

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
 Data File : BF137073.D
 Acq On : 15 Jan 2024 20:05
 Operator : CG\JU
 Sample : P1140-01 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-309-0-2

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137073.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	4	7	13	rVB5	5395	7893	1.21%	0.124%
2	5.004	493	496	508	rBV	27102	31962	4.90%	0.501%
3	5.428	565	568	584	rBV	401122	412942	63.30%	6.476%
4	6.434	736	739	757	rBV	340238	383268	58.75%	6.011%
5	6.781	795	798	802	rBV	253386	213808	32.77%	3.353%
6	7.345	890	894	905	rBV	262298	242936	37.24%	3.810%
7	8.057	1012	1015	1024	rBV	281757	244885	37.54%	3.841%
8	9.134	1195	1198	1201	rBV	623206	467061	71.59%	7.325%
9	9.210	1208	1211	1215	rBV	13991	12045	1.85%	0.189%
10	9.681	1288	1291	1294	rBV	12682	11442	1.75%	0.179%
11	9.745	1299	1302	1304	rBV	20269	15204	2.33%	0.238%
12	9.816	1310	1314	1318	rBV	331376	264570	40.55%	4.149%
13	10.245	1384	1387	1389	rVB	12885	9357	1.43%	0.147%
14	10.369	1404	1408	1412	rVB	8253	8113	1.24%	0.127%
15	10.610	1446	1449	1462	rVB	314809	287349	44.05%	4.507%
16	10.722	1465	1468	1474	rBV4	7890	14201	2.18%	0.223%
17	10.792	1477	1480	1482	rBV	7317	7512	1.15%	0.118%
18	10.828	1482	1486	1489	rVB3	6867	9250	1.42%	0.145%
19	10.980	1508	1512	1515	rBV4	6596	9210	1.41%	0.144%
20	11.051	1522	1524	1532	rVB5	5716	8162	1.25%	0.128%
21	11.204	1546	1550	1555	rVB4	6478	8451	1.30%	0.133%
22	11.310	1564	1568	1570	rBV	397678	311728	47.78%	4.889%
23	11.333	1570	1572	1576	rVV	105425	83541	12.81%	1.310%
24	11.386	1578	1581	1584	rVB	21527	18221	2.79%	0.286%
25	11.810	1650	1653	1656	rBV2	42419	54086	8.29%	0.848%
26	11.845	1656	1659	1665	rVV2	110605	132082	20.25%	2.071%
27	11.892	1665	1667	1670	rVV	13729	14044	2.15%	0.220%
28	11.927	1670	1673	1675	rVV	33500	33243	5.10%	0.521%
29	11.951	1675	1677	1681	rVB2	12614	10981	1.68%	0.172%
30	12.110	1702	1704	1708	rBV	13763	11894	1.82%	0.187%
31	12.145	1708	1710	1714	rVB3	9408	8849	1.36%	0.139%
32	12.263	1725	1730	1733	rBV5	5026	8518	1.31%	0.134%
33	12.369	1744	1748	1750	rBV	15999	15729	2.41%	0.247%
34	12.404	1750	1754	1756	rVV5	9170	10904	1.67%	0.171%
35	12.457	1760	1763	1767	rVB4	10125	12040	1.85%	0.189%
36	12.533	1770	1776	1779	rBV	204939	201638	30.91%	3.162%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.569	1779	1782	1785	rVB5	7305	9819	1.51%	0.154%
38	12.633	1790	1793	1798	rBV2	22280	28687	4.40%	0.450%
39	12.716	1805	1807	1809	rVB	12591	8251	1.26%	0.129%
40	12.763	1809	1815	1821	rVV	200344	200601	30.75%	3.146%

41	12.816	1821	1824	1827	rVB3	9204	9740	1.49%	0.153%
42	12.904	1835	1839	1842	rBV	762743	652378	100.00%	10.232%
43	12.927	1842	1843	1848	rVB	26001	16690	2.56%	0.262%
44	12.980	1848	1852	1856	rBV3	17844	28435	4.36%	0.446%
45	13.069	1864	1867	1868	rBV2	16243	15662	2.40%	0.246%

46	13.092	1868	1871	1874	rVB2	35004	36868	5.65%	0.578%
47	13.133	1874	1878	1880	rBV2	11009	12338	1.89%	0.194%
48	13.157	1880	1882	1885	rVV	24671	19532	2.99%	0.306%
49	13.198	1885	1889	1892	rVV2	23230	24081	3.69%	0.378%
50	13.292	1902	1905	1908	rBV2	16715	13097	2.01%	0.205%

51	13.321	1908	1910	1913	rVB	13782	12393	1.90%	0.194%
52	13.445	1929	1931	1933	rVB	22025	15996	2.45%	0.251%
53	13.474	1933	1936	1939	rBV3	9852	12507	1.92%	0.196%
54	13.610	1956	1959	1963	rVB	20627	20335	3.12%	0.319%
55	13.716	1975	1977	1980	rBV	17525	16831	2.58%	0.264%

