

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
 Data File : BF130566.D
 Acq On : 06 Oct 2022 23:43
 Operator : CG\JU
 Sample : N5012-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OE-3-100522

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.787	455	459	472	rBV	316030	371142	24.27%	2.679%
2	5.222	529	533	545	rBV	1421169	1339306	87.58%	9.668%
3	5.622	598	601	606	rVB	25442	21804	1.43%	0.157%
4	6.263	707	710	728	rBV	1190204	1233748	80.67%	8.906%
5	6.457	738	743	747	rVB2	16894	18870	1.23%	0.136%
6	6.616	767	770	774	rBV	479290	387358	25.33%	2.796%
7	7.187	863	867	870	rBV	838862	739594	48.36%	5.339%
8	7.898	985	988	992	rBV	565388	438749	28.69%	3.167%
9	8.975	1167	1171	1174	rBV	1642732	1243315	81.30%	8.975%
10	9.510	1259	1262	1266	rBV	52457	41260	2.70%	0.298%
11	9.651	1282	1286	1289	rBV	520079	459983	30.08%	3.320%
12	10.433	1416	1419	1428	rBV	999408	878786	57.46%	6.343%
13	11.027	1517	1520	1525	rVB2	12860	18823	1.23%	0.136%
14	11.127	1534	1537	1539	rBV	611894	498699	32.61%	3.600%
15	11.151	1539	1541	1545	rVB	187288	141885	9.28%	1.024%
16	11.204	1545	1550	1553	rBV	73081	61479	4.02%	0.444%
17	11.533	1602	1606	1610	rVB2	56357	53254	3.48%	0.384%
18	11.627	1620	1622	1625	rBV	41778	39489	2.58%	0.285%
19	11.657	1625	1627	1632	rVV2	68285	89699	5.87%	0.647%
20	11.704	1632	1635	1638	rVV2	31512	33438	2.19%	0.241%
21	11.739	1638	1641	1644	rVV	105285	112336	7.35%	0.811%
22	11.763	1644	1645	1651	rVB	41372	27896	1.82%	0.201%
