LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101822\
Data File : BF130703.D
Acq On : 18 Oct 2022 17:48
Operator : CG\JU
Sample : N5171-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-101722

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-BF101122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130703.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.739	481	485	500	rBV	114981	165692	2.41%	0.533%
2	5.181	557	560	583	rBV	1217721	1251909	18.20%	4.025%
3	6.228	735	738	756	rBV	1225697	1157541	16.83%	3.722%
4	6.575	794	797	805	rVB	437277	371216	5.40%	1.194%
5	7.145	890	894	906	rBV	890022	753426	10.96%	2.423%
6	7.857	1011	1015	1018	rBV	532633	424568	6.17%	1.365%
7	8.933	1194	1198	1201	rBV	1454059	1233602	17.94%	3.967%
8	9.604	1308	1312	1315	rBV	442081	380199	5.53%	1.222%
9	10.392	1442	1446	1457	rVB	758925	654724	9.52%	2.105%
10	11.080	1560	1563	1565	rBV	379695	337313	4.90%	1.085%
11	11.104	1565	1567	1571	rVV	427807	389445	5.66%	1.252%
12	11.157	1571	1576	1580	rVB	112904	117103	1.70%	0.377%
13	11.321	1599	1604	1610	rBV2	67418	99047	1.44%	0.318%
14	11.492	1629	1633	1636	rBV	2111100	1722094	25.04%	5.537%
15	11.586	1645	1649	1651	rBV	76751	72068	1.05%	0.232%
16	11.616	1651	1654	1655	rBV	90958	89958	1.31%	0.289%
17	11.633	1655	1657	1660	rVV	134126	133003	1.93%	0.428%
18	11.692	1664	1667	1670	rBV	141866	151419	2.20%	0.487%
19	11.916	1702	1705	1708	rVB	91006	83720	1.22%	0.269%
20	12.186	1745	1751	1752	rBV	5670573	6877100	100.00%	22.113%
21	12.204	1752	1754	1760	rVV2	4793707	4313585	62.72%	13.870%
22	12.280	1764	1767	1768	rBV	1184259	989284	14.39%	3.181%
23	12.292	1768	1769	1772	rVB	948230	746670	10.86%	2.401%
24	12.521	1803	1808	1811	rVV	942726	1024351	14.90%	3.294%
25	12.668	1830	1833	1841	rVB	1402163	1267539	18.43%	4.076%
26	12.739	1841	1845	1850	rBV2	71993	128127	1.86%	0.412%
27	12.851	1857	1864	1868	rBV	203291	268996	3.91%	0.865%
28	12.915	1871	1875	1878	rVV	190854	216553	3.15%	0.696%
29	12.957	1878	1882	1887	rVV3	135132	202854	2.95%	0.652%
30	13.004	1887	1890	1893	rVB2	97169	99712	1.45%	0.321%
31	13.110	1905	1908	1911	rVV2	97725	91601	1.33%	0.295%
32	13.145	1911	1914	1921	rVB2	106125	134318	1.95%	0.432%
33	13.468	1966	1969	1971	rBV	92573	75517	1.10%	0.243%
34	13.574	1984	1987	1990	rBV	84112	71690	1.04%	0.231%
35	13.668	2000	2003	2005	rBV	98023	75375	1.10%	0.242%
36	13.715	2005	2011	2014	rVV2	880107	1374662	19.99%	4.420%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101822\
Data File : BF130703.D
Acq On : 18 Oct 2022 17:48
Operator : CG\JU
Sample : N5171-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-101722

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-BF101122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.745	2014	2016	2023	rVV	715337	586993	8.54%	1.887%
38	13.821	2026	2029	2032	rVB	161174	145088	2.11%	0.467%
39	14.109	2073	2078	2080	rVB2	136959	182955	2.66%	0.588%
40	14.315	2111	2113	2117	rVB	120746	119534	1.74%	0.384%
41	14.721	2178	2182	2184	rBV	611295	738416	10.74%	2.374%
42	14.815	2196	2198	2202	rVB	96856	90977	1.32%	0.293%
43	14.986	2224	2227	2233	rVB	291506	315754	4.59%	1.015%
44	15.045	2233	2237	2241	rVB	459297	506346	7.36%	1.628%
45	15.098	2242	2246	2249	rBV	349145	392264	5.70%	1.261%
46	16.392	2461	2466	2475	rBV	142377	279318	4.06%	0.898%
47	16.780	2527	2532	2540	rVB	101877	196646	2.86%	0.632%

