LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HD-02-101023

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-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135764.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	486	489	508	rVB	100887	161687	7.56%	0.908%
2	5.369	555	558	576	rBV	1895610	2137762	100.00%	12.005%
3	6.387	728	731	744	rBV	2084462	2090077	97.77%	11.738%
4	6.734	787	790	797	rBV	653742	584894	27.36%	3.285%
5	7.304	883	887	896	rBV	1502633	1303911	60.99%	7.323%
6	8.016	1005	1008	1014	rBV	814173	691518	32.35%	3.883%
7	9.092	1188	1191	1194	rBV	2550463	2017640	94.38%	11.331%
8	9.169	1200	1204	1208	rVB4	25404	28670	1.34%	0.161%
9	9.210	1208	1211	1215	rBV	37040	39763	1.86%	0.223%
10	9.639	1280	1284	1287	rBV	43138	48205	2.25%	0.271%
11	9.775	1303	1307	1310	rBV	768294	683606	31.98%	3.839%
12	9.804	1310	1312	1320	rVB	38695	41543	1.94%	0.233%
13	10.328	1398	1401	1405	rVB	42002	41000	1.92%	0.230%
14	10.569	1439	1442	1453	rBV	1120615	1010770	47.28%	5.676%
15	10.692	1459	1463	1466	rVB2	31305	34701	1.62%	0.195%
16	11.163	1539	1543	1550	rVB2	41990	63270	2.96%	0.355%
17	11.269	1557	1561	1563	rBV	738587	604056	28.26%	3.392%
18	11.292	1563	1565	1570	rVV	342313	290410	13.58%	1.631%
19	11.351	1572	1575	1578	rVB	68275	63708	2.98%	0.358%
20	11.516	1600	1603	1608	rBV3	27931	30541	1.43%	0.172%
21	11.775	1644	1647	1649	rBV	46050	38773	1.81%	0.218%
22	11.804	1649	1652	1659	rVV	279347	274606	12.85%	1.542%
23	11.886	1663	1666	1669	rBV	121069	104519	4.89%	0.587%
24	12.074	1695	1698	1702	rVB	33846	30714	1.44%	0.172%
25	12.116	1703	1705	1708	rVB	28483	25954	1.21%	0.146%
26	12.327	1738	1741	1743	rBV	41610	36321	1.70%	0.204%
27	12.492	1766	1769	1775	rBV	691316	605249	28.31%	3.399%
28	12.592	1784	1786	1792	rBV4	56171	73373	3.43%	0.412%
29	12.645	1792	1795	1798	rVV	53243	52862	2.47%	0.297%
30	12.722	1802	1808	1815	rVV	615966	672670	31.47%	3.778%
31	12.780	1815	1818	1822	rVV2	27564	31746	1.49%	0.178%
32	12.863	1828	1832	1836	rBV	1718745	1599413	74.82%	8.982%
33	12.892	1836	1837	1842	rVB	28025	33453	1.56%	0.188%
34	12.945	1842	1846	1850	rBV2	44053	84046	3.93%	0.472%
35	13.033	1858	1861	1863	rBV3	44428	61056	2.86%	0.343%
36	13.057	1863	1865	1868	rVB	63291	54842	2.57%	0.308%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

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-BF101323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.121	1874	1876	1879	rVB2	42638	35478	1.66%	0.199%
38	13.163	1880	1883	1890	rVB3	64557	77205	3.61%	0.434%
39	13.257	1897	1899	1901	rVB	39532	28331	1.33%	0.159%
40	13.286	1902	1904	1907	rBV2	37434	40430	1.89%	0.227%
41	13.739	1978	1981	1983	rBV	54885	68033	3.18%	0.382%
42	13.933	2010	2014	2017	rBV2	604133	739167	34.58%	4.151%
43	13.963	2017	2019	2023	rVB	240065	202266	9.46%	1.136%
44	14.986	2190	2193	2196	rBV	187010	235036	10.99%	1.320%
45	15.292	2242	2245	2249	rVB	99670	120150	5.62%	0.675%
46	15.351	2253	2255	2260	rVB	134659	156655	7.33%	0.880%
47	15.415	2262	2266	2270	rBV	297904	356550	16.68%	2.002%