23	11.927	1669	1673	1675	rBV	28515	29945	1.96%	0.216%
24	11.951	1675	1677	1680	rVB	18733	18917	1.24%	0.137%
25	12.180	1712	1716	1718	rBV	49087	56423	3.69%	0.407%
26	12.216	1718	1722	1724	rVV2	41937	57564	3.76%	0.416%
27	12.239	1724	1726	1728	rVV	69321	56257	3.68%	0.406%
28	12.263	1728	1730	1734	rVV2	41840	45837	3.00%	0.331%
29	12.339	1738	1743	1746	rBV	716828	591985	38.71%	4.273%
30	12.433	1756	1759	1762	rBV	50771	41693	2.73%	0.301%
31	12.563	1776	1781	1785	rBV	583577	603747	39.48%	4.358%
32	12.622	1788	1791	1796	rVB2	25047	30627	2.00%	0.221%
33	12.686	1798	1802	1803	rBV2	37888	35466	2.32%	0.256%
34	12.716	1803	1807	1810	rVV	1898839	1529314	100.00%	11.039%
35	12.786	1814	1819	1822	rBV2	45693	75186	4.92%	0.543%
36	12.892	1831	1837	1841	rBV2	94843	137495	8.99%	0.992%

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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-BF091422.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.963	1845	1849	1851	rVB	69036	64327	4.21%	0.464%
38	12.998	1851	1855	1859	rBV	66780	72396	4.73%	0.523%
39	13.086	1868	1870	1873	rVB	35821	30973	2.03%	0.224%
40	13.121	1873	1876	1878	rBV	39721	41629	2.72%	0.300%
41	13.404	1922	1924	1928	rVB	32046	29409	1.92%	0.212%
42	13.510	1940	1942	1945	rVB	55540	45580	2.98%	0.329%
43	13.539	1945	1947	1949	rBV	42620	35308	2.31%	0.255%
44	13.610	1957	1959	1963	rVB2	34345	39315	2.57%	0.284%
45	13.763	1980	1985	1987	rBV2	621049	783545	51.24%	5.656%