Sum of corrected areas: 31100272

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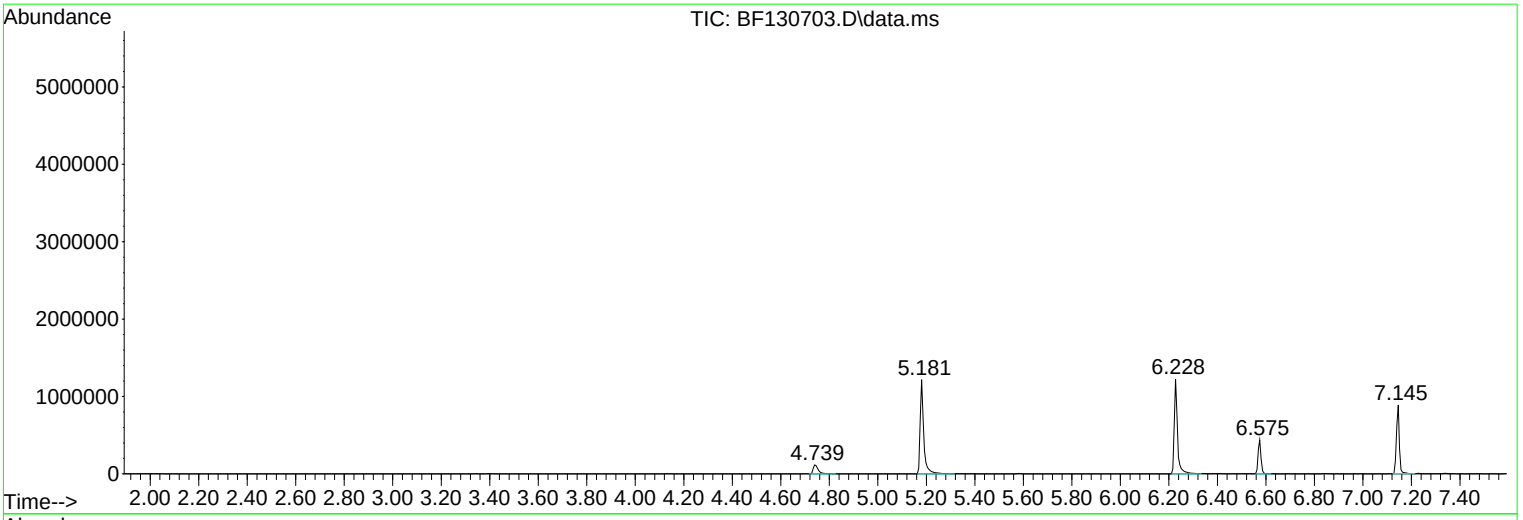
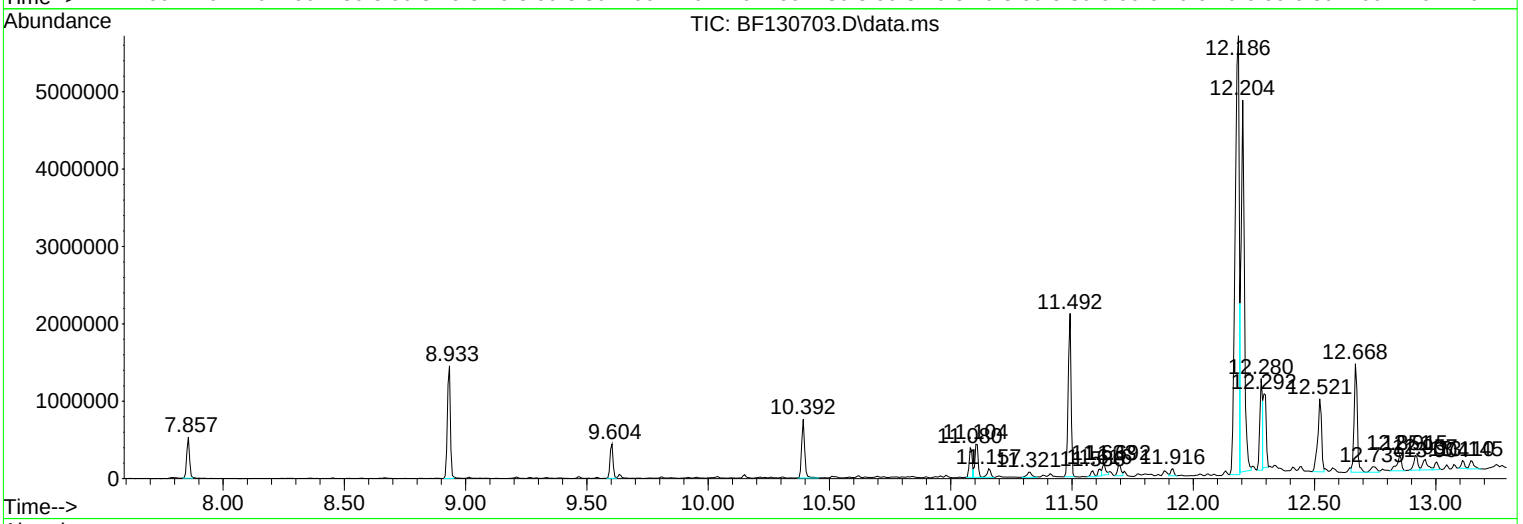
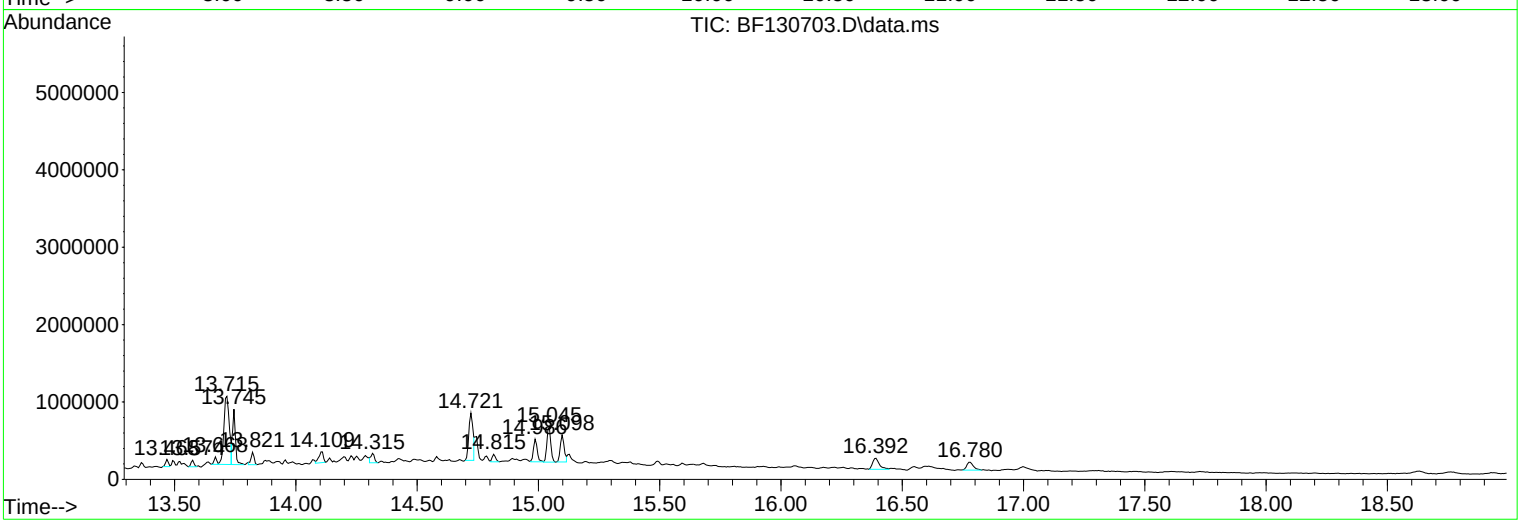
ClientSampleId :
NB-08-101722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.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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Data File : BF130703.D
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Operator : CG\JU
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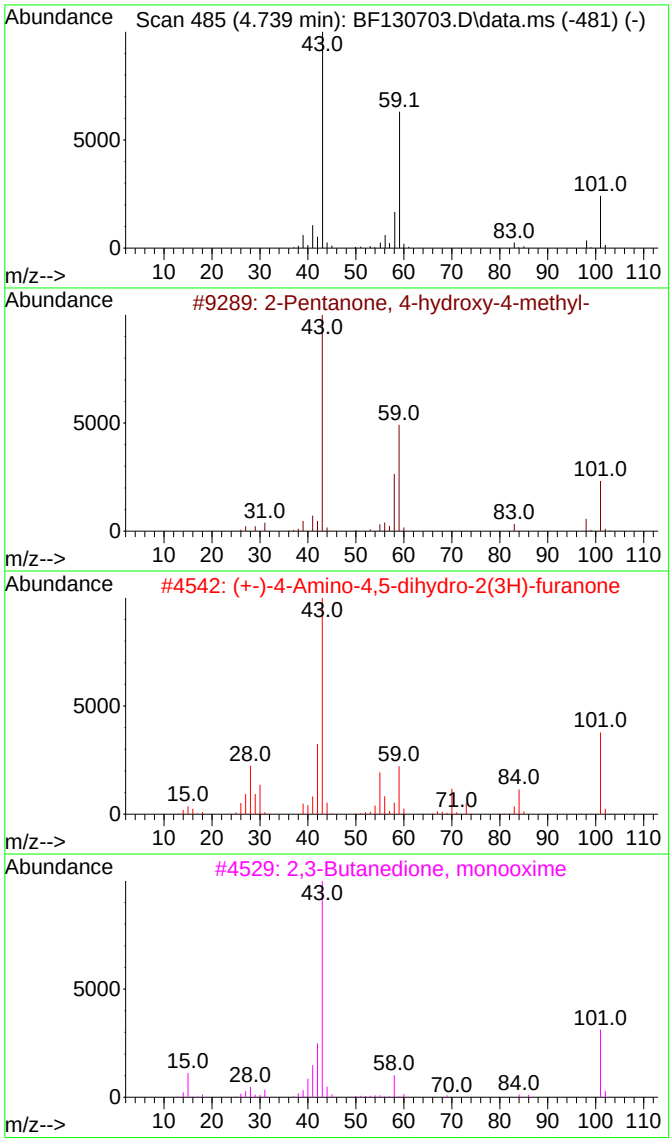
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

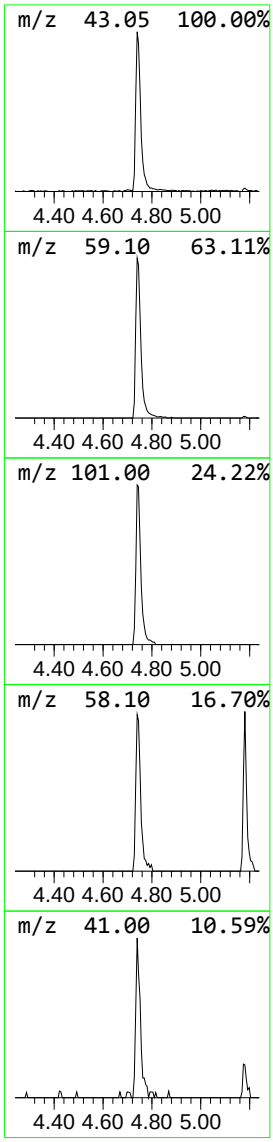
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.739	8.93 ng	165692	1,4-Dichlorobenzene-d4	6.575