Sum of corrected areas: 17806630

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
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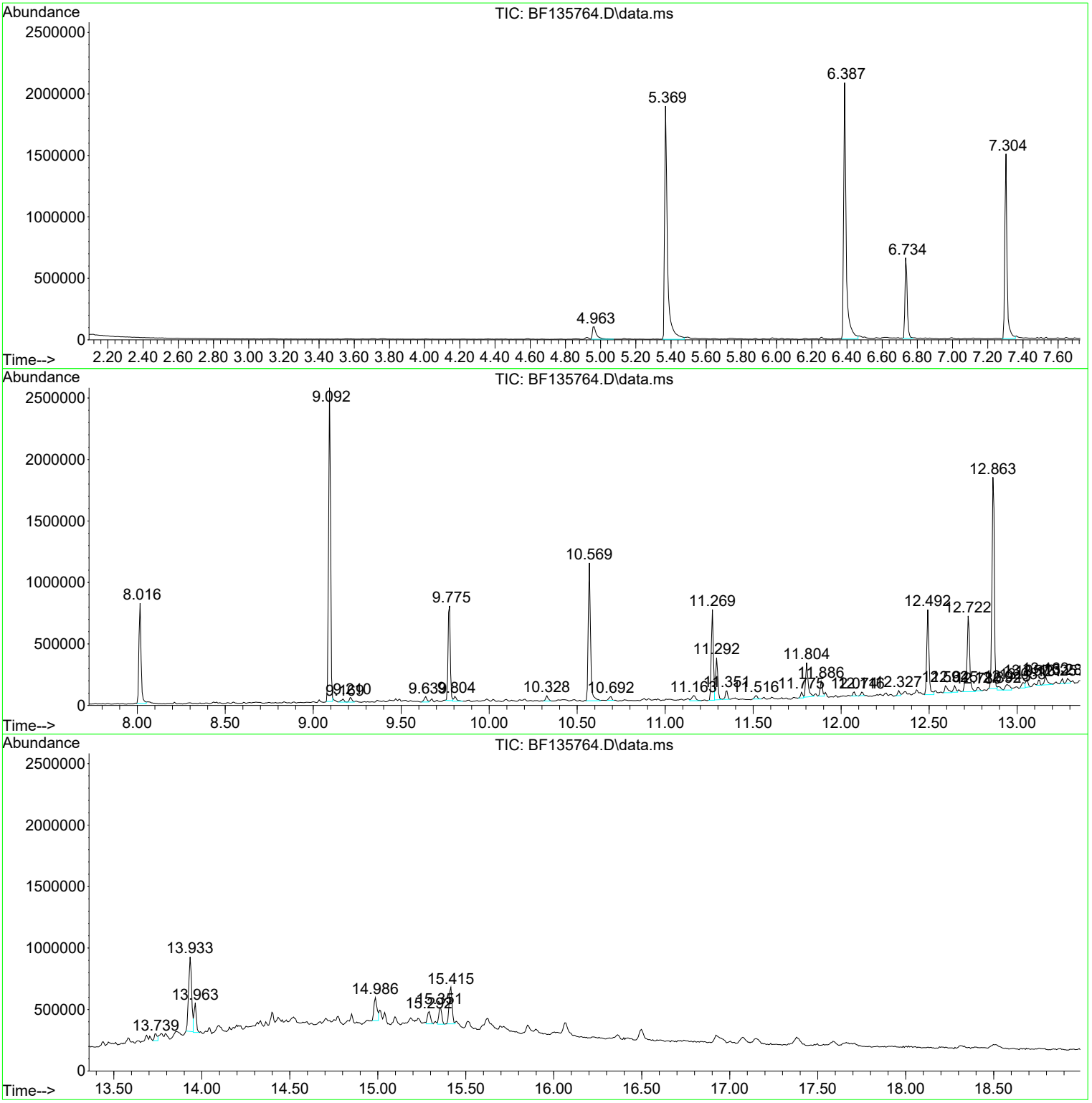
Instrument :
BNA_F
ClientSampleId :
HD-02-101023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

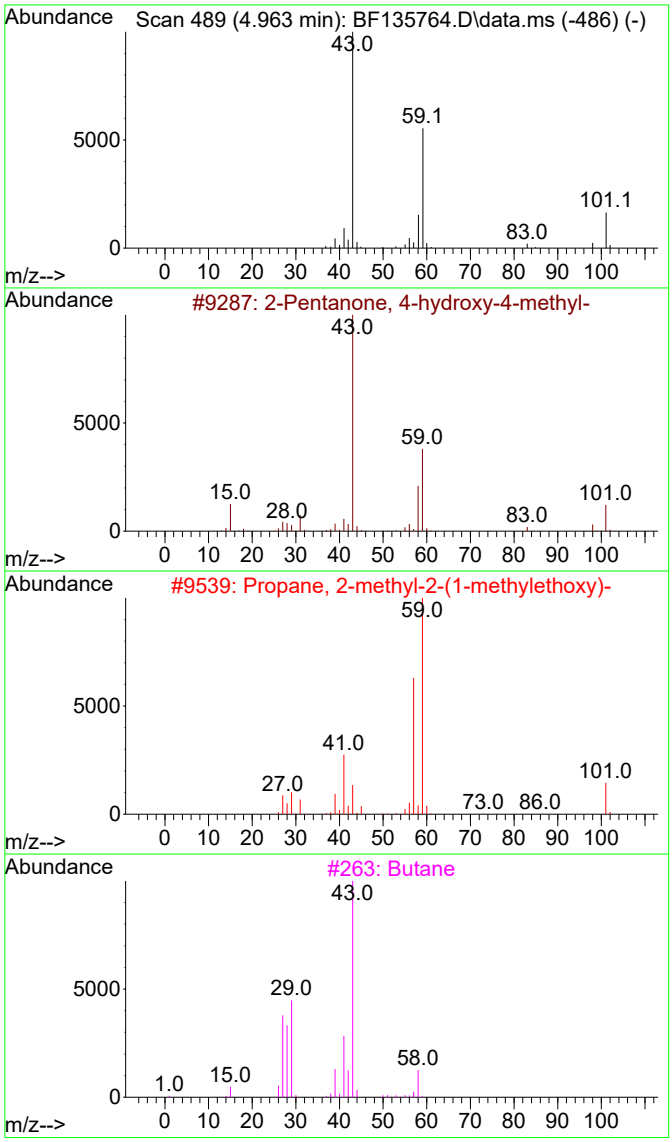
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