46	13.786	1987	1989	1992	rVB	244950	192796	12.61%	1.392%
47	13.910	2008	2010	2012	rBV	36394	32846	2.15%	0.237%
48	14.763	2152	2155	2162	rVB	195826	319834	20.91%	2.309%
49	15.033	2199	2201	2207	rVB	104467	118513	7.75%	0.855%
50	15.092	2208	2211	2216	rVB	161815	173601	11.35%	1.253%
51	15.145	2217	2220	2224	rBV	262764	312098	20.41%	2.253%

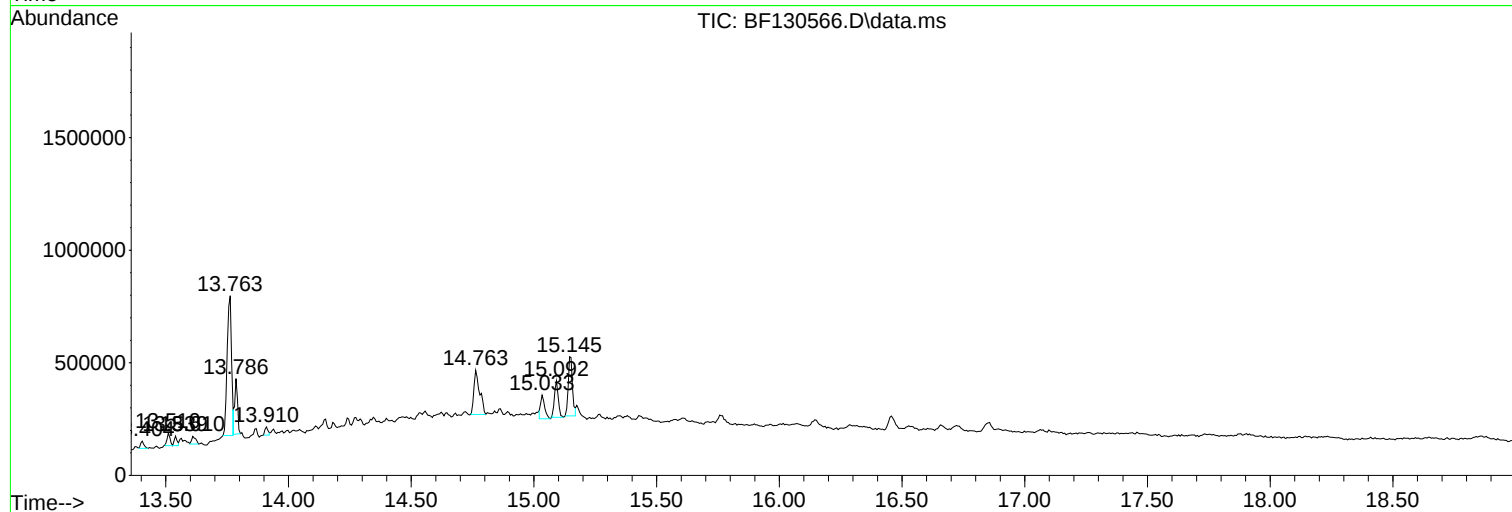
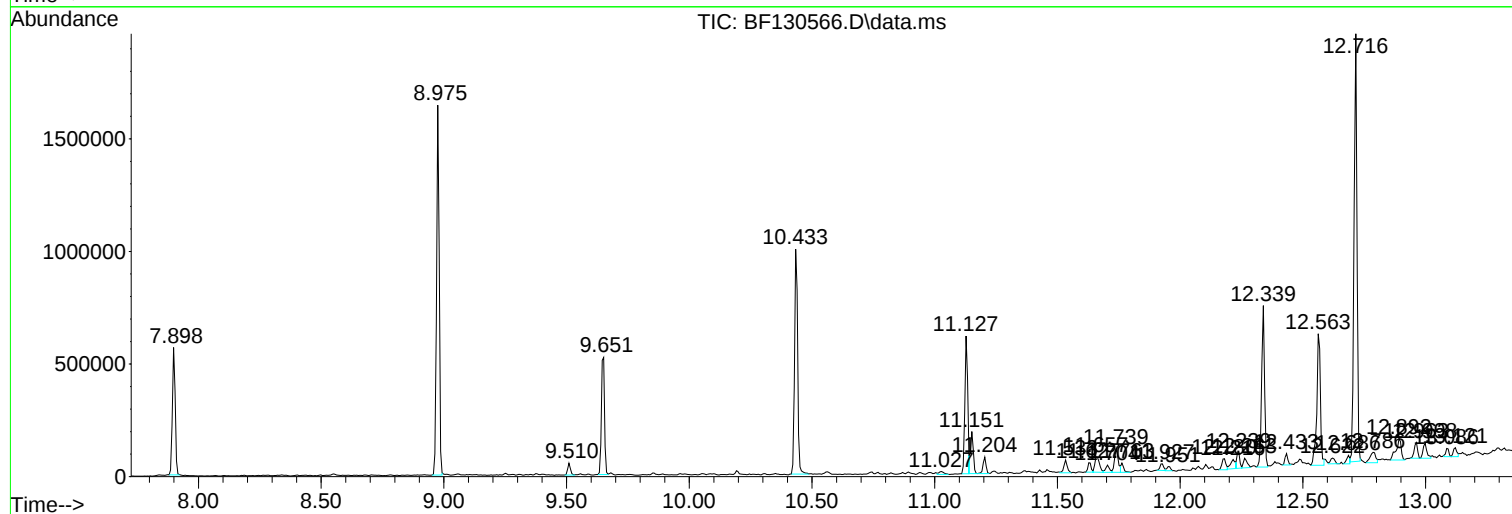
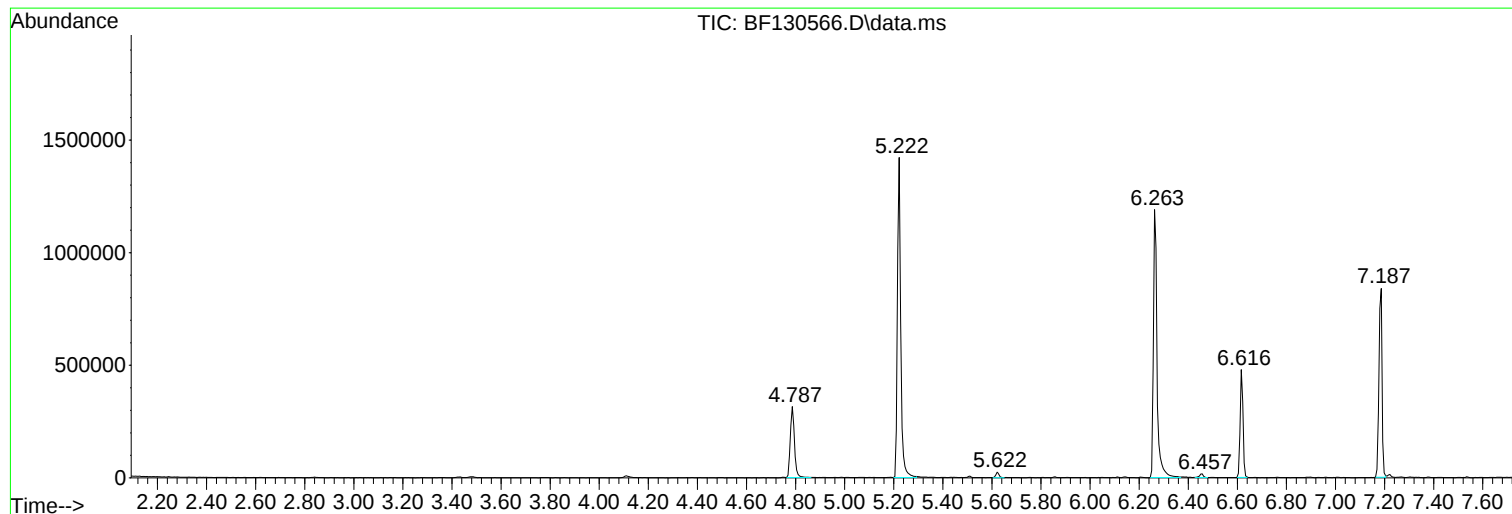
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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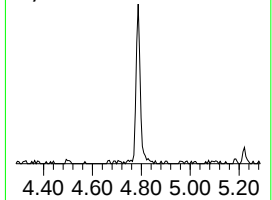
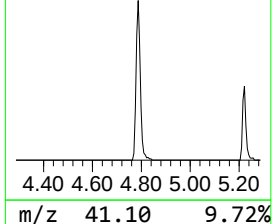
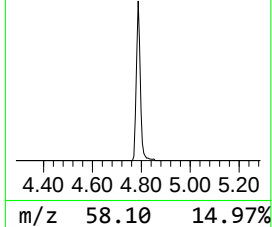
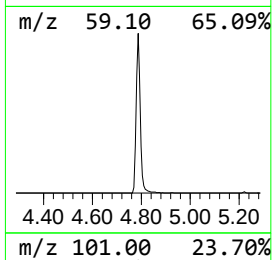
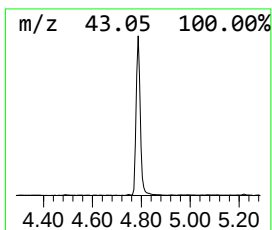
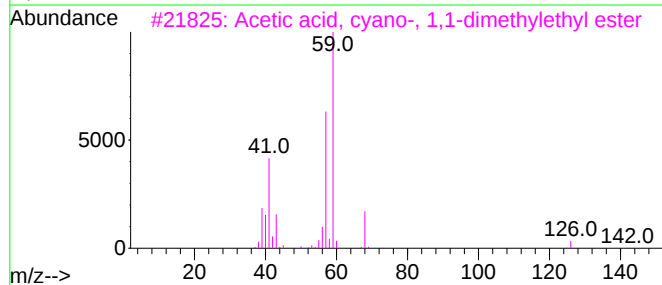
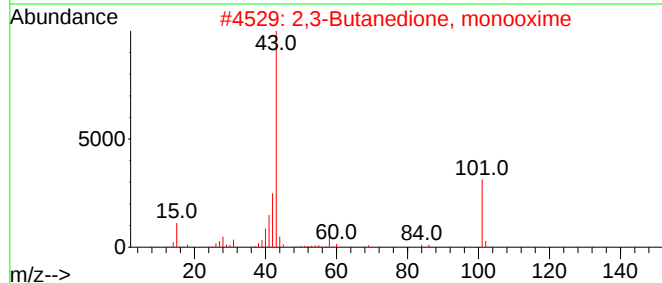
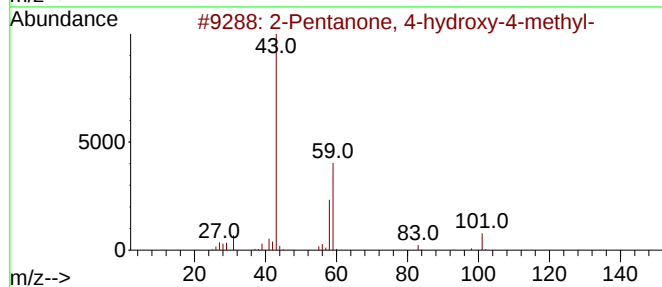
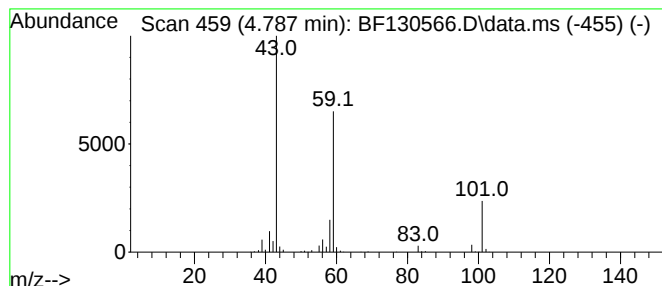
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.787	19.16 ng	371142	1,4-Dichlorobenzene-d4	6.616

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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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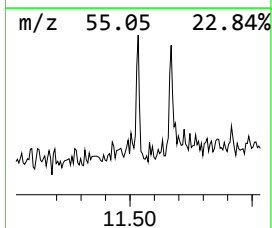
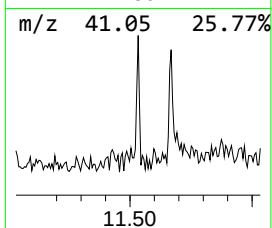
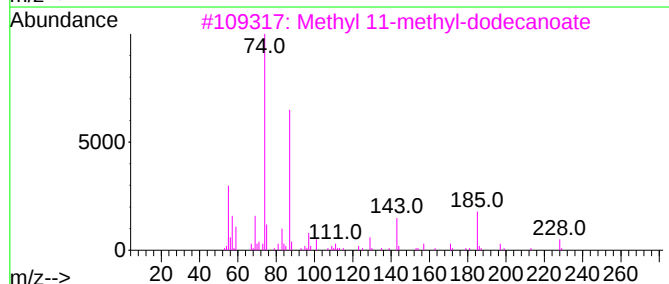
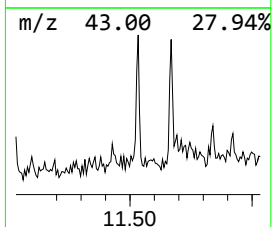
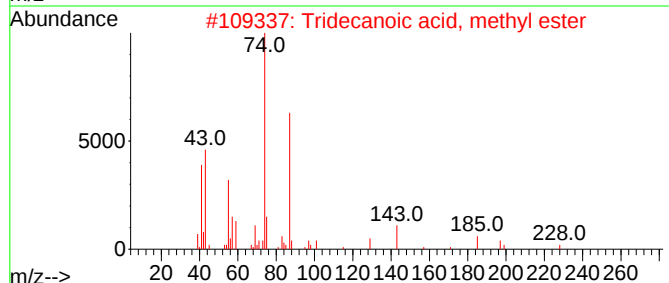
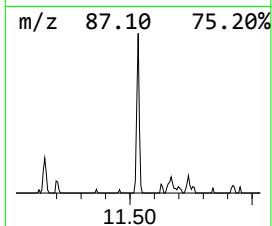