56	13.745	1980	1982	1984	rVB	19521	15532	2.38%	0.244%
57	13.769	1984	1986	1987	rBV	17480	14866	2.28%	0.233%
58	13.821	1992	1995	1997	rBV	24103	28178	4.32%	0.442%
59	13.969	2012	2020	2023	rBV2	448189	542027	83.08%	8.501%
60	13.992	2023	2024	2033	rVB	109526	93812	14.38%	1.471%

61	14.057	2033	2035	2036	rBV2	17071	12692	1.95%	0.199%
62	14.127	2044	2047	2050	rBV3	14823	17663	2.71%	0.277%
63	14.251	2066	2068	2071	rVB3	9992	7732	1.19%	0.121%
64	14.321	2078	2080	2082	rBV3	12011	11107	1.70%	0.174%
65	14.357	2082	2086	2090	rVV	23312	33765	5.18%	0.530%

66	14.392	2090	2092	2095	rBV2	15315	15027	2.30%	0.236%
67	14.433	2097	2099	2101	rVV3	16383	15218	2.33%	0.239%
68	14.486	2105	2108	2110	rBV3	19776	22854	3.50%	0.358%
69	14.892	2174	2177	2180	rVB3	24970	28280	4.33%	0.444%
70	15.021	2195	2199	2202	rBV	86438	124907	19.15%	1.959%

71	15.086	2207	2210	2214	rVB2	29217	39998	6.13%	0.627%
72	15.333	2248	2252	2259	rVB	47060	60481	9.27%	0.949%
73	15.392	2259	2262	2267	rBV	65393	80618	12.36%	1.264%
74	15.457	2269	2273	2278	rBV	217483	302019	46.30%	4.737%
75	15.921	2348	2352	2356	rBV3	27186	38525	5.91%	0.604%