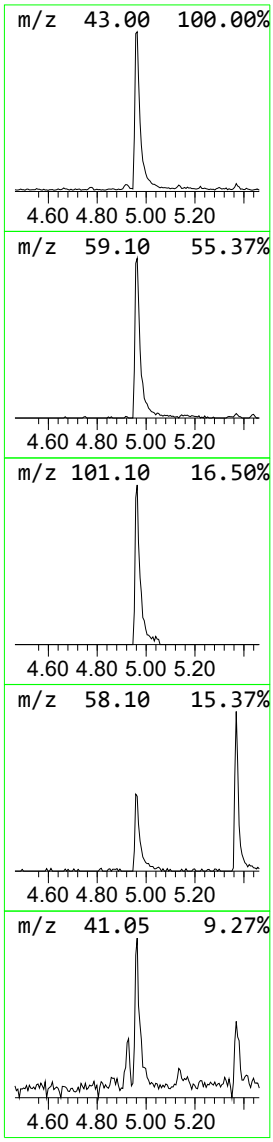
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	5.53 ng	161687	1,4-Dichlorobenzene-d4	6.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Butane	58	C4H10	000106-97-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

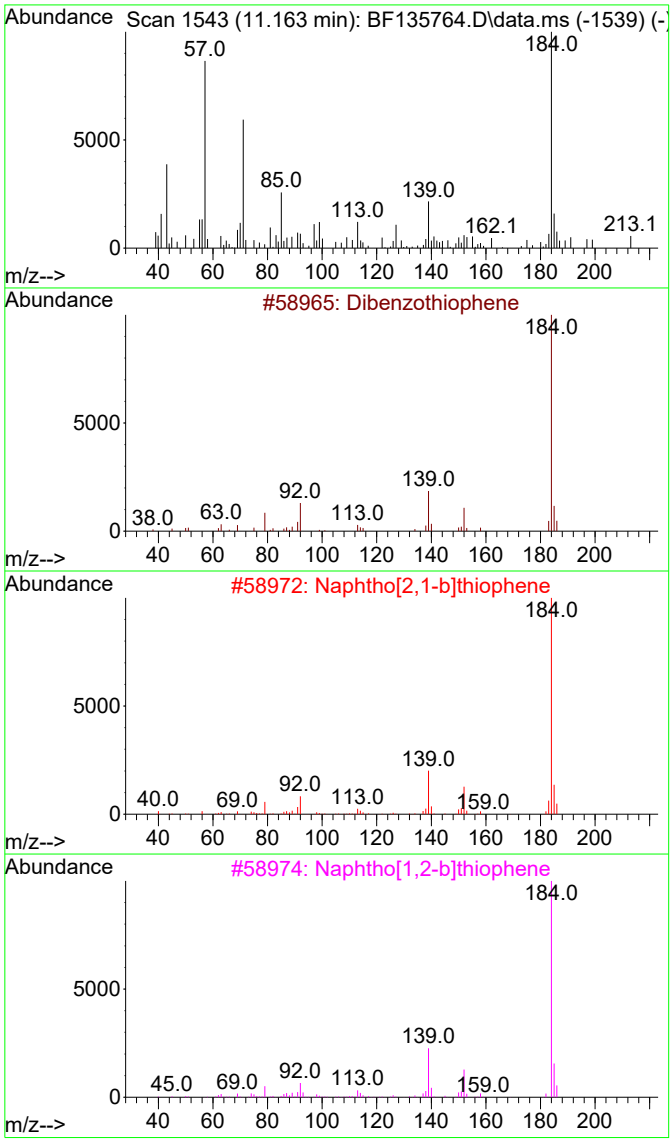
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