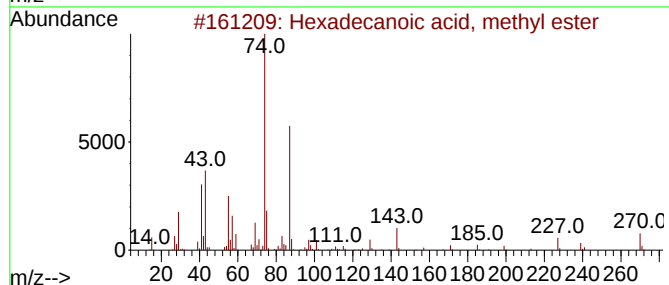
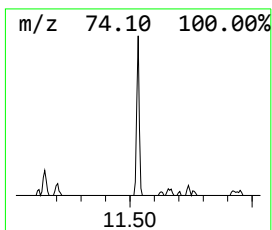
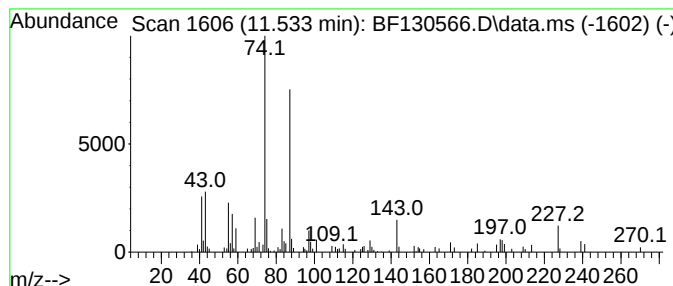
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.533	2.14 ng	53254	Phenanthrene-d10		11.128	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	91
2	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	90
3	Methyl 11-methyl-dodecanoate		228	C14H28O2	1000336-45-1	83
4	Tridecanoic acid, 12-methyl-, me...		242	C15H30O2	005129-58-8	80
5	Methyl tetradecanoate		242	C15H30O2	000124-10-7	80



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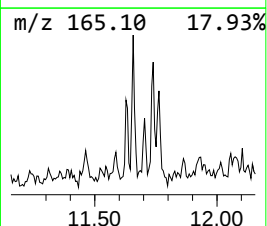
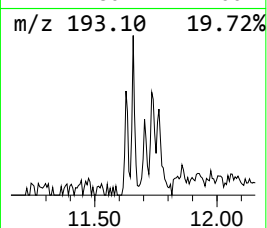
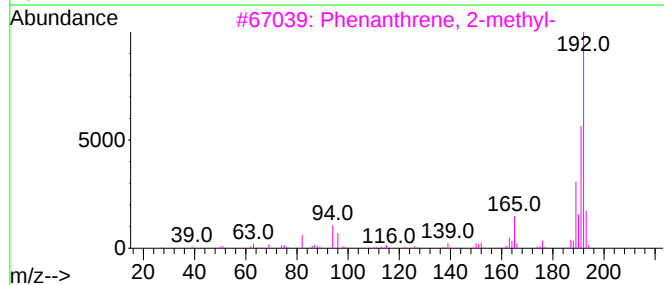
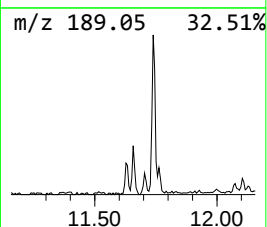
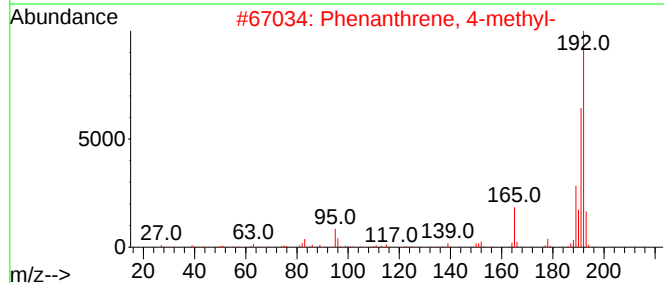
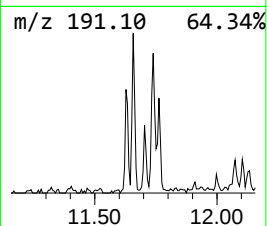
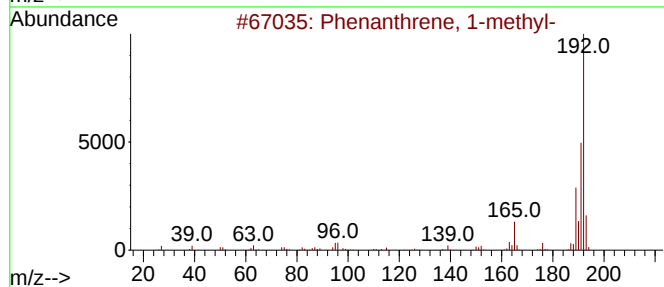
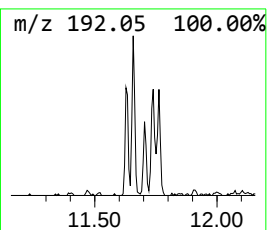
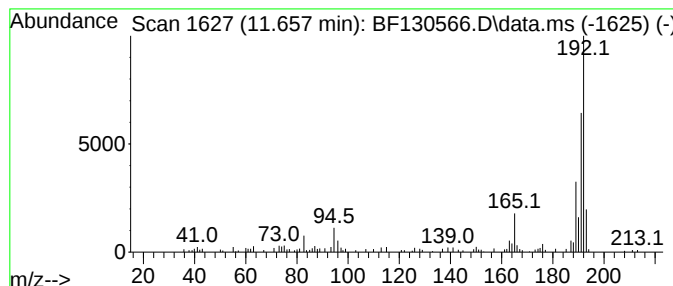
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.657	3.60 ng	89699	Phenanthrene-d10	11.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91



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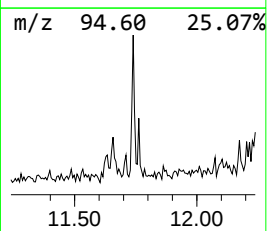
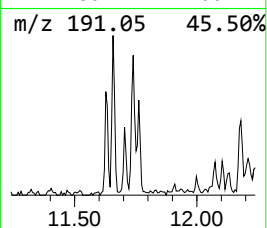
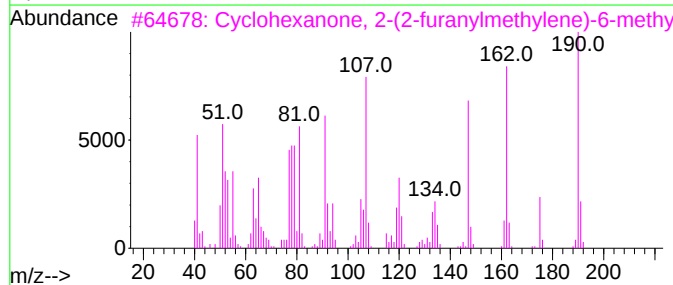
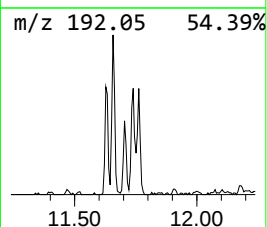
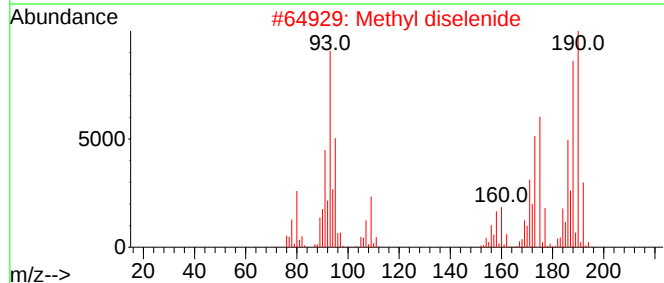
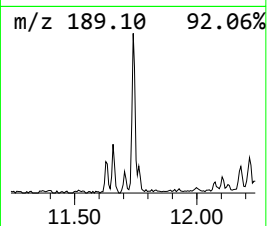
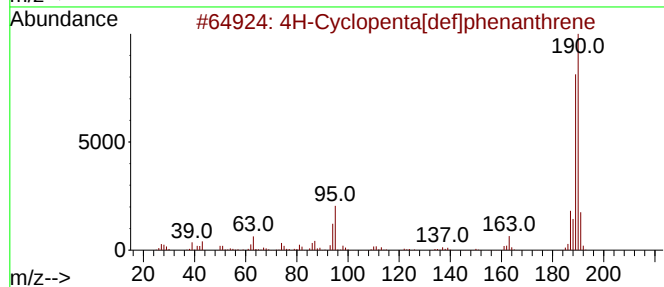