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Acq On : 18 Oct 2022 17:48
Operator : CG\JU
Sample : N5171-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-101722

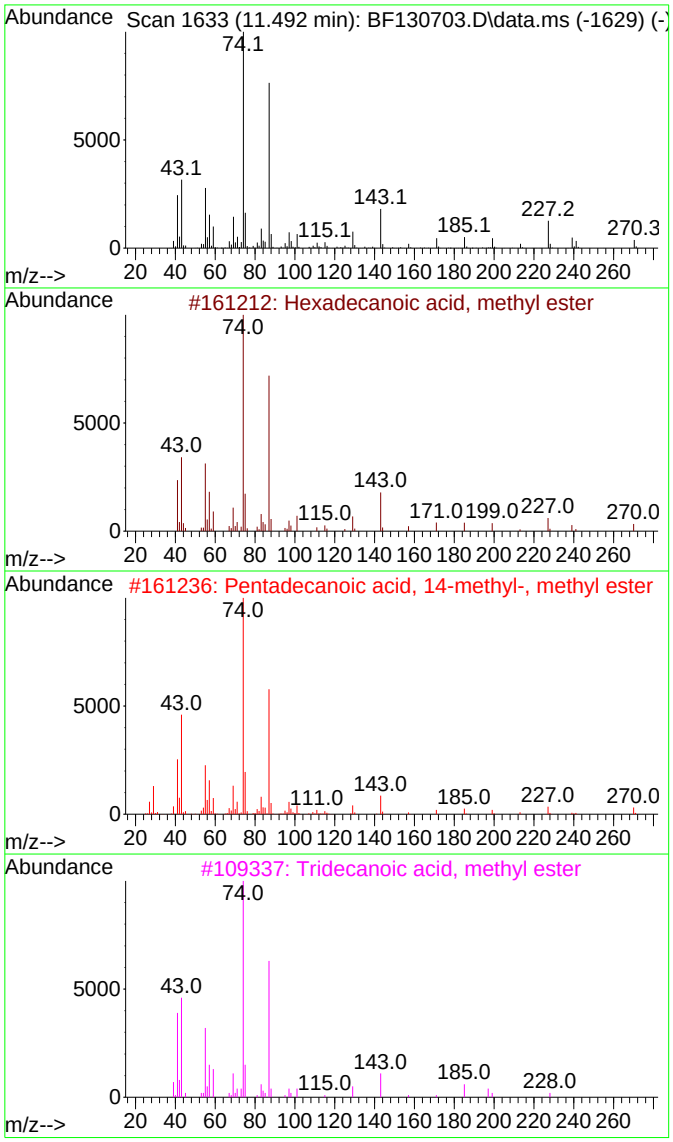
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

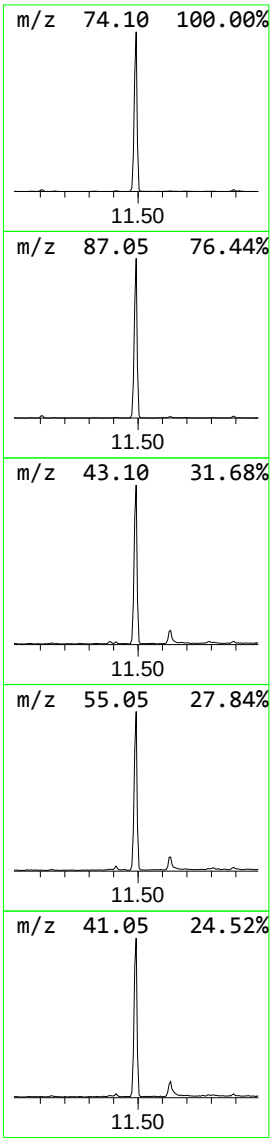
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.492	102.11 ng	1722090	Phenanthrene-d10	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83





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Data File : BF130703.D
Acq On : 18 Oct 2022 17:48
Operator : CG\JU
Sample : N5171-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-101722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

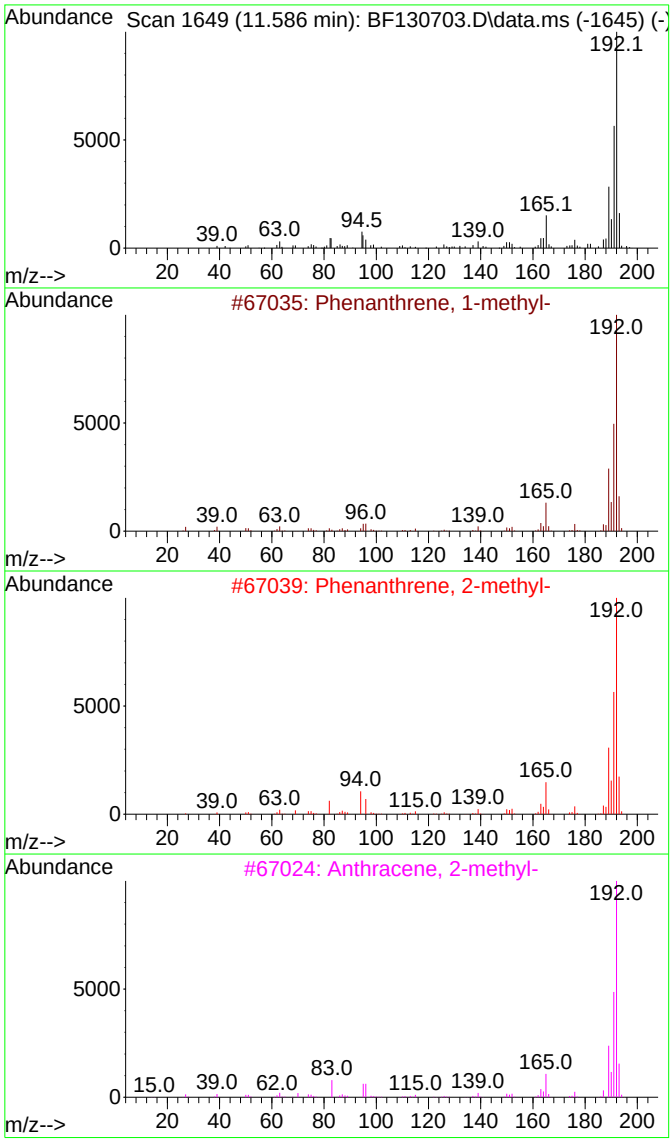
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

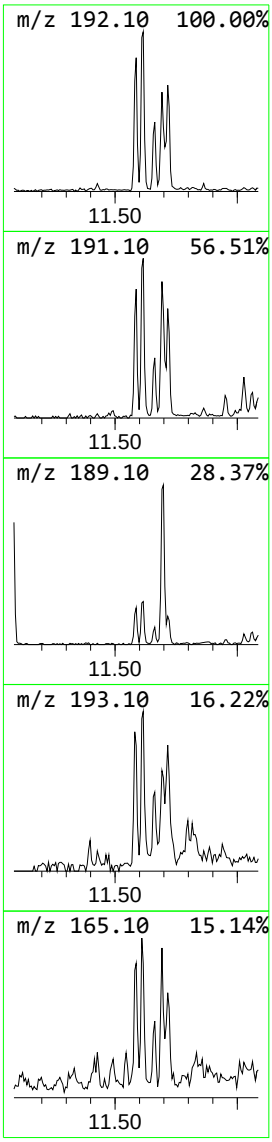
****

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.586	4.27 ng	72068	Phenanthrene-d10	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-101722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