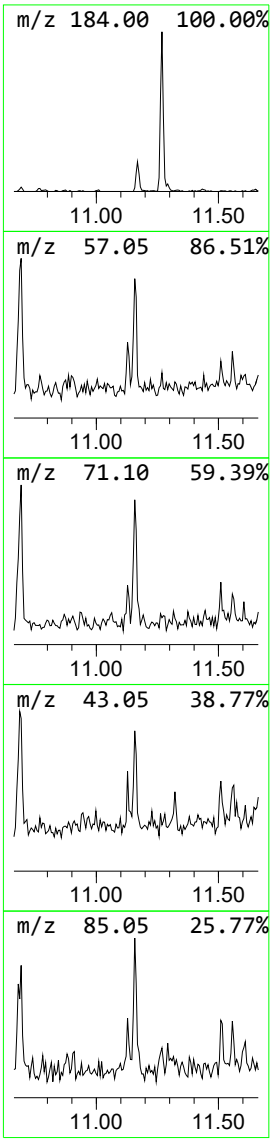
****

Peak Number 2 Dibenzothiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.163	2.09 ng	63270	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	55
2	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	55
3	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	55
4	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	46
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

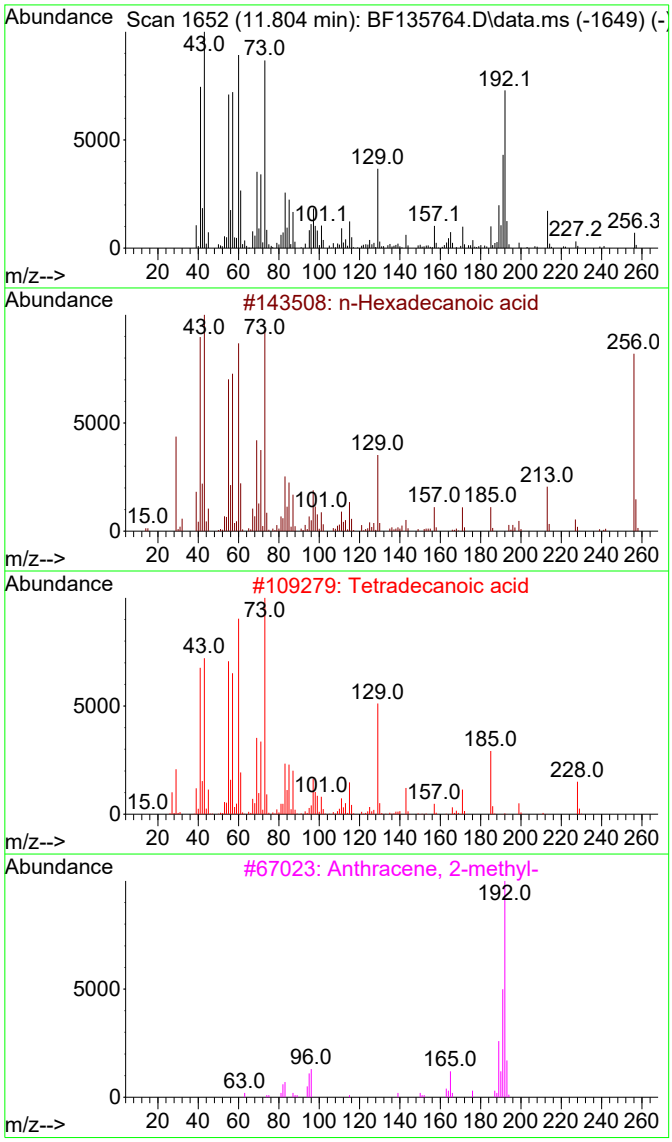
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

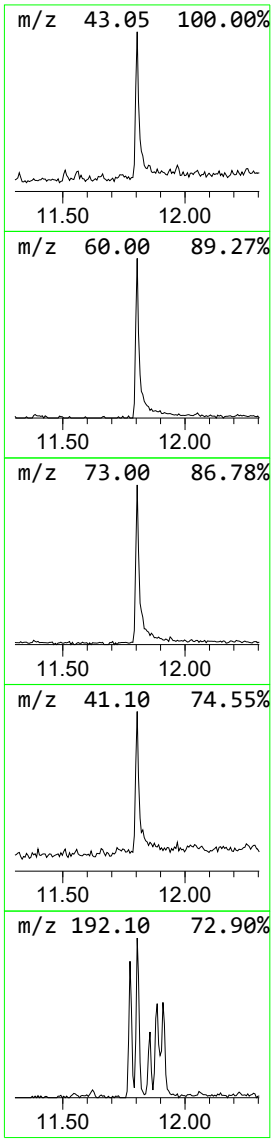
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	9.09 ng	274606	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	89
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