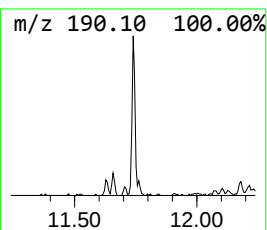
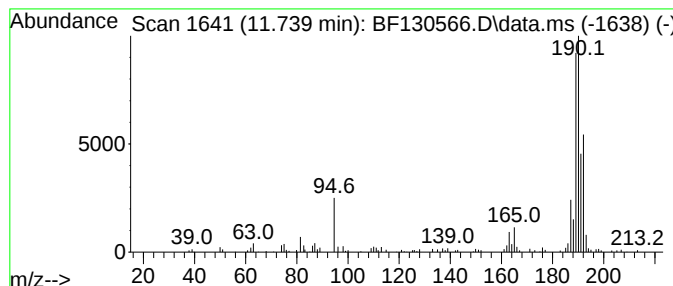
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	4.51 ng	112336	Phenanthrene-d10	11.128

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	45
3			Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22
4			5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	18
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	18



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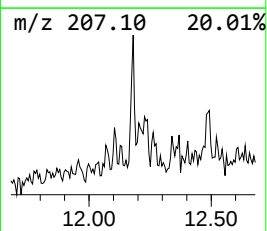
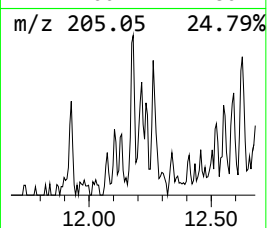
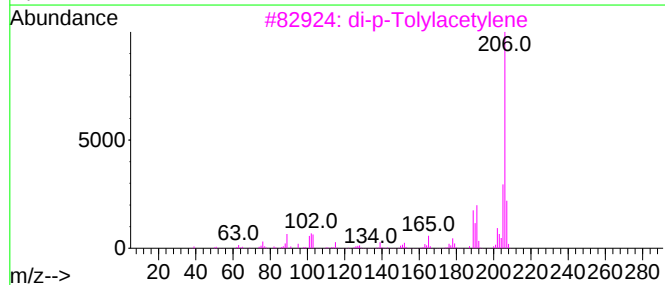
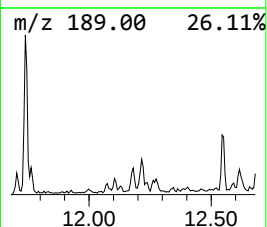
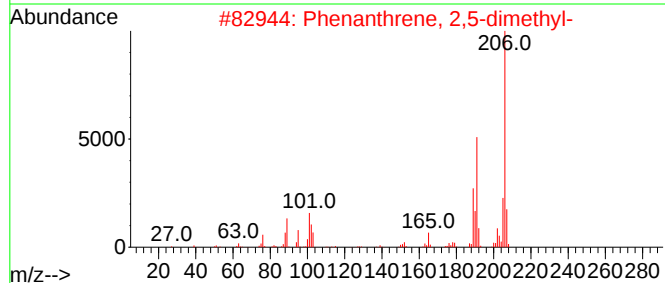
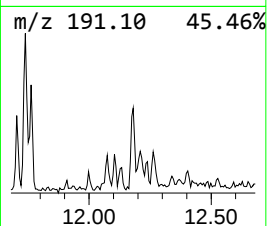
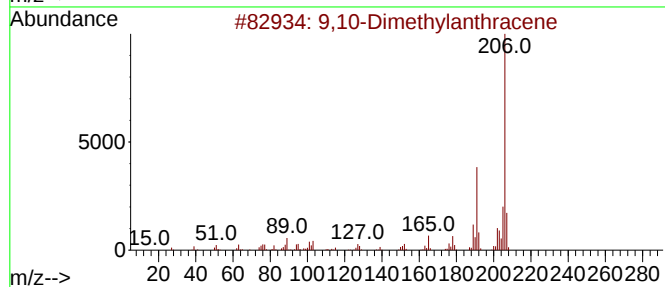
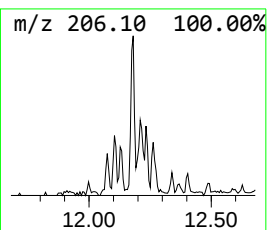
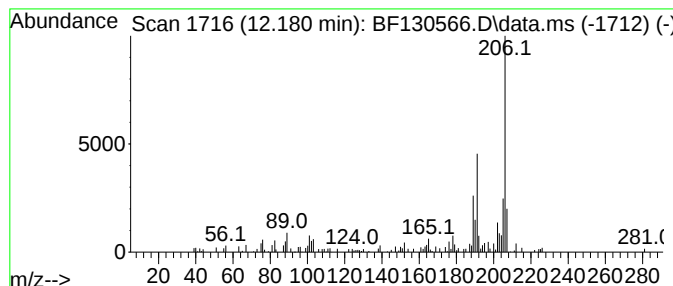
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9,10-Dimethylantracene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.180	2.26 ng	56423	Phenanthrene-d10	11.128

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,10-Dimethylantracene	206	C16H14	000781-43-1	94
2		Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
3		di-p-Tolylacetylene	206	C16H14	002789-88-0	92
4		3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	91
5		Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130566.D
Acq On : 06 Oct 2022 23:43
Operator : CG\JU
Sample : N5012-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OE-3-100522