76	16.986	2528	2533	2540	rVB2	30740	67876	10.40%	1.065%
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	17.451	2607	2612	2622	rVB3	22141	51619	7.91%	0.810%
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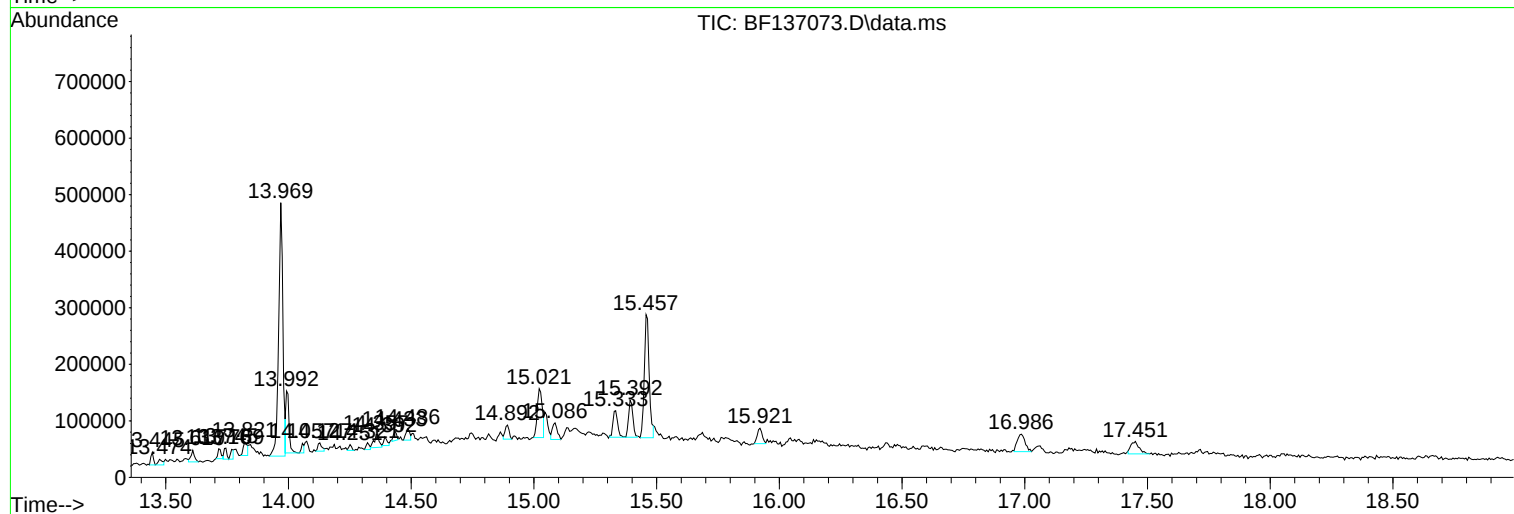
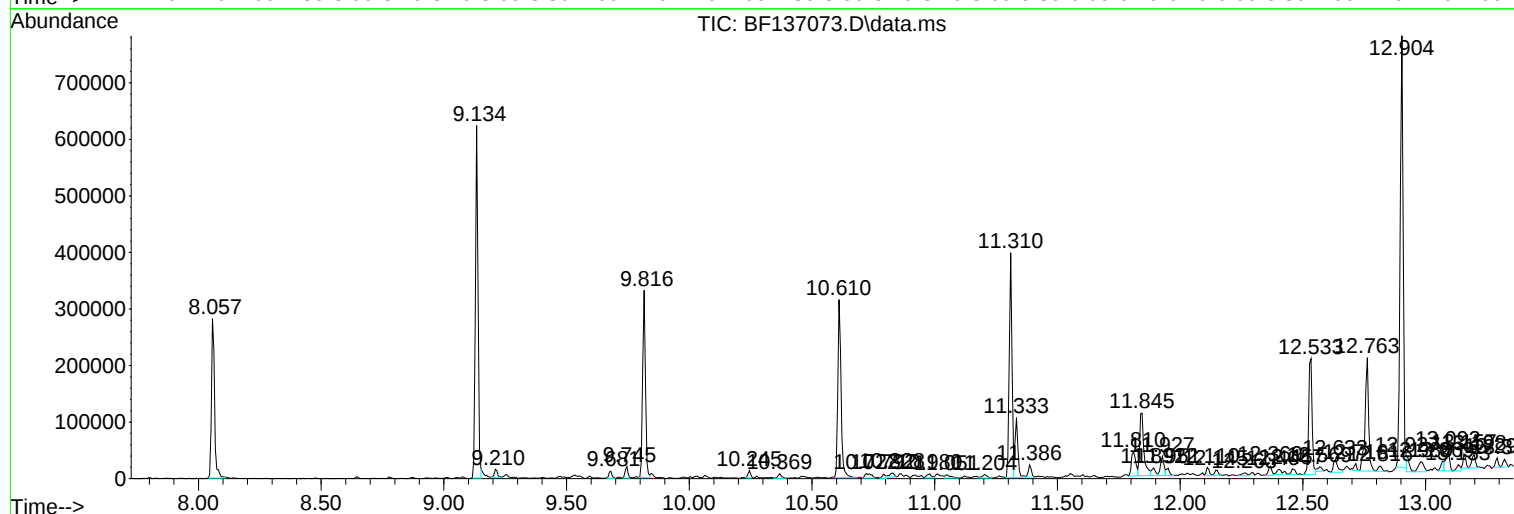
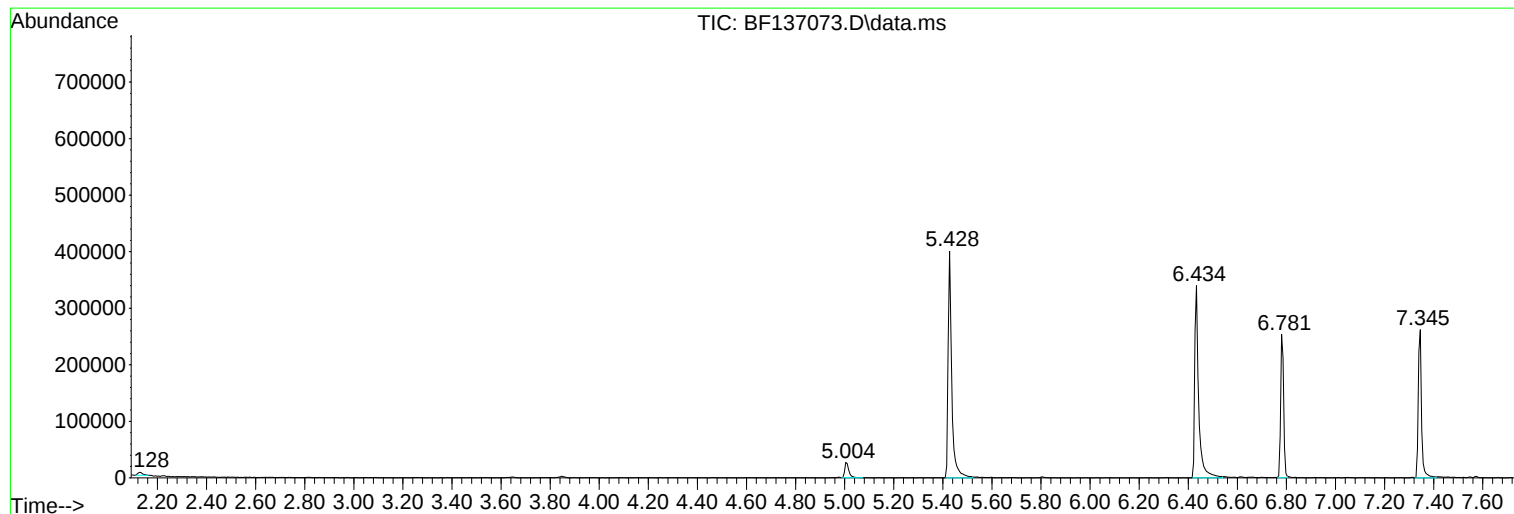
Sum of corrected areas: 6376156