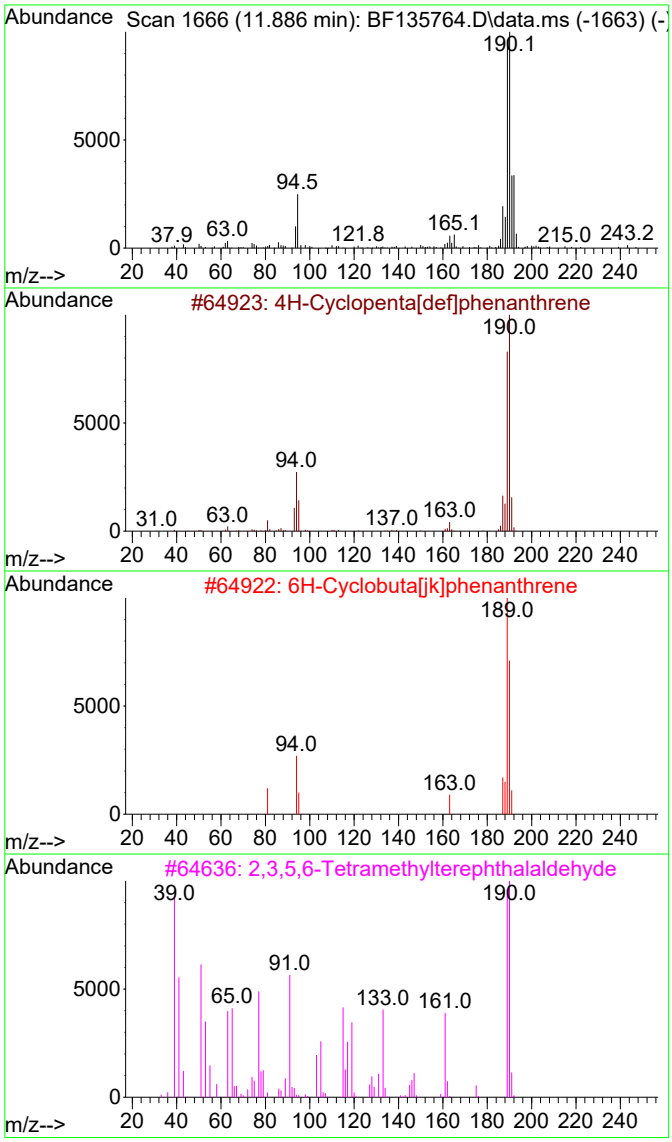
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

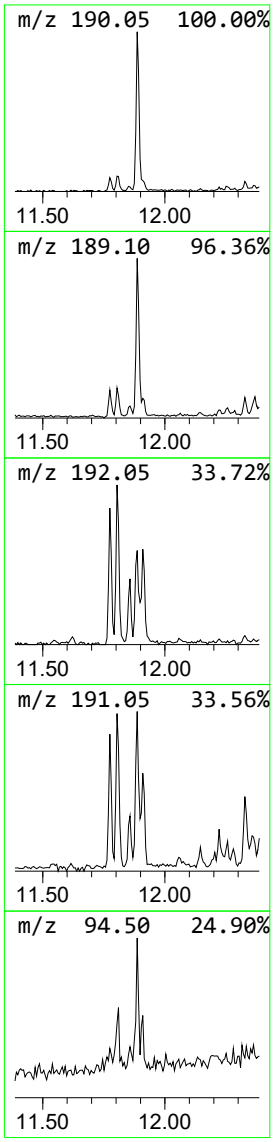
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.46 ng	104519	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
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Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