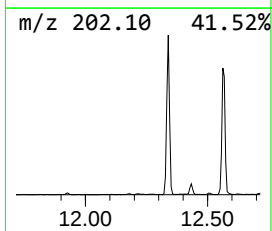
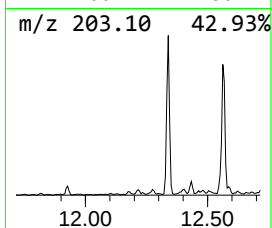
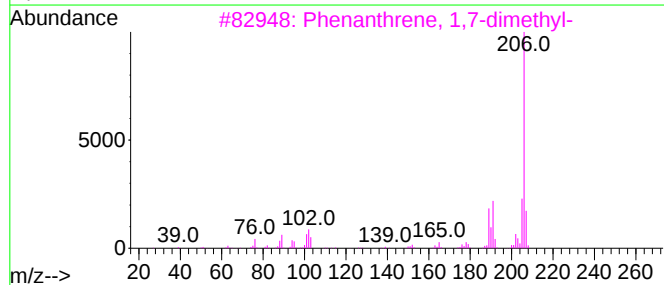
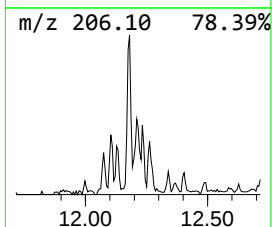
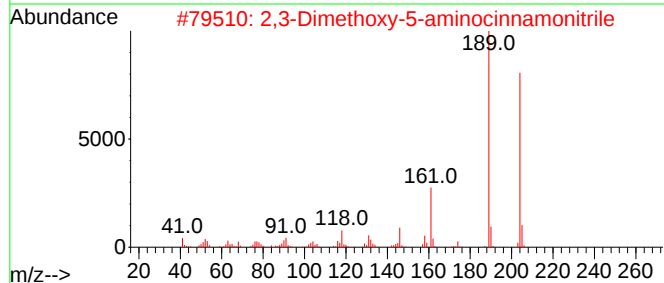
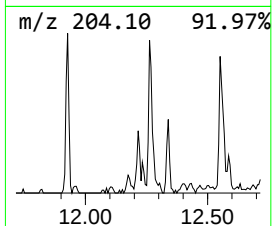
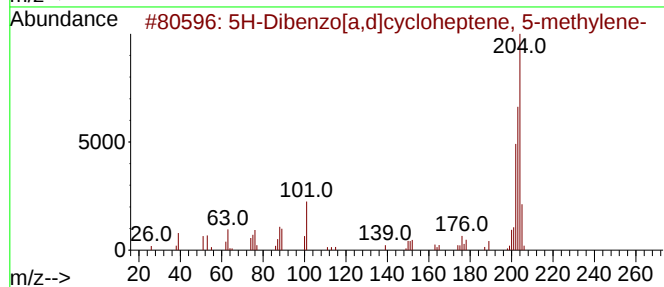
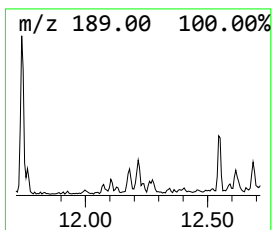
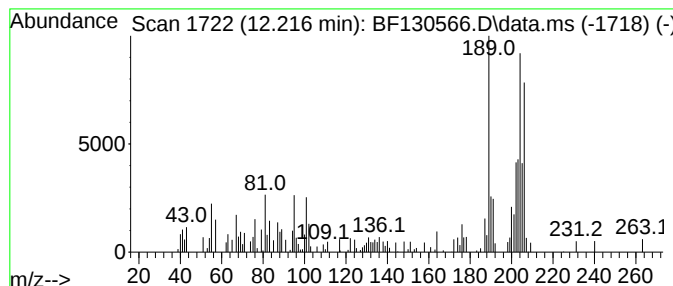
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.216 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.216	2.31 ng	57564	Phenanthrene-d10	11.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5H-Dibenzo[a,d]cycloheptene, 5-m...	204	C16H12	002975-79-3	38
2			2,3-Dimethoxy-5-aminocinnamitrile	204	C11H12N2O2	1000214-46-5	27
3			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	27
4			6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	27
5			1H-Indol-6-ylamine, TMS derivative	204	C11H16N2Si	1000484-86-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130566.D
Acq On : 06 Oct 2022 23:43
Operator : CG\JU
Sample : N5012-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OE-3-100522

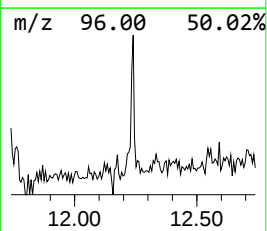
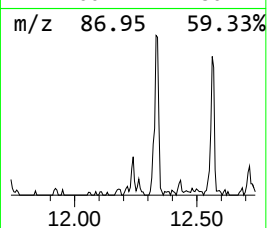
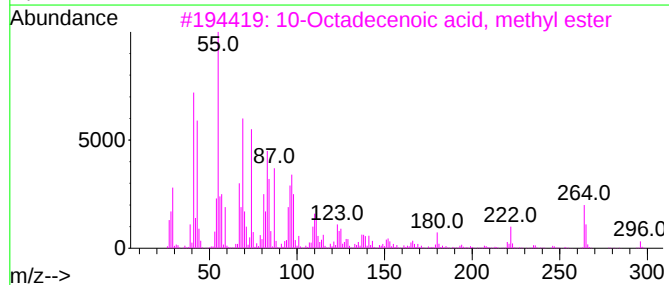
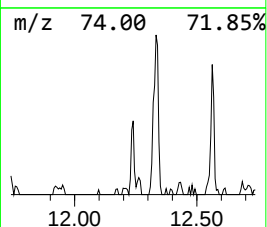
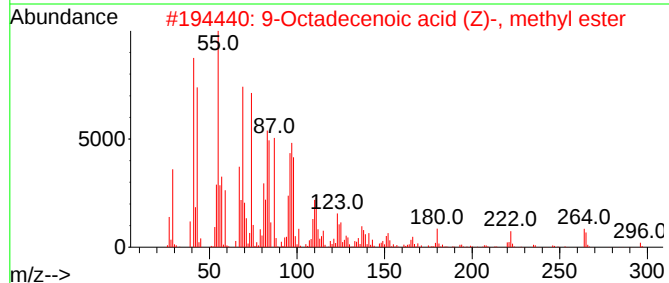
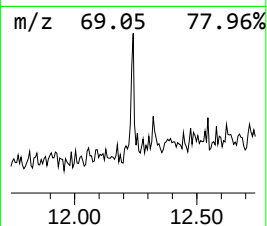
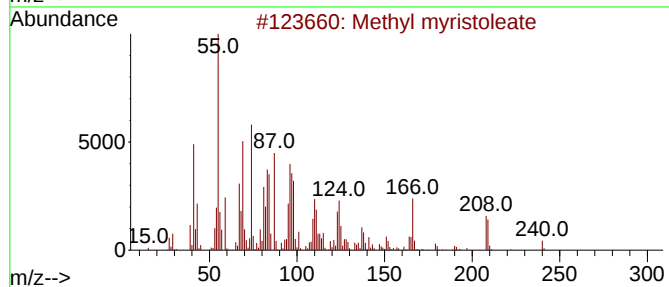
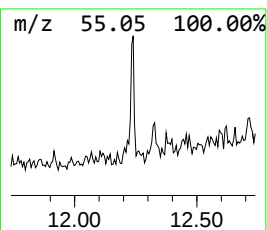