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Misc :
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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
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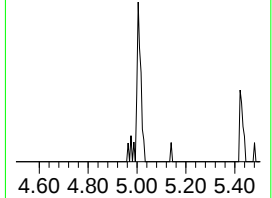
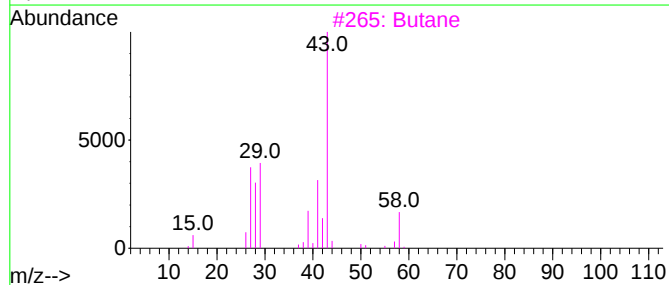
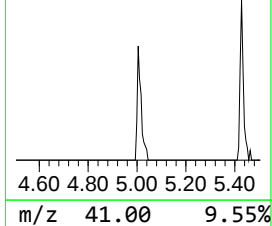
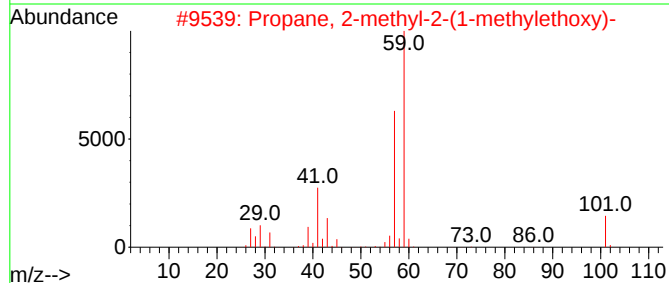
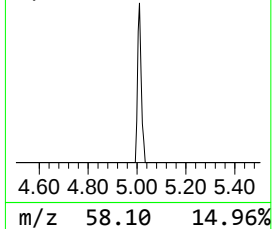
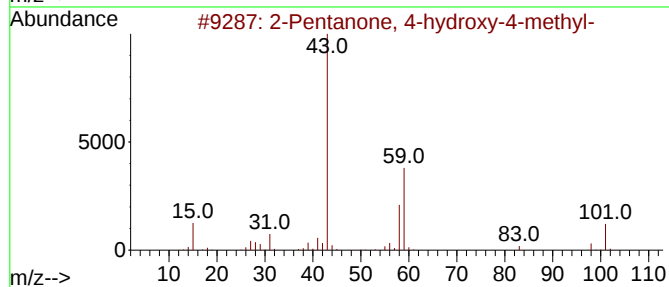
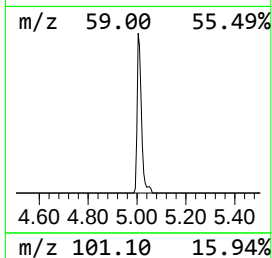
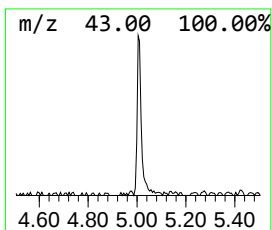
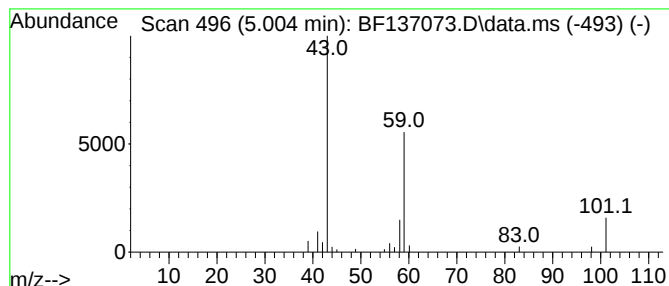
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.99 ng	31962	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	Butane	58	C4H10	000106-97-8	9		
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9		
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9		