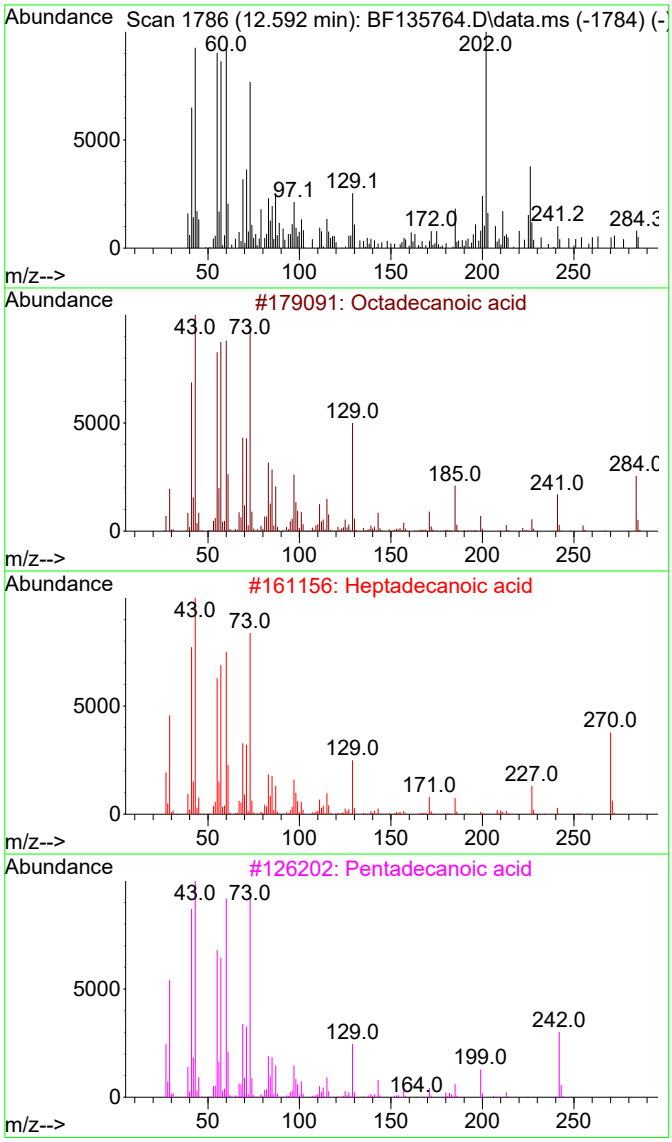
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

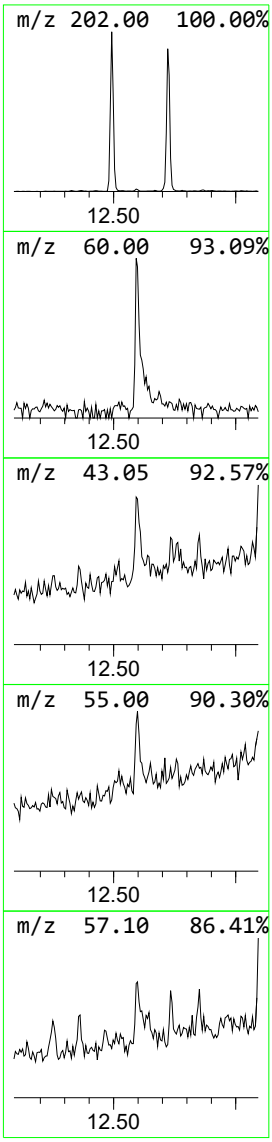
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.592	2.43 ng	73373	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	55
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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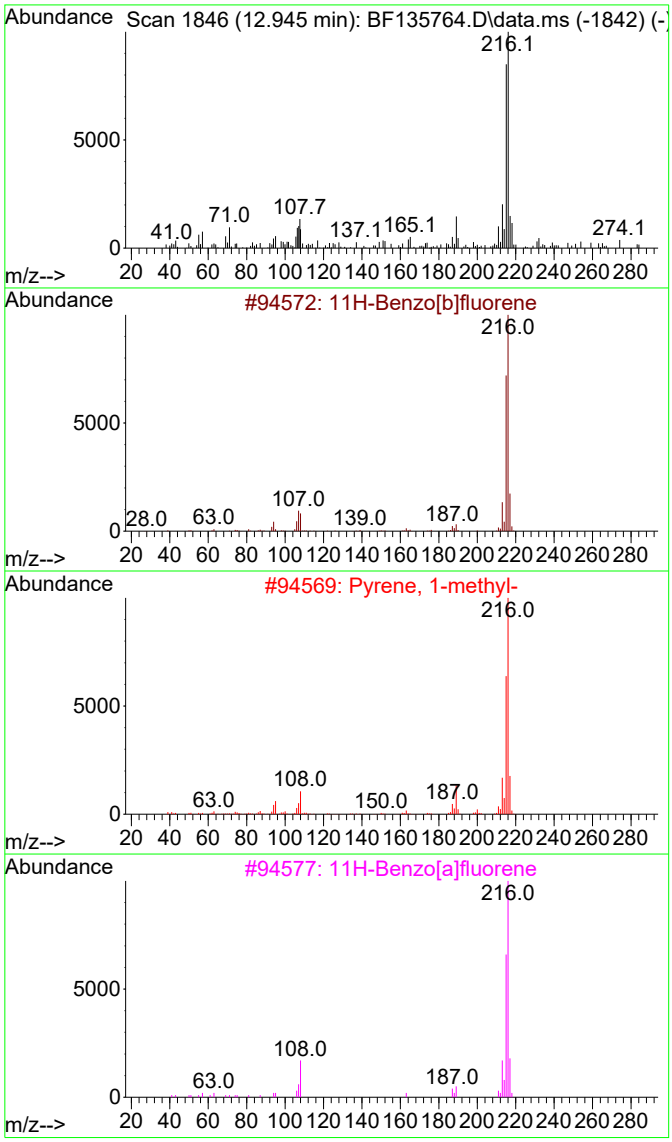
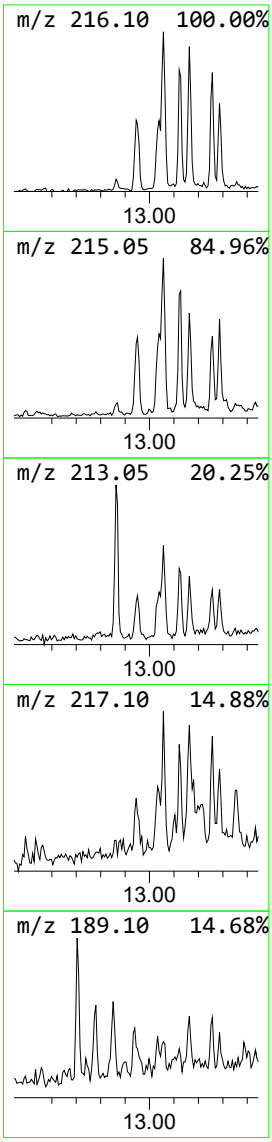
Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.945	2.27 ng	84046	Chrysene-d12	13.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	76
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	68
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	64
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