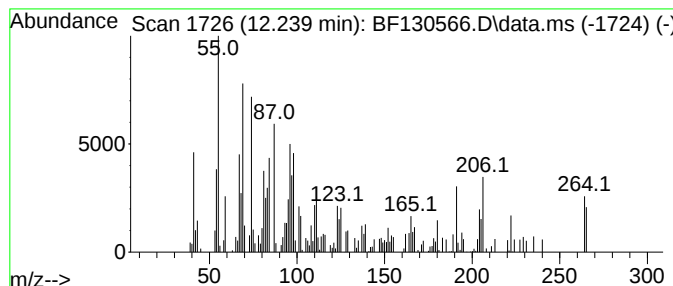
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl myristoleate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.239	2.26 ng	56257	Phenanthrene-d10	11.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl myristoleate	240	C15H28O2	056219-06-8	83
2			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	83
3			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	53
4			Oleic Acid	282	C18H34O2	000112-80-1	47
5			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130566.D
Acq On : 06 Oct 2022 23:43
Operator : CG\JU
Sample : N5012-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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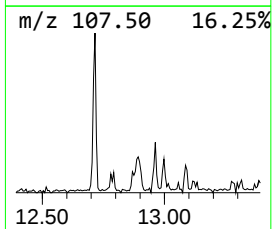
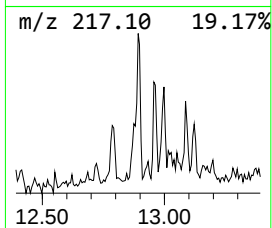
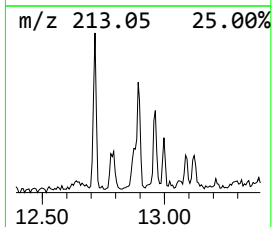
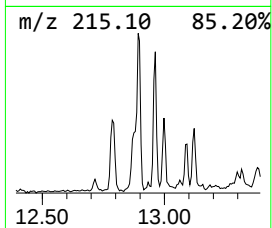
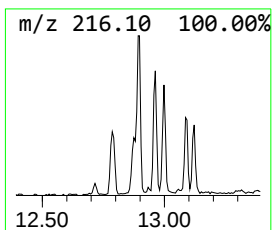
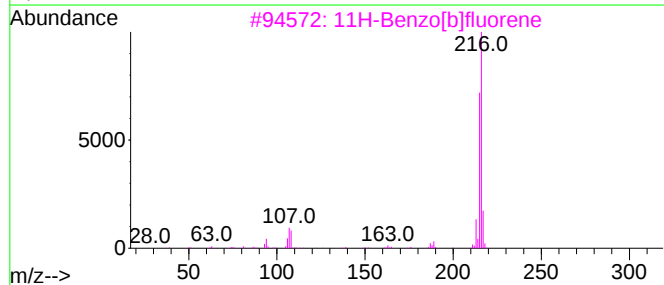
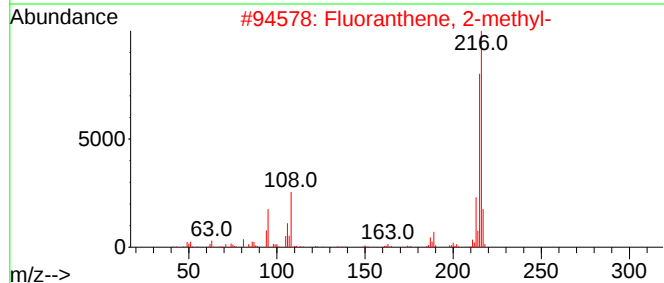
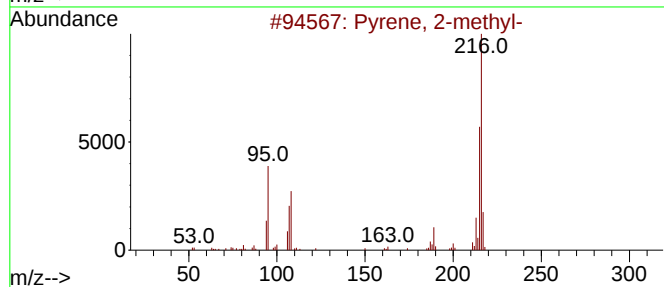
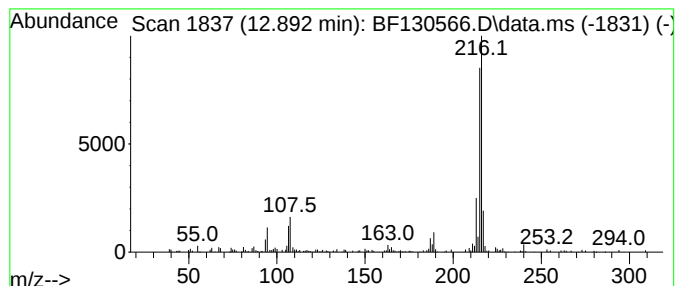
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pyrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.892	3.51 ng	137495	Chrysene-d12	13.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
2		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	94
3		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
5		Pyrene, 1-methyl-	216	C17H12	002381-21-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130566.D