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Instrument :
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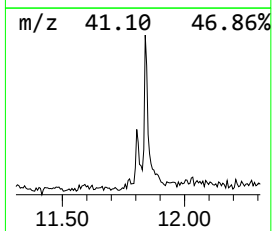
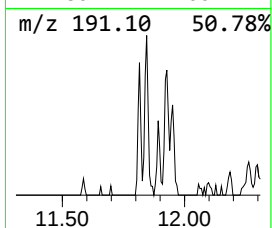
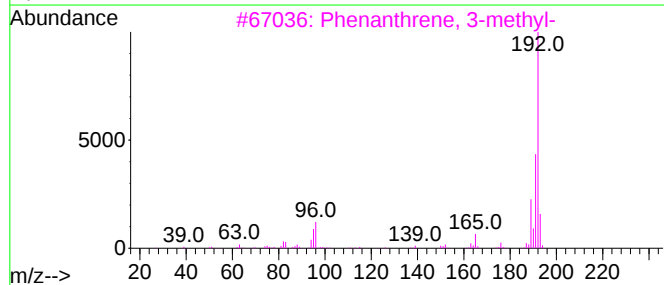
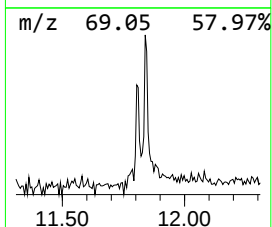
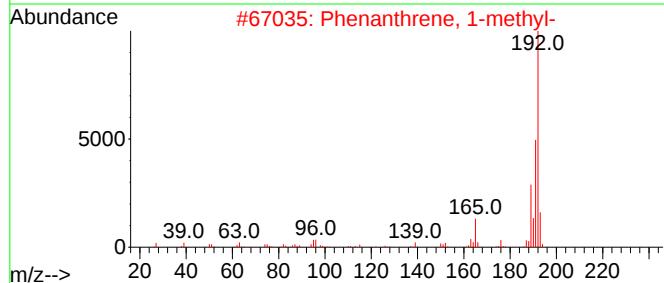
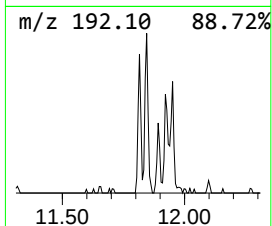
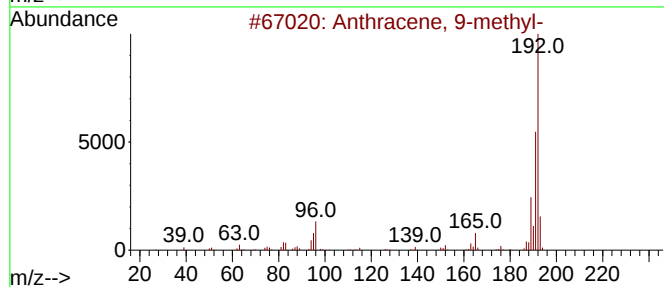
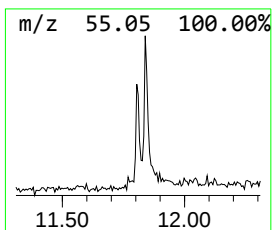
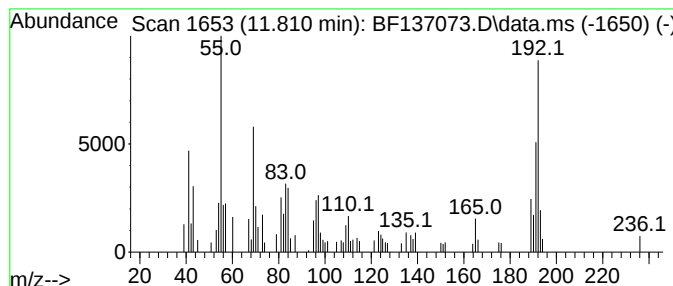
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Anthracene, 9-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	3.47 ng	54086	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	70
3			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	64
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	64
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	62



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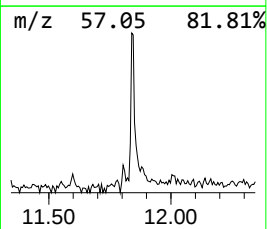
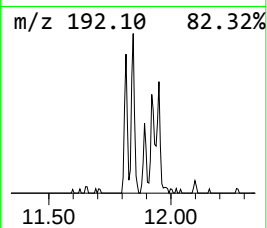
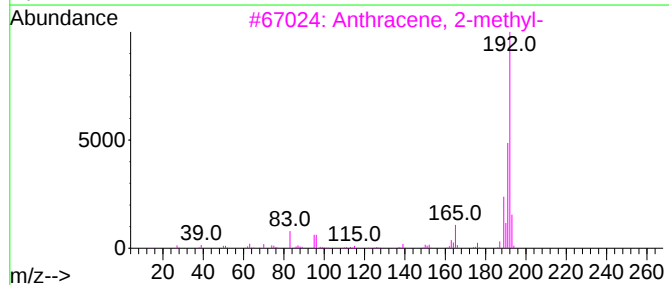
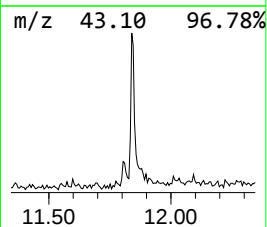
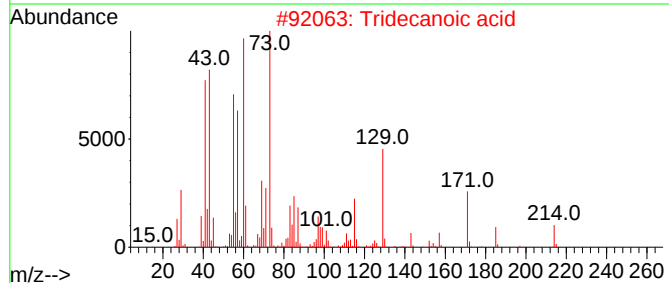
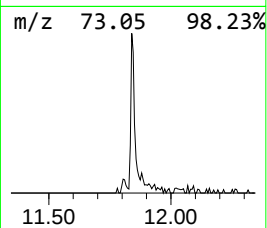
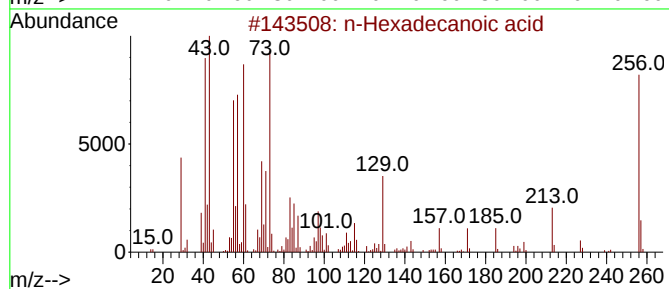
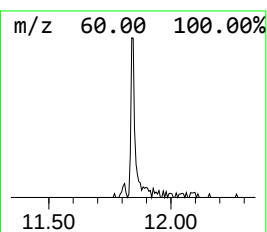
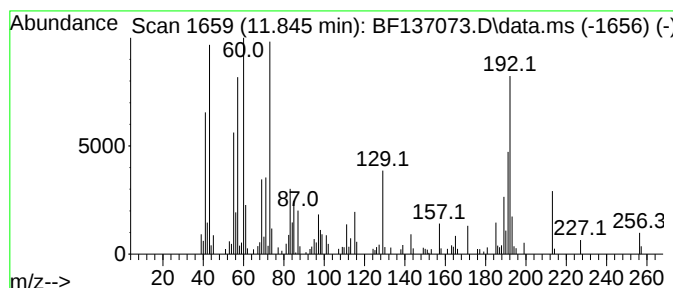
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.845	8.47 ng	132082	Phenanthrene-d10		11.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	96
2	Tridecanoic acid		214	C13H26O2	000638-53-9	89
3	Anthracene, 2-methyl-		192	C15H12	000613-12-7	64
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	55
5	Phenanthrene, 2-methyl-		192	C15H12	002531-84-2	53



