LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020223\
Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-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-BF013123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132313.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.248	236	240	246	rVB	30794	37771	1.27%	0.119%
2	5.307	414	420	428	rBV	931285	1067068	35.97%	3.361%
3	5.690	480	485	488	rBV	2795825	2686096	90.54%	8.461%
4	6.678	648	653	656	rBV	2570552	2526283	85.15%	7.957%
5	6.889	685	689	693	rBV3	32322	33463	1.13%	0.105%
6	7.066	715	719	722	rBV	1140642	896791	30.23%	2.825%
7	7.625	810	814	817	rBV	1911184	1713938	57.77%	5.399%
8	8.354	934	938	941	rBV	1251404	1100900	37.11%	3.468%
9	9.430	1117	1121	1124	rBV	3298238	2966827	100.00%	9.345%
10	9.977	1211	1214	1218	rBV	63569	59927	2.02%	0.189%
11	10.119	1234	1238	1241	rBV	1222788	1053571	35.51%	3.319%
12	10.148	1241	1243	1246	rVB	69213	50668	1.71%	0.160%
13	10.319	1269	1272	1275	rVB2	41071	38828	1.31%	0.122%
14	10.530	1304	1308	1312	rVB3	34397	41568	1.40%	0.131%
15	10.666	1328	1331	1337	rVB	88031	76602	2.58%	0.241%
16	10.830	1355	1359	1362	rVB2	102954	94318	3.18%	0.297%
17	10.907	1368	1372	1376	rBV	1961965	1658910	55.92%	5.225%
18	11.007	1387	1389	1399	rVB6	31671	64577	2.18%	0.203%
19	11.219	1420	1425	1427	rBV4	34694	51060	1.72%	0.161%
20	11.413	1456	1458	1461	rVB3	32988	32888	1.11%	0.104%
21	11.460	1463	1466	1469	rBV2	38278	37952	1.28%	0.120%
22	11.613	1489	1492	1495	rBV	1059390	996697	33.59%	3.139%
23	11.636	1495	1496	1500	rVB	576522	423746	14.28%	1.335%
24	11.689	1500	1505	1508	rBV	189336	167520	5.65%	0.528%
25	12.119	1575	1578	1581	rBV	467296	473314	15.95%	1.491%
26	12.148	1581	1583	1586	rVB	187870	147744	4.98%	0.465%
27	12.195	1588	1591	1594	rVB	77712	64798	2.18%	0.204%
28	12.236	1594	1598	1600	rBV2	214881	261388	8.81%	0.823%
29	12.301	1606	1609	1611	rBV2	42329	36059	1.22%	0.114%
30	12.413	1625	1628	1631	rBV	98763	93834	3.16%	0.296%
31	12.442	1631	1633	1638	rVB2	48915	49644	1.67%	0.156%