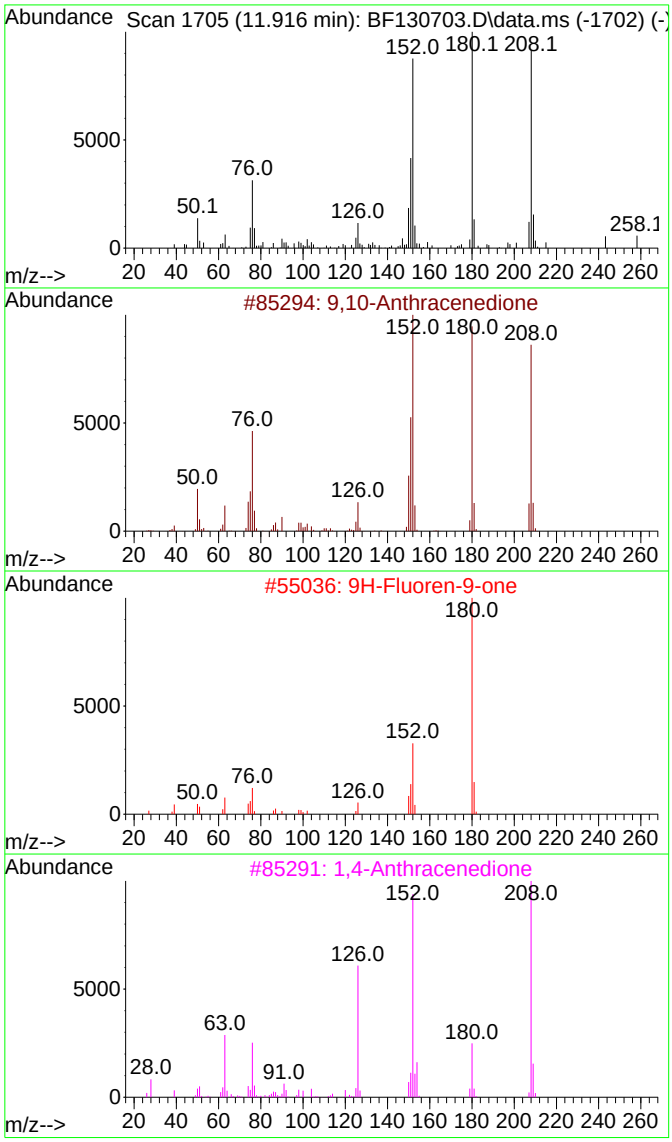
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

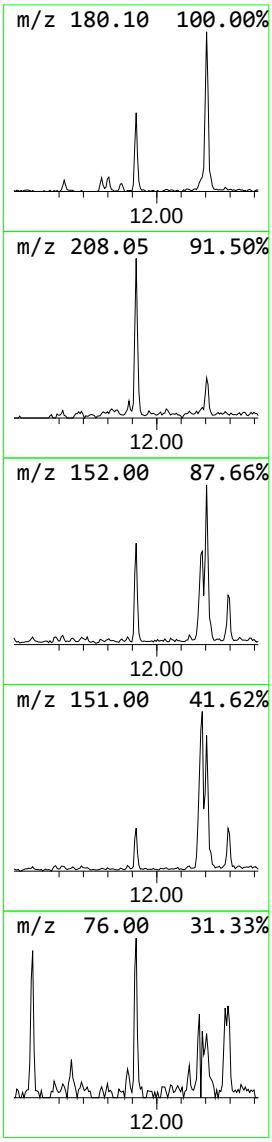
****

Peak Number 4 9,10-Anthracenedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.96 ng	83720	Phenanthrene-d10	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	98
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	64
3	1,4-Anthracenedione	208	C14H8O2	000635-12-1	64
4	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	64
5	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	58





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Instrument :
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ClientSampleId :
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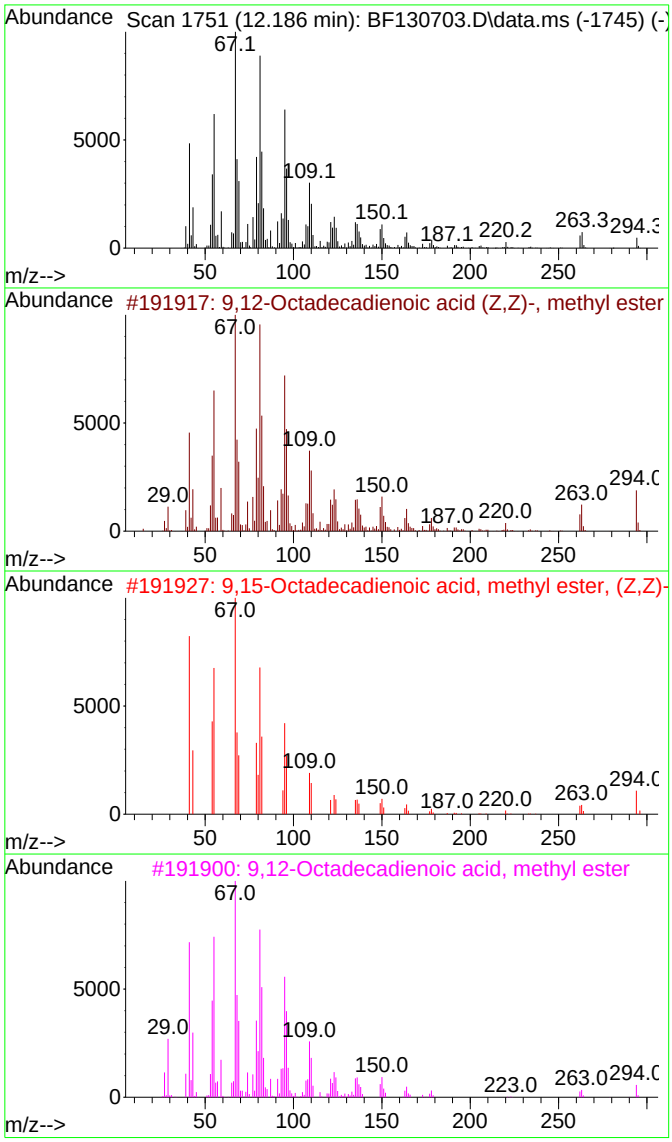
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

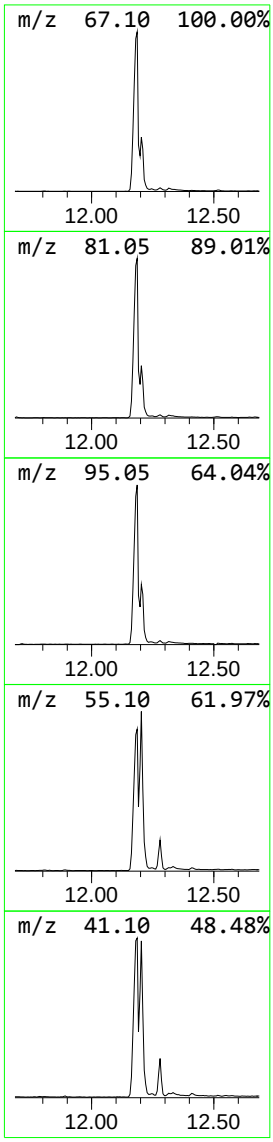
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.186	407.76 ng	6877100	Phenanthrene-d10	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99