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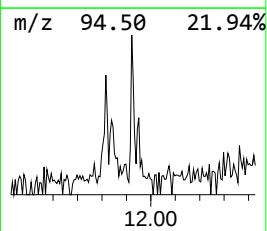
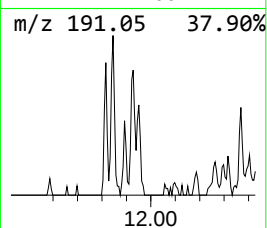
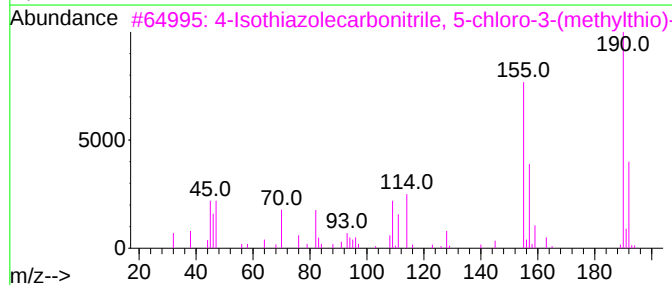
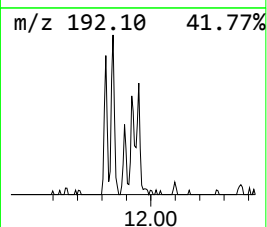
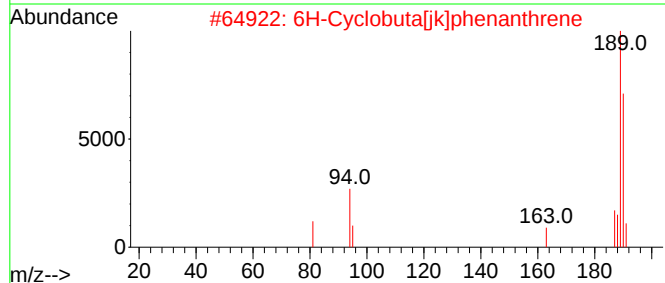
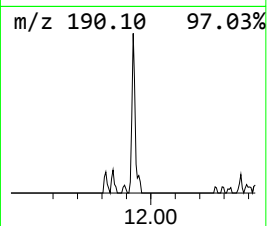
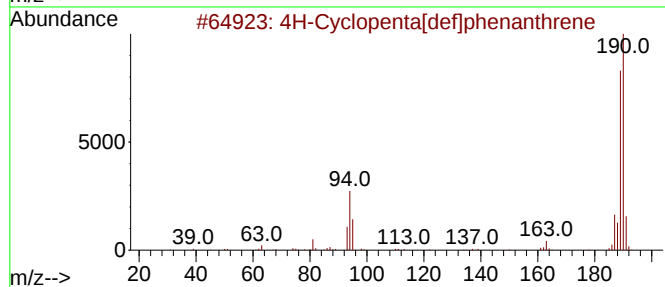
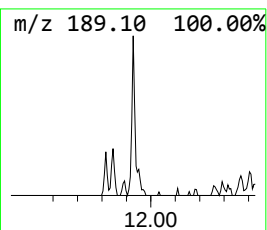
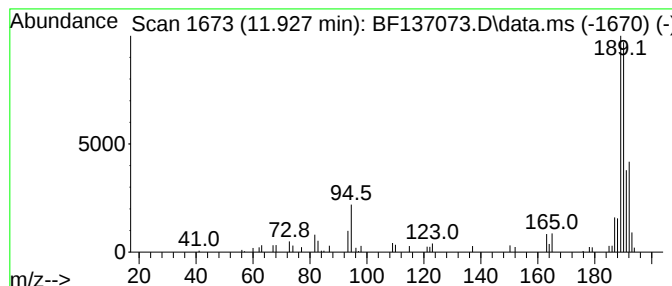
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	2.13 ng	33243	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3			4-Isothiazolecarbonitrile, 5-chl...	190	C5H3ClN2S2	054798-93-5	17
4			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	16
5			Isoquinoline, 1-chloro-3-ethyl-	191	C11H10ClN	055150-52-2	13



