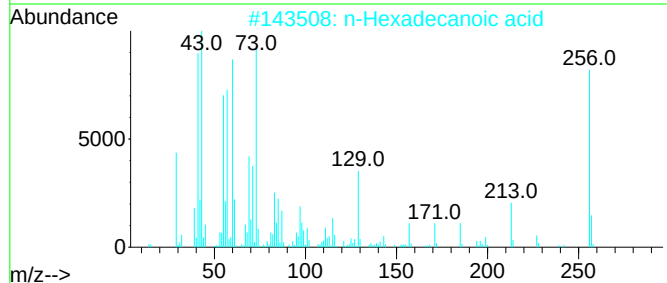
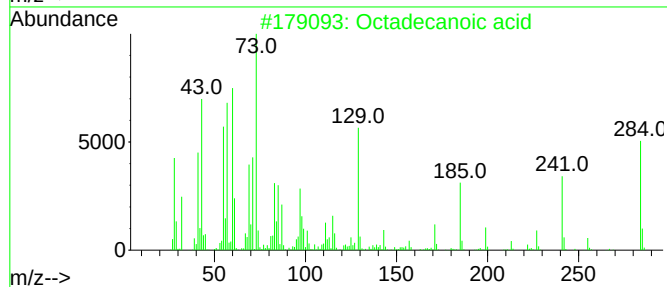
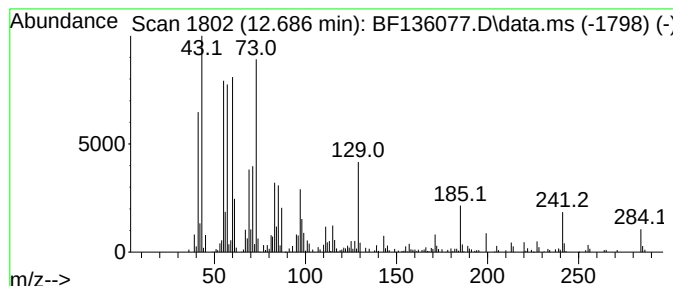
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	3.80 ng	223554	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
Data File : BF136077.D
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Operator : CG\JU
Sample : 05138-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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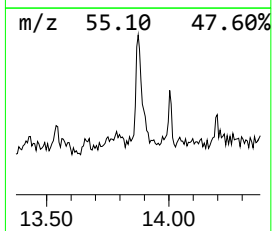
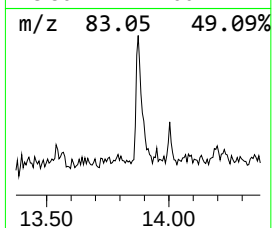
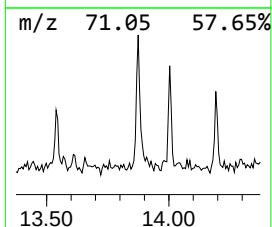
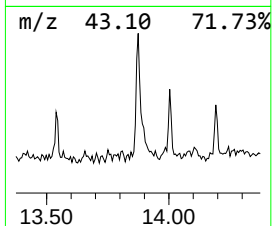
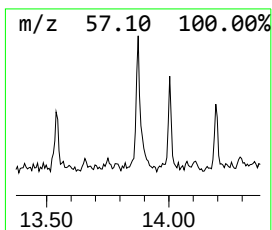
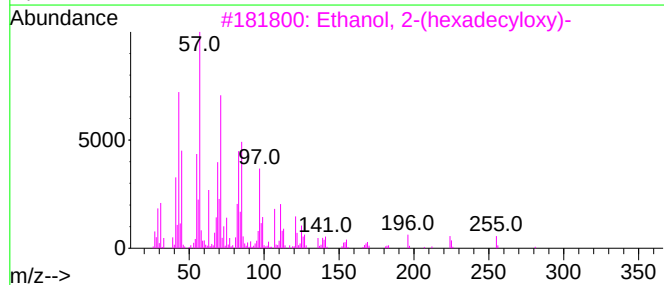
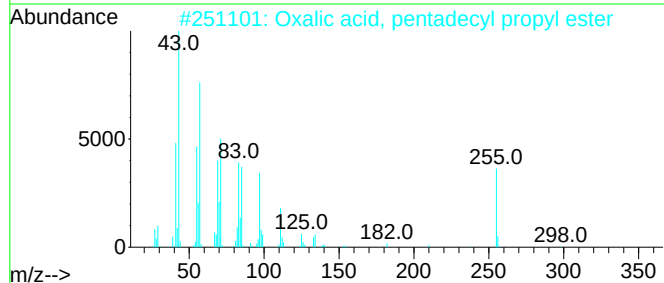
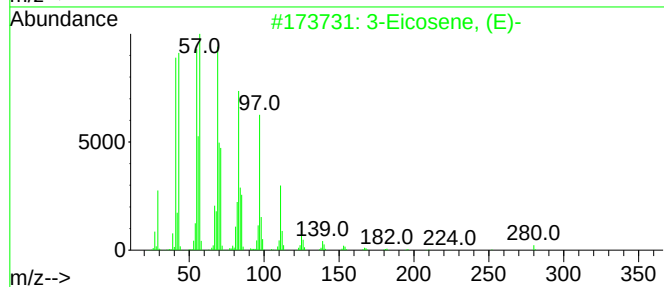
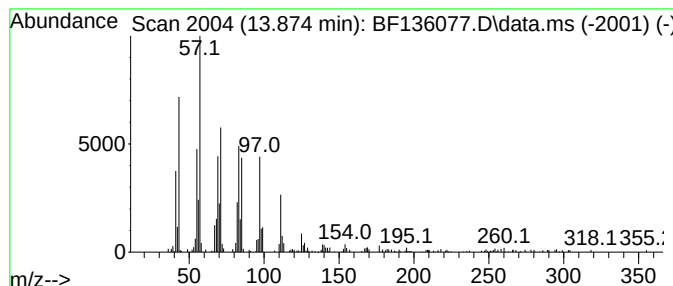
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.19 ng	187735	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	92
2			Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	91
3			Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
4			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
5			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
Data File : BF136077.D
Acq On : 01 Nov 2023 15:27