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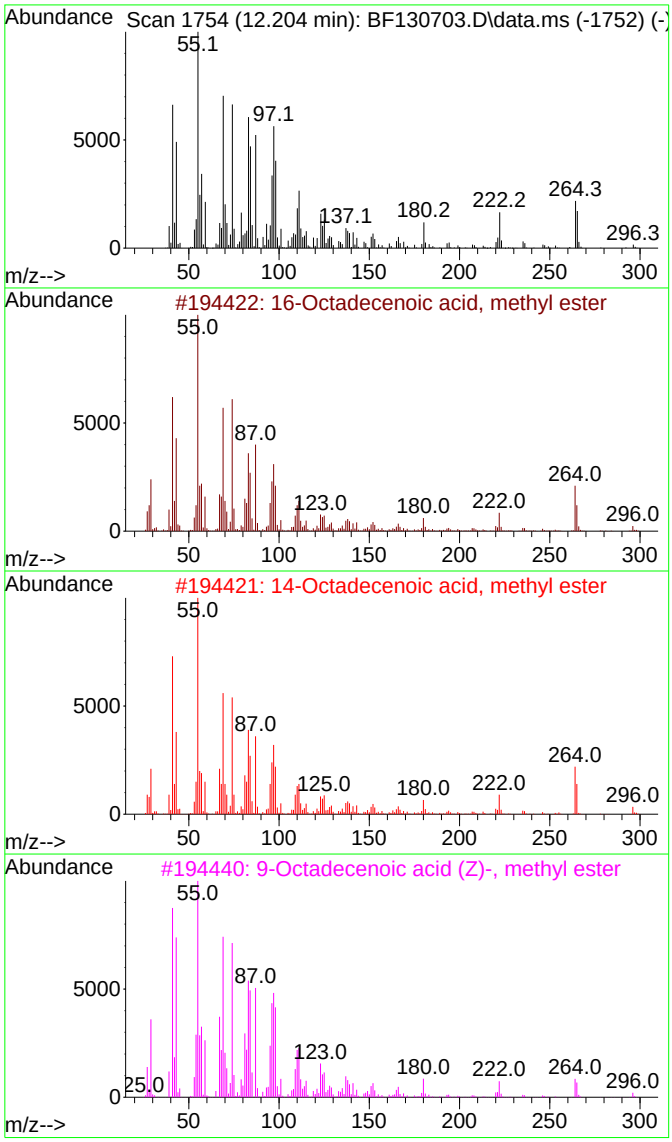
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

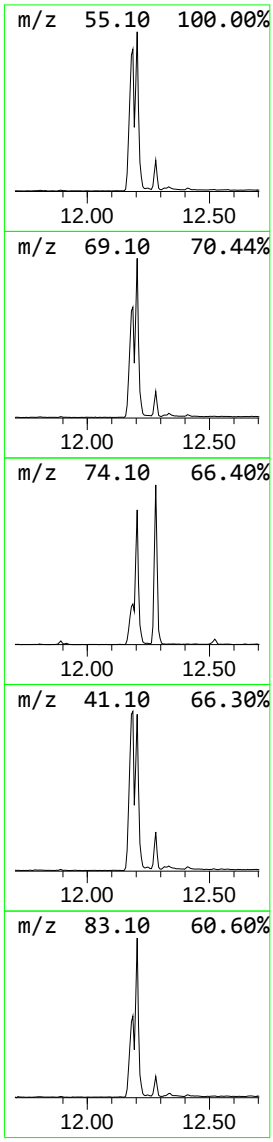
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 16-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.204	255.76 ng	4313590	Phenanthrene-d10	11.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	96
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	95
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	94
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

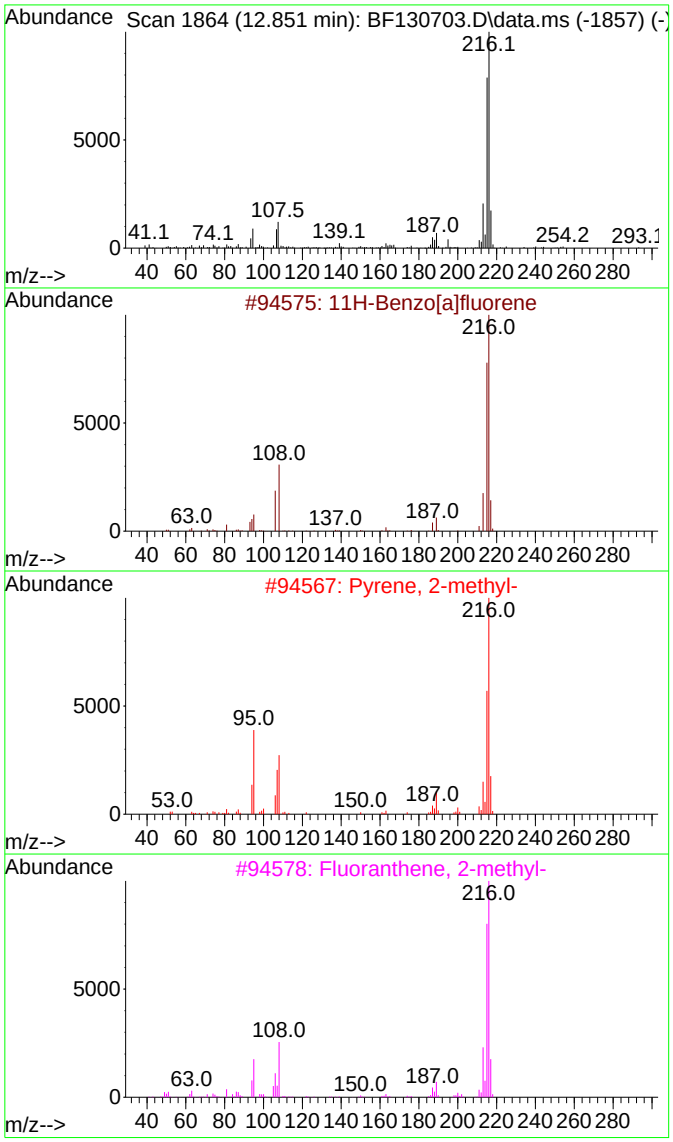
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

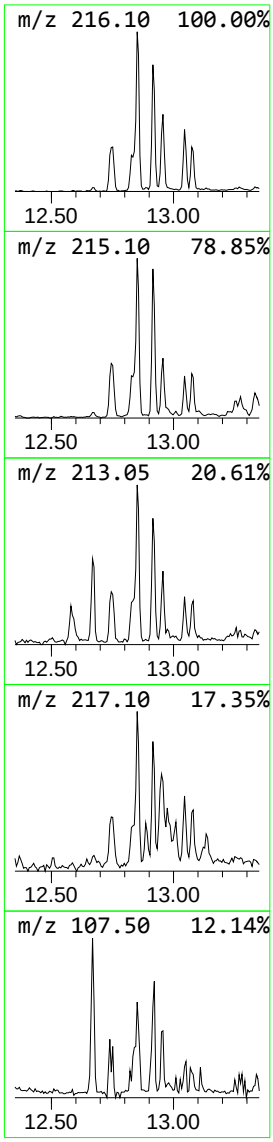
****

Peak Number 7 11H-Benzo[a]fluorene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.851	3.91 ng	268996	Chrysene-d12	13.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91





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Data File : BF130703.D
Acq On : 18 Oct 2022 17:48
Operator : CG\JU
Sample : N5171-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-101722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