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137073.D
Acq On : 15 Jan 2024 20:05
Operator : CG\JU
Sample : P1140-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-309-0-2

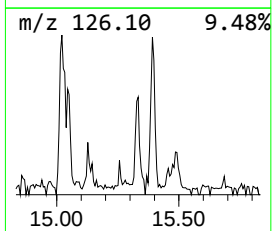
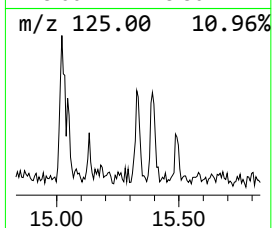
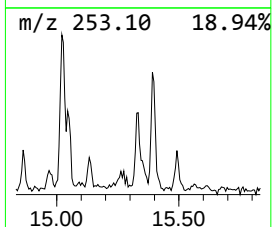
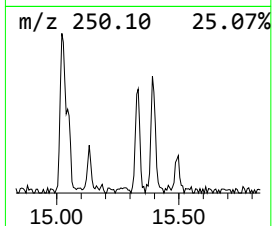
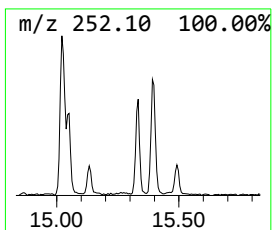
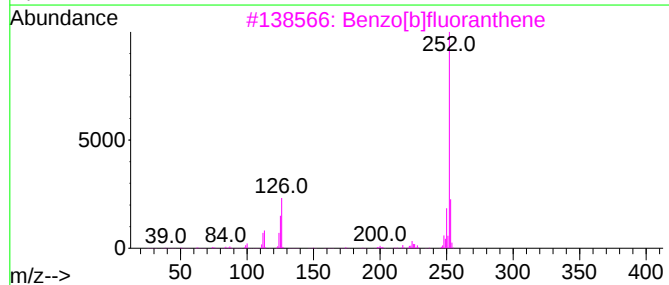
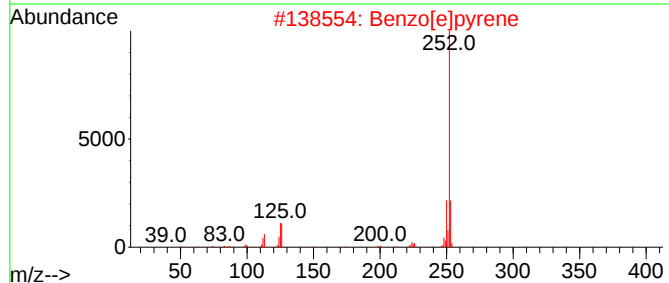
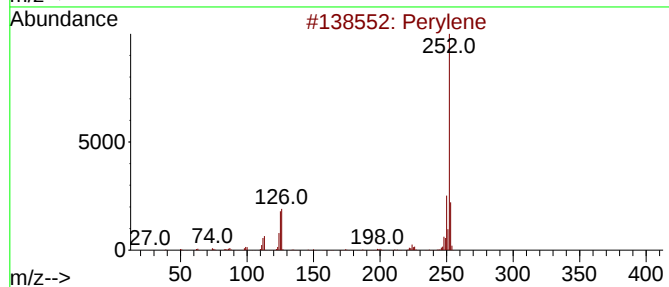
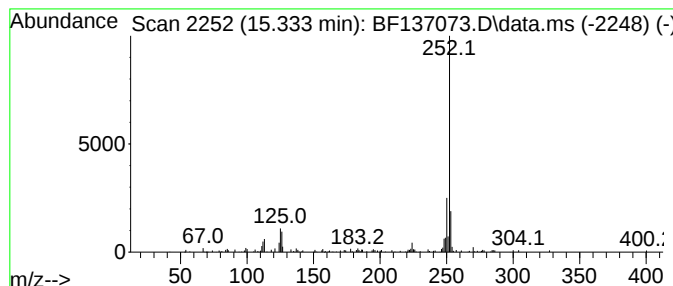
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	4.01 ng	60481	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	95
2			Benzo[e]pyrene	252	C20H12	000192-97-2	93
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	90
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137073.D
Acq On : 15 Jan 2024 20:05
Operator : CG\JU
Sample : P1140-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-309-0-2