32	12.566	1652	1654	1656	rVB2	47948	32705	1.10%	0.103%
33	12.671	1669	1672	1674	rBV	138701	136525	4.60%	0.430%
34	12.760	1684	1687	1693	rBV2	104774	137259	4.63%	0.432%
35	12.836	1697	1700	1704	rBV	1187470	1111884	37.48%	3.502%
36	12.913	1709	1713	1715	rBV2	129462	134300	4.53%	0.423%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020223\
Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-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-BF013123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.995	1725	1727	1728	rBV	46671	34036	1.15%	0.107%
38	13.071	1734	1740	1745	rBV	1461615	1494662	50.38%	4.708%
39	13.118	1745	1748	1752	rVB2	77459	93944	3.17%	0.296%
40	13.207	1759	1763	1770	rVB	2623590	2389545	80.54%	7.527%
41	13.289	1773	1777	1784	rBV4	120367	222937	7.51%	0.702%
42	13.377	1789	1792	1793	rVV3	95514	108455	3.66%	0.342%
43	13.401	1793	1796	1798	rVB	215326	210669	7.10%	0.664%
44	13.465	1804	1807	1810	rBV	164419	130796	4.41%	0.412%
45	13.507	1811	1814	1816	rVB3	186330	164708	5.55%	0.519%
46	13.601	1827	1830	1832	rBV	146135	121806	4.11%	0.384%
47	13.630	1832	1835	1838	rVV	140502	118097	3.98%	0.372%
48	13.907	1880	1882	1887	rVB	116748	127950	4.31%	0.403%
49	14.054	1905	1907	1909	rBV	146321	100027	3.37%	0.315%
50	14.095	1909	1914	1917	rBV3	375361	519552	17.51%	1.637%
51	14.277	1940	1945	1948	rBV2	1170452	1740262	58.66%	5.482%
52	14.307	1948	1950	1955	rVB	737432	626422	21.11%	1.973%
53	14.389	1961	1964	1967	rBV	100295	99041	3.34%	0.312%
54	14.671	2010	2012	2015	rVB	171233	135892	4.58%	0.428%
55	15.389	2130	2134	2138	rBV	543700	922891	31.11%	2.907%
56	15.730	2188	2192	2198	rVB	370735	482485	16.26%	1.520%
57	15.801	2200	2204	2210	rVB	461170	635794	21.43%	2.003%
58	15.871	2211	2216	2219	rBV	520934	710252	23.94%	2.237%

Sum of corrected areas: 31747646

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Data File : BF132313.D
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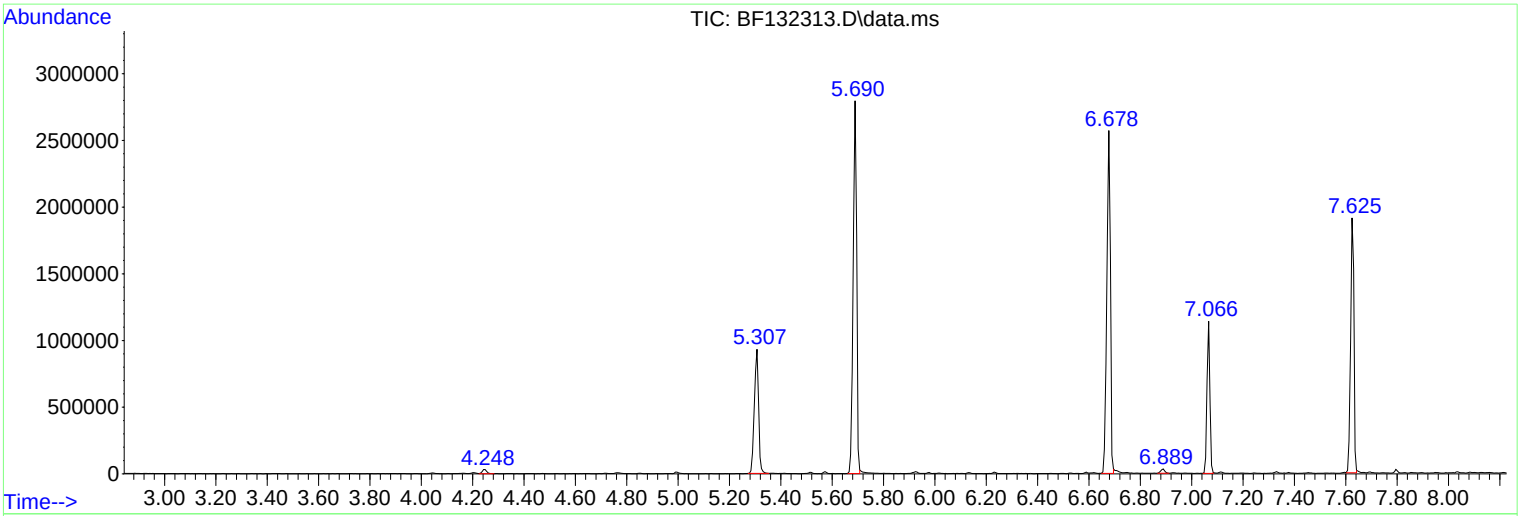