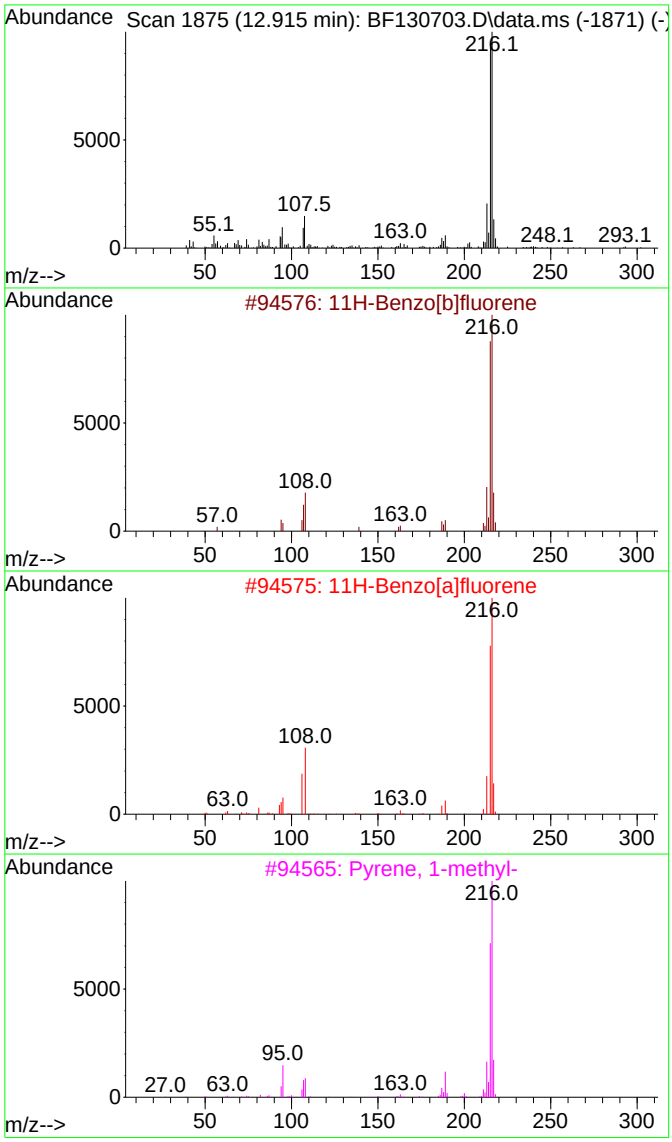
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

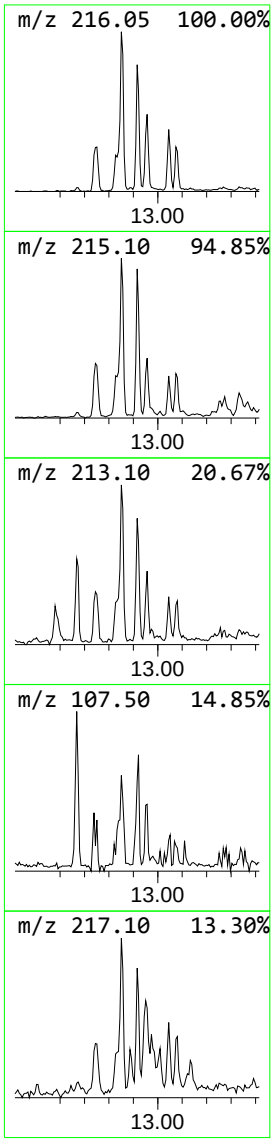
****

Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.915	3.15 ng	216553	Chrysene-d12	13.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	62





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Data File : BF130703.D
Acq On : 18 Oct 2022 17:48
Operator : CG\JU
Sample : N5171-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-101722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.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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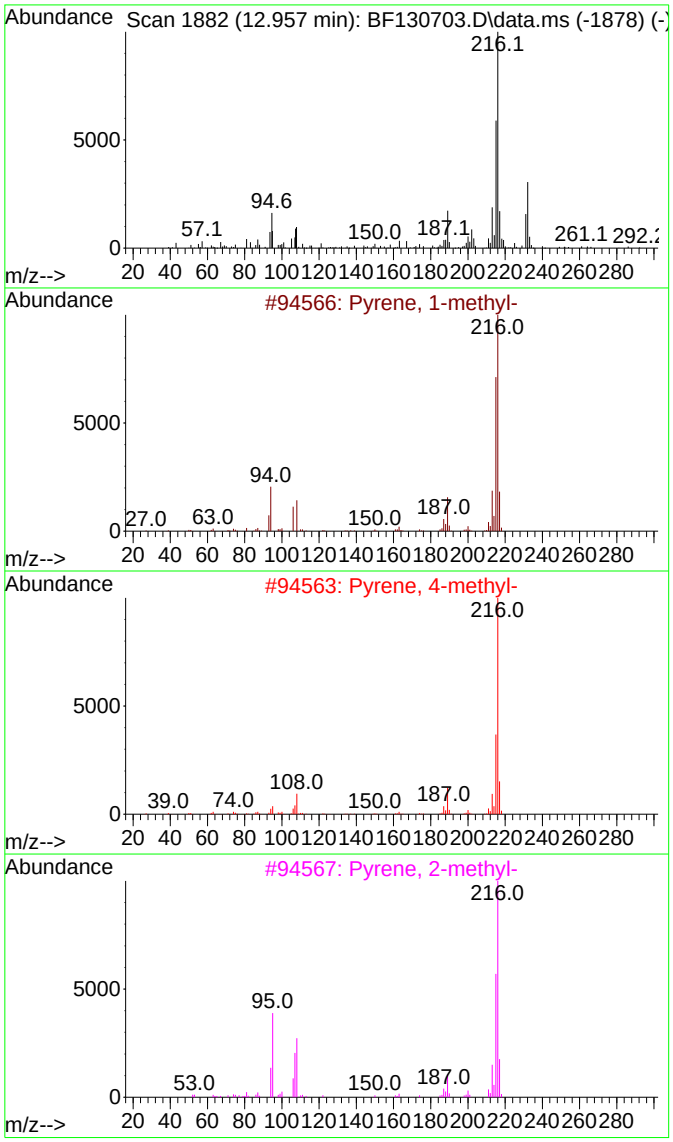
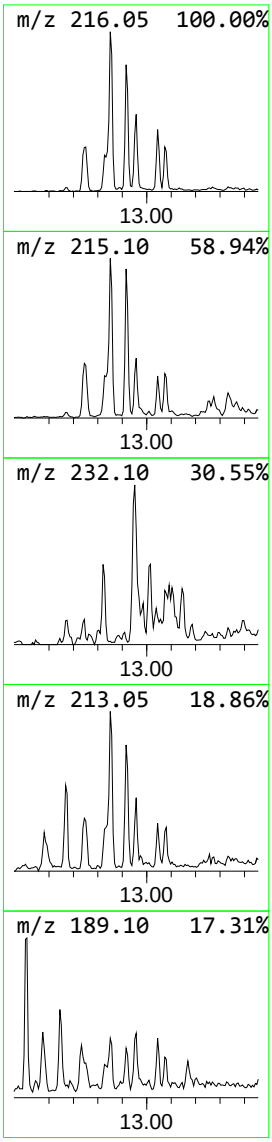
Peak Number 9 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.957	2.95 ng	202854	Chrysene-d12	13.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	Pyrene, 4-methyl-	216	C17H12	003353-12-6	92
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	74





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Operator : CG\JU
Sample : N5171-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.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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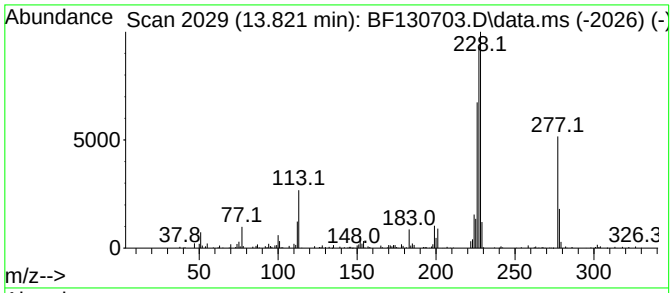
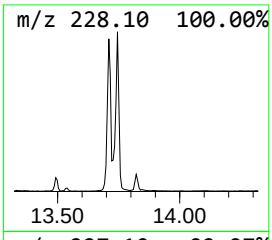
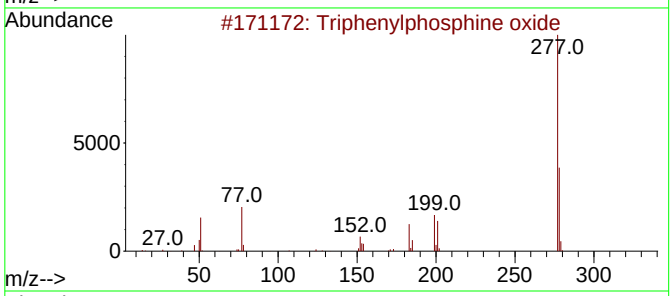
Peak Number 10 unknown13.821 Concentration Rank 13