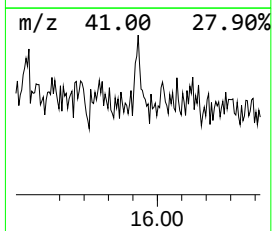
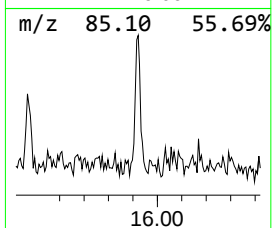
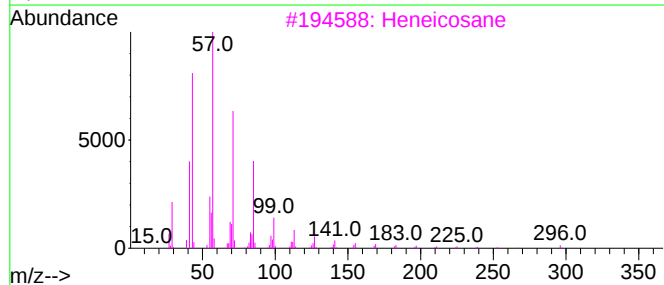
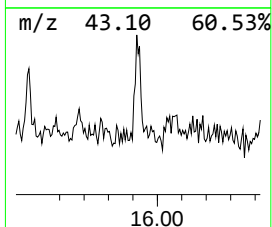
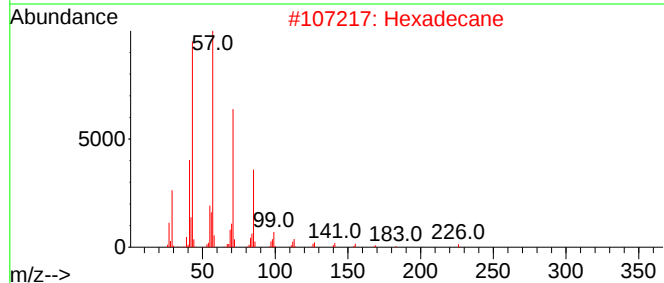
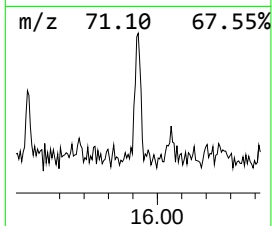
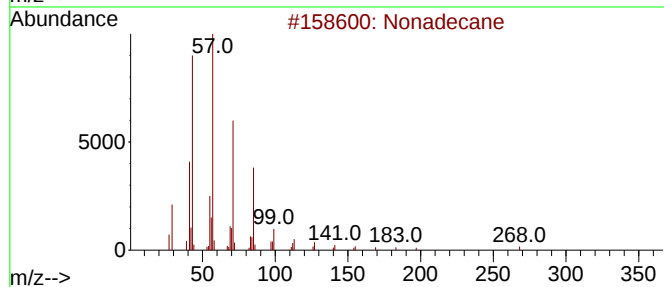
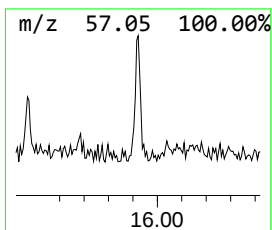
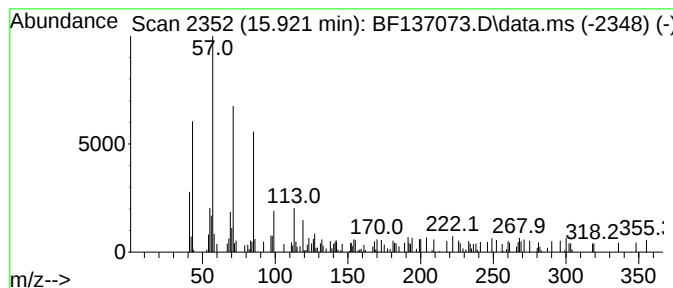
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	2.55 ng	38525	Perylene-d12	15.457

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	92
2		Hexadecane	226	C16H34	000544-76-3	78
3		Heneicosane	296	C21H44	000629-94-7	70
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
5		Eicosane	282	C20H42	000112-95-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011524\
Data File : BF137073.D
Acq On : 15 Jan 2024 20:05
Operator : CG\JU
Sample : P1140-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-309-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-...	5.004	3.0	ng	31962	1	6.781	213808	20.0
Anthracene, 9-m...	11.810	3.5	ng	54086	4	11.310	311728	20.0
n-Hexadecanoic ...	11.845	8.5	ng	132082	4	11.310	311728	20.0
4H-Cyclopenta[d...	11.928	2.1	ng	33243	4	11.310	311728	20.0
Perylene	15.333	4.0	ng	60481	6	15.457	302019	20.0
Nonadecane	15.921	2.5	ng	38525	6	15.457	302019	20.0