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Sample : 05138-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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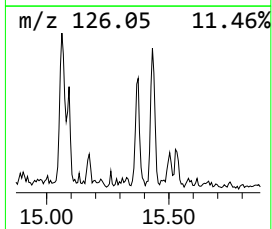
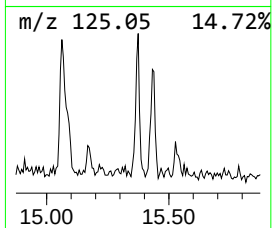
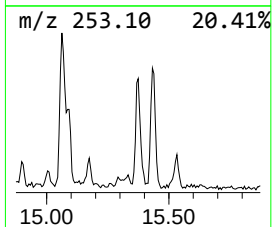
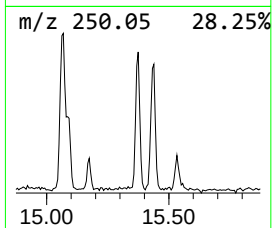
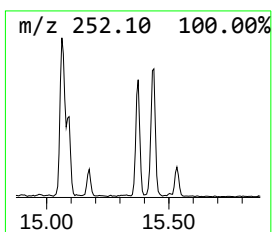
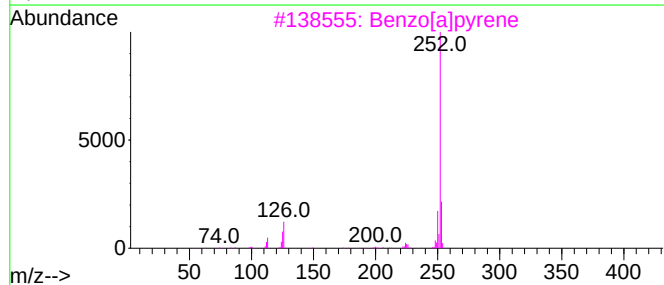
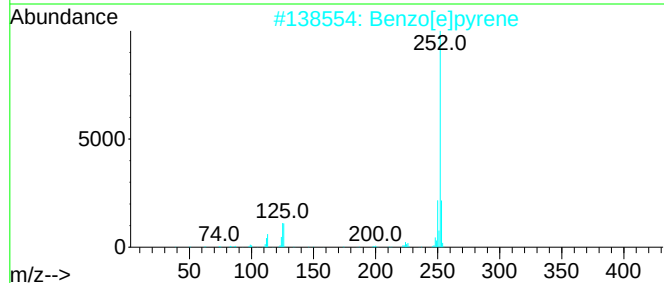
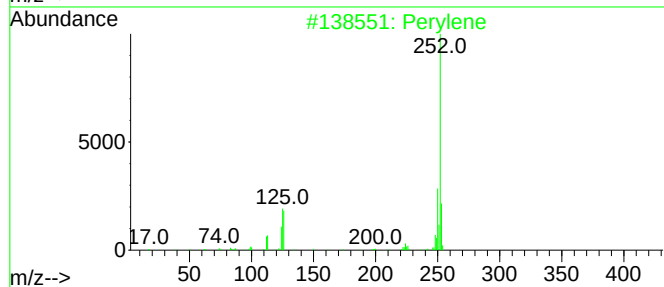
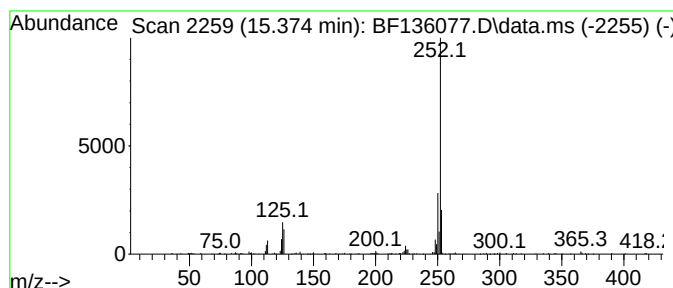
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	3.05 ng	119550	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	96
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	93
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
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Operator : CG\JU
Sample : 05138-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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-...	5.057	2.4	ng	101557	1	6.822	855325	20.0
unknown6.651	6.651	2.8	ng	121392	1	6.822	855325	20.0
1H-Indene-1,2-d...	9.551	2.5	ng	149695	3	9.863	1186110	20.0
n-Hexadecanoic ...	11.892	9.8	ng	543500	4	11.351	1112040	20.0
Naphtho[1,2-b]n...	11.969	2.7	ng	150970	4	11.351	1112040	20.0
Octadecanoic acid	12.686	3.8	ng	223554	5	14.010	1176790	20.0
3-Eicosene, (E)-	13.874	3.2	ng	187735	5	14.010	1176790	20.0
Perylene	15.374	3.0	ng	119550	6	15.504	783540	20.0