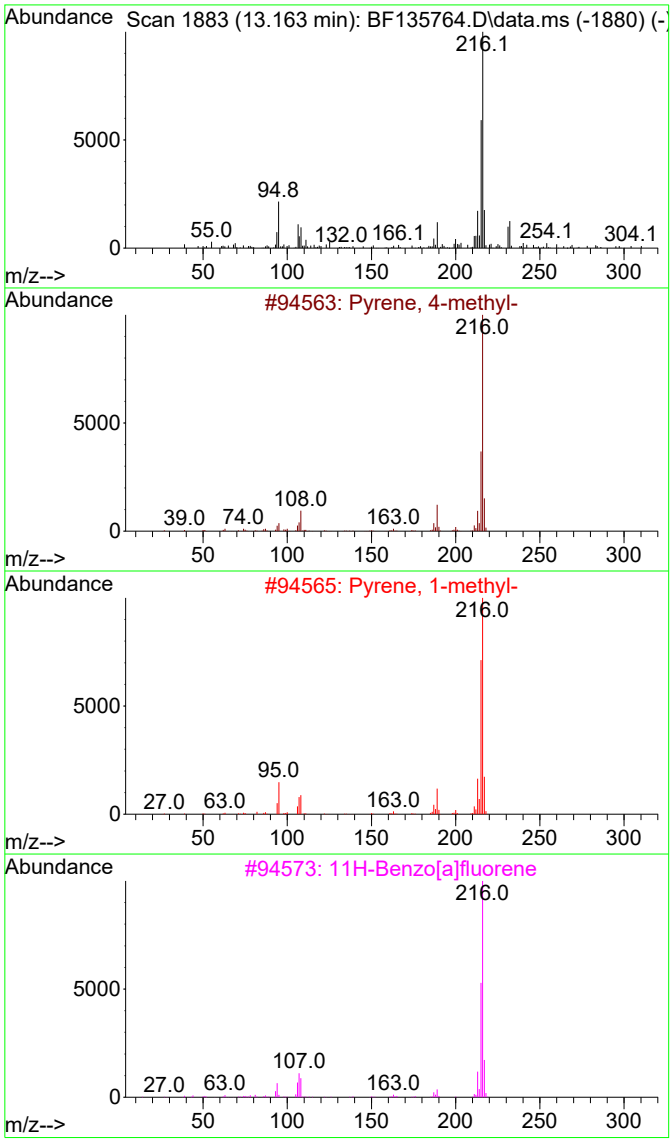
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