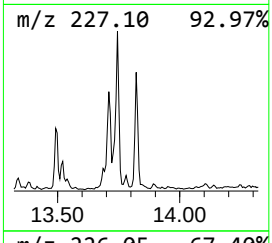
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	2.11 ng	145088	Chrysene-d12	13.721

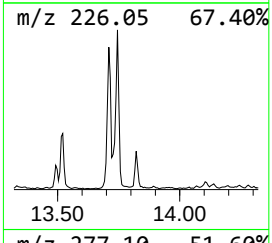
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	44
2	Pyrazole-4-carboxaldehyde-, 3,5-...	228	C14H16N2O	1000272-54-8	43
3	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	42
4	Isothiazol-5-amine, 4-bromo-3-ch...	226	C4H4BrClN2S	1000272-59-9	38
5	Triphenylene	228	C18H12	000217-59-4	27

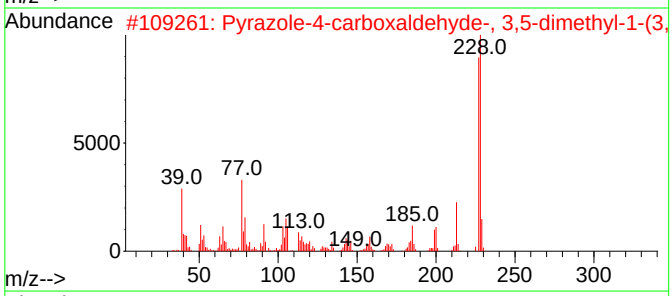


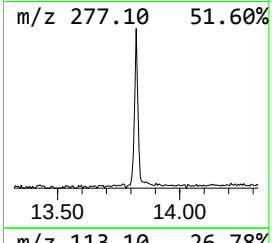


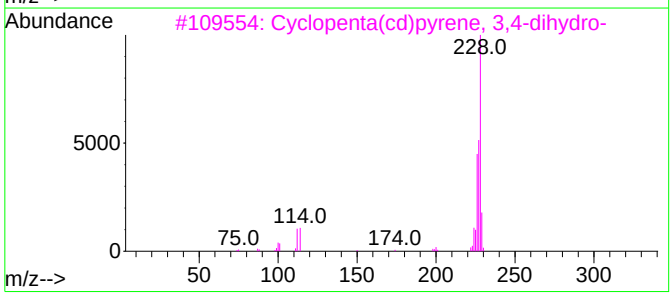


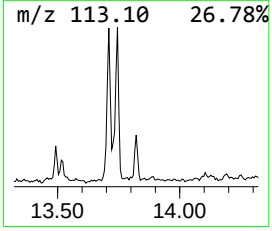












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Acq On : 18 Oct 2022 17:48
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-101722

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.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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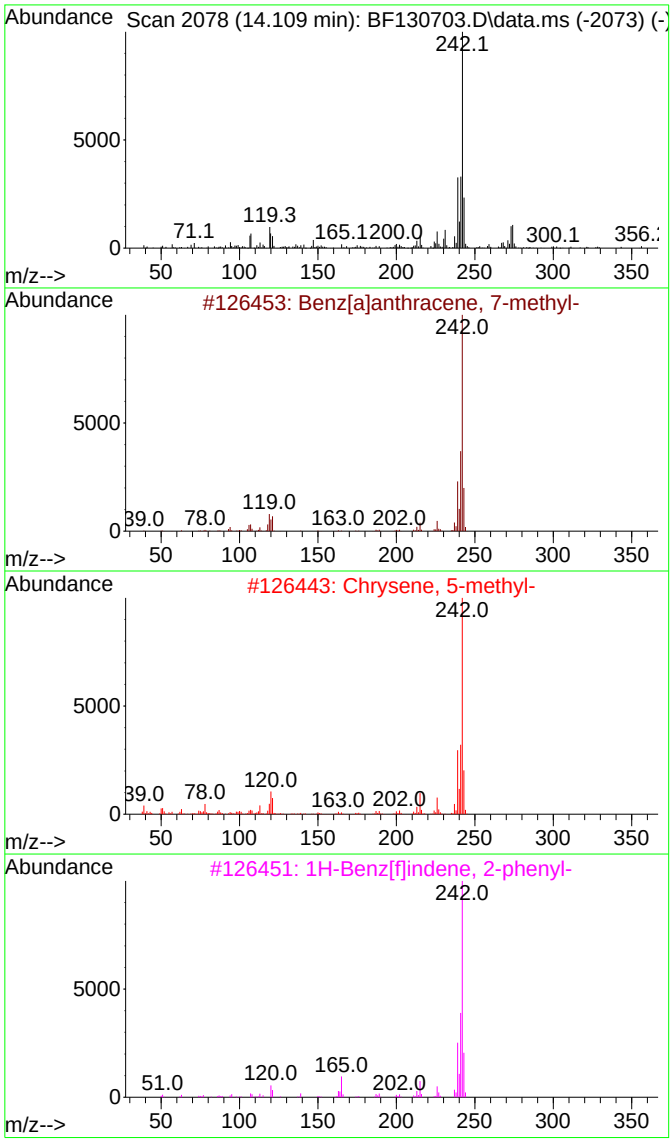
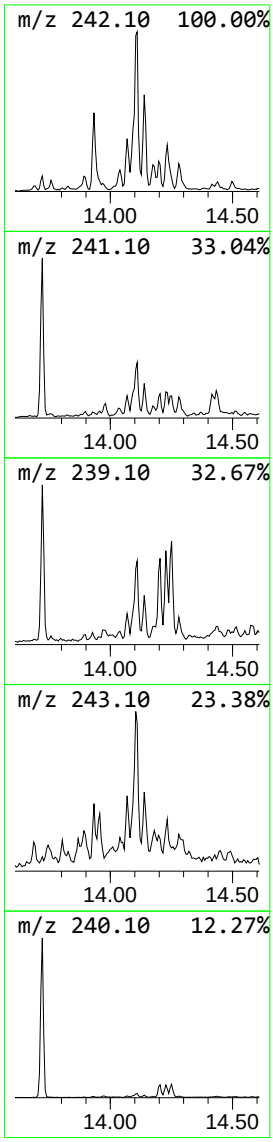
Peak Number 11 Benz[a]anthracene, 7-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	2.66 ng	182955	Chrysene-d12	13.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	96
2	Chrysene, 5-methyl-	242	C19H14	003697-24-3	93
3	1H-Benz[f]indene, 2-phenyl-	242	C19H14	1000305-22-4	92
4	2-Methylchrysene	242	C19H14	003351-32-4	90
5	Chrysene, 1-methyl-	242	C19H14	003351-28-8	89