Acq On : 06 Oct 2022 23:43
Operator : CG\JU
Sample : N5012-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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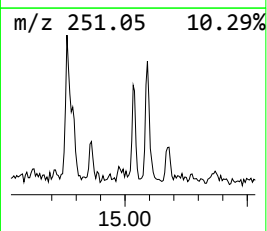
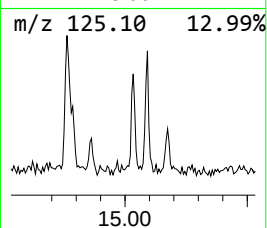
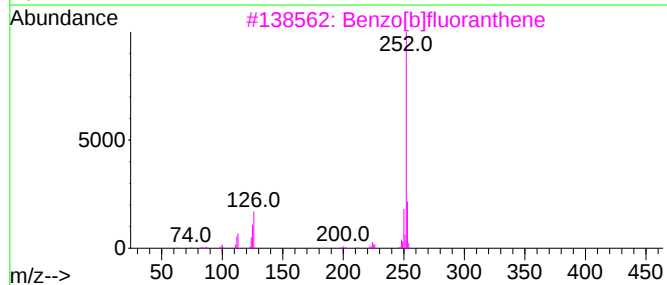
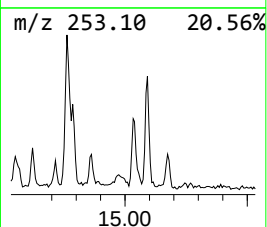
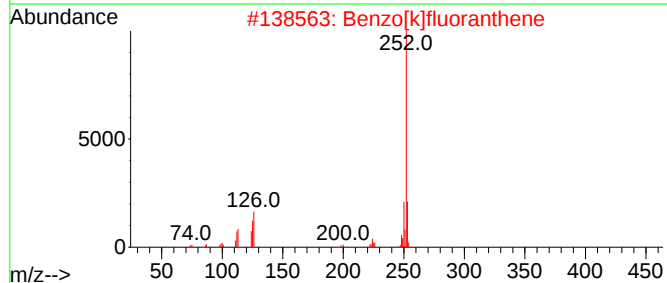
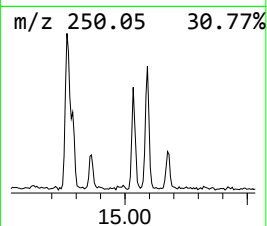
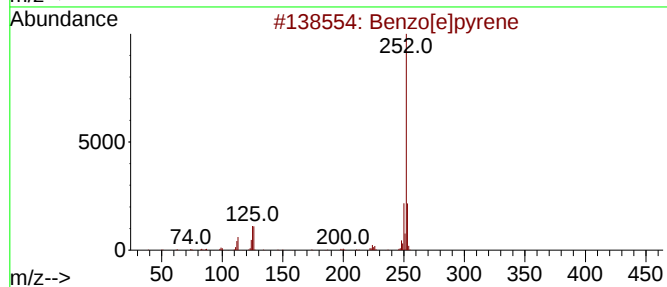
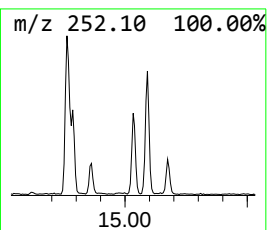
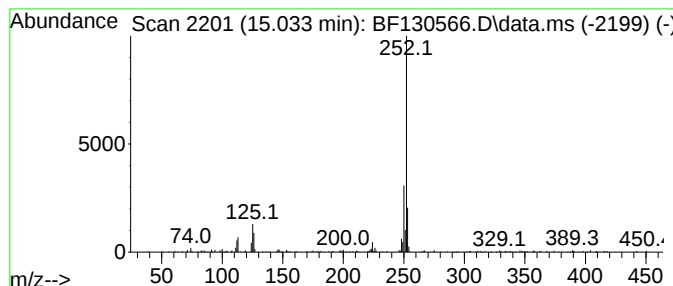
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	7.59 ng	118513	Perylene-d12	15.151

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100622\
Data File : BF130566.D
Acq On : 06 Oct 2022 23:43
Operator : CG\JU
Sample : N5012-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OE-3-100522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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Hexadecanoic ac...	11.533	2.1	ng	53254	4	11.128	498699	20.0
Phenanthrene, 1...	11.657	3.6	ng	89699	4	11.128	498699	20.0
4H-Cyclopenta[d...	11.739	4.5	ng	112336	4	11.128	498699	20.0
9,10-Dimethylan...	12.180	2.3	ng	56423	4	11.128	498699	20.0
unknown12.216	12.216	2.3	ng	57564	4	11.128	498699	20.0
Methyl myristol...	12.239	2.3	ng	56257	4	11.128	498699	20.0
Pyrene, 2-methyl-	12.892	3.5	ng	137495	5	13.763	783545	20.0
Benzo[e]pyrene	15.033	7.6	ng	118513	6	15.151	312098	20.0