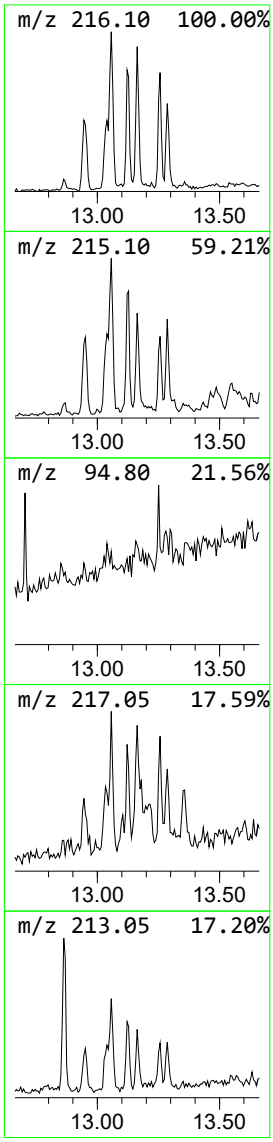
****

Peak Number 7 Pyrene, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	2.09 ng	77205	Chrysene-d12	13.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 4-methyl-	216	C17H12	003353-12-6	92
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	76
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	70
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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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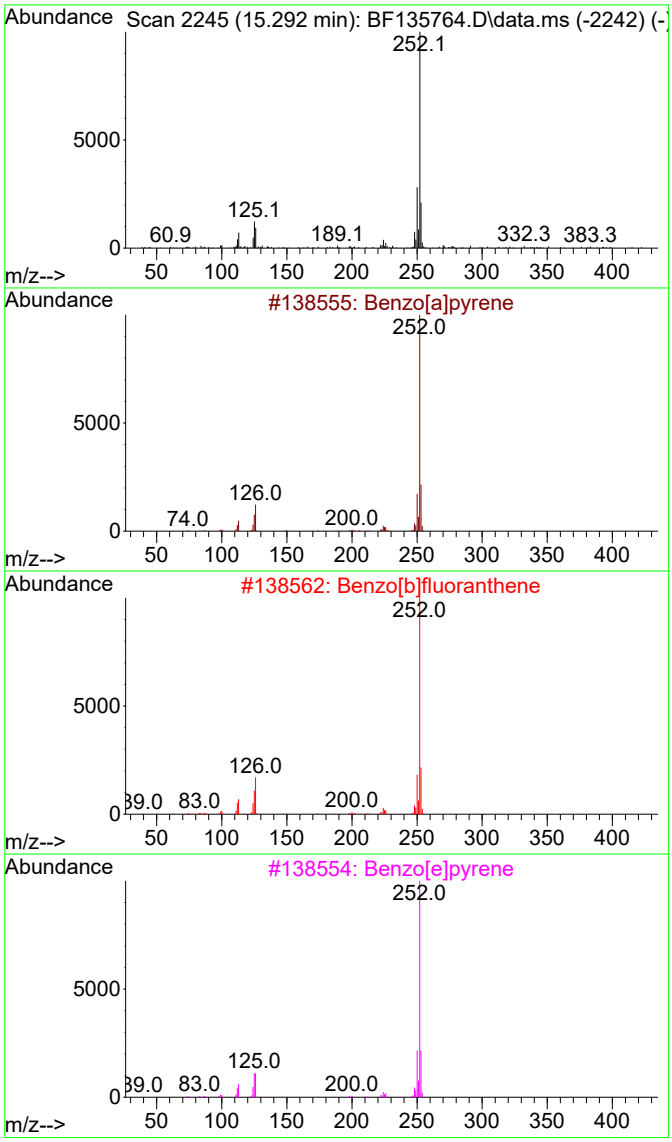
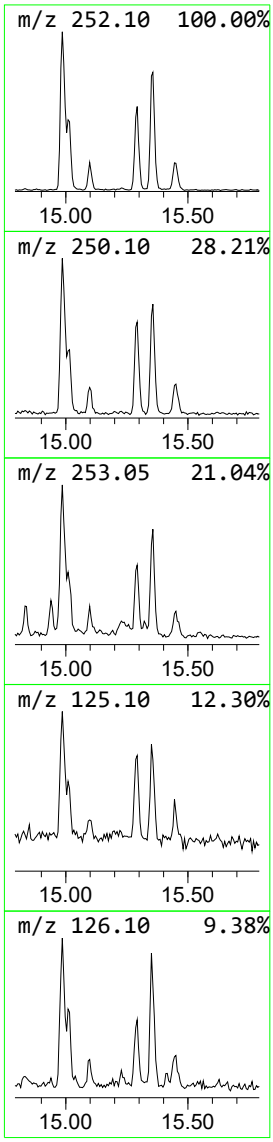
Peak Number 8 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	6.74 ng	120150	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	95
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3	Benzo[e]pyrene	252	C20H12	000192-97-2	91
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5	Perylene	252	C20H12	000198-55-0	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101323\
Data File : BF135764.D
Acq On : 13 Oct 2023 21:13
Operator : CG\JU
Sample : 04839-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-101023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
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-...	4.963	5.5	ng	161687	1	6.734	584894	20.0
Dibenzothiophene	11.163	2.1	ng	63270	4	11.269	604056	20.0
n-Hexadecanoic ...	11.804	9.1	ng	274606	4	11.269	604056	20.0
4H-Cyclopenta[d...	11.886	3.5	ng	104519	4	11.269	604056	20.0
Octadecanoic acid	12.592	2.4	ng	73373	4	11.269	604056	20.0
11H-Benzo[b]flu...	12.945	2.3	ng	84046	5	13.933	739167	20.0
Pyrene, 4-methyl-	13.163	2.1	ng	77205	5	13.933	739167	20.0
Benzo[e]pyrene	15.292	6.7	ng	120150	6	15.416	356550	20.0