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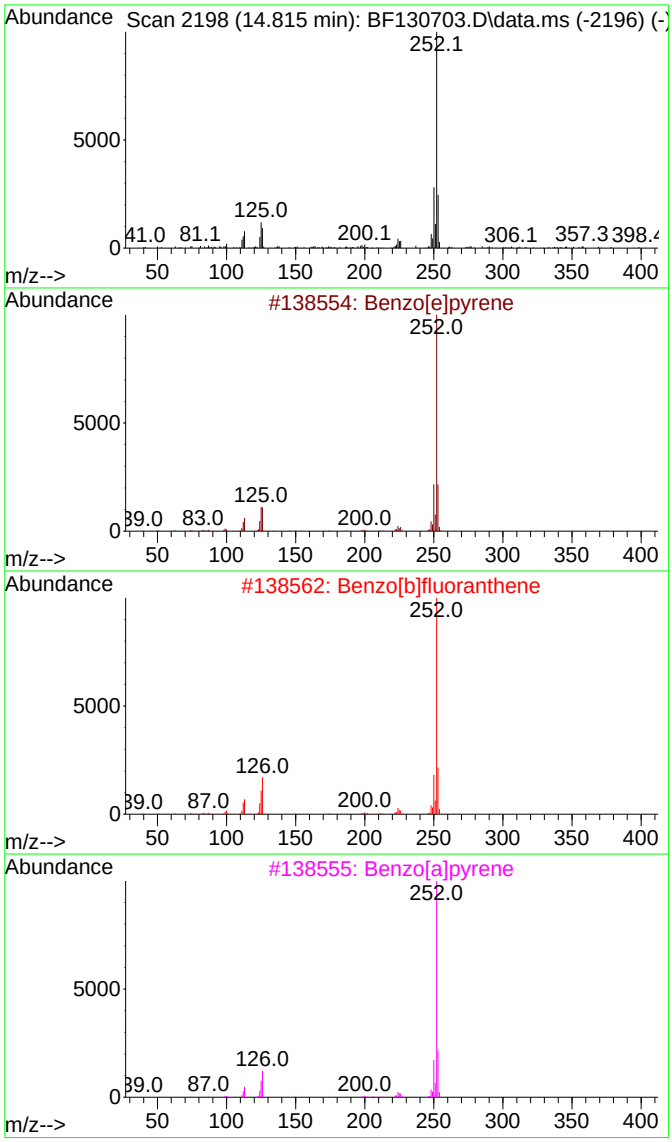
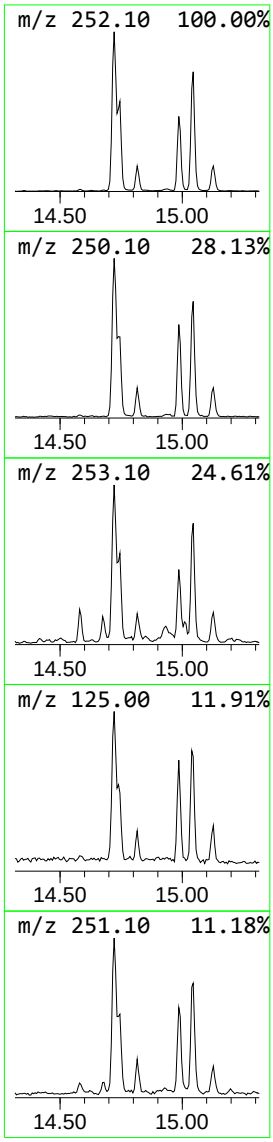
Peak Number 12 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	4.64 ng	90977	Perylene-d12	15.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





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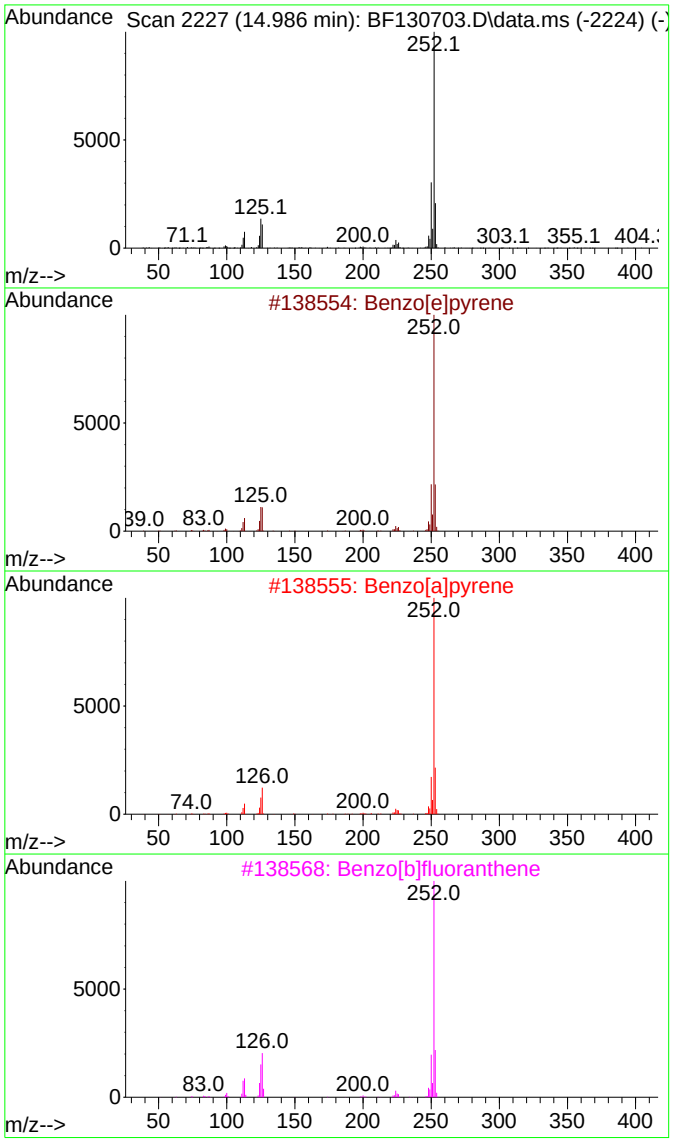
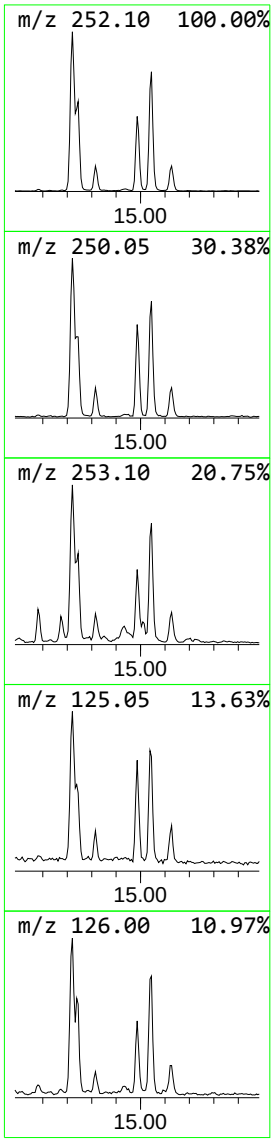
Peak Number 13 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	16.10 ng	315754	Perylene-d12	15.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.739	8.9	ng	165692	1	6.575	371216	20.0
Hexadecanoic ac...	11.492	102.1	ng	1722090	4	11.080	337313	20.0
Phenanthrene, 1...	11.586	4.3	ng	72068	4	11.080	337313	20.0
9,10-Anthracene...	11.916	5.0	ng	83720	4	11.080	337313	20.0
9,12-Octadecadi...	12.186	407.8	ng	6877100	4	11.080	337313	20.0
16-Octadecenoic...	12.204	255.8	ng	4313590	4	11.080	337313	20.0
11H-Benzo[a]flu...	12.851	3.9	ng	268996	5	13.721	1374660	20.0
11H-Benzo[b]flu...	12.915	3.1	ng	216553	5	13.721	1374660	20.0
Pyrene, 1-methyl-	12.957	3.0	ng	202854	5	13.721	1374660	20.0
unknown13.821	13.821	2.1	ng	145088	5	13.721	1374660	20.0
Benz[a]anthrace...	14.110	2.7	ng	182955	5	13.721	1374660	20.0
Benzo[e]pyrene	14.815	4.6	ng	90977	6	15.098	392264	20.0
Perylene	14.986	16.1	ng	315754	6	15.098	392264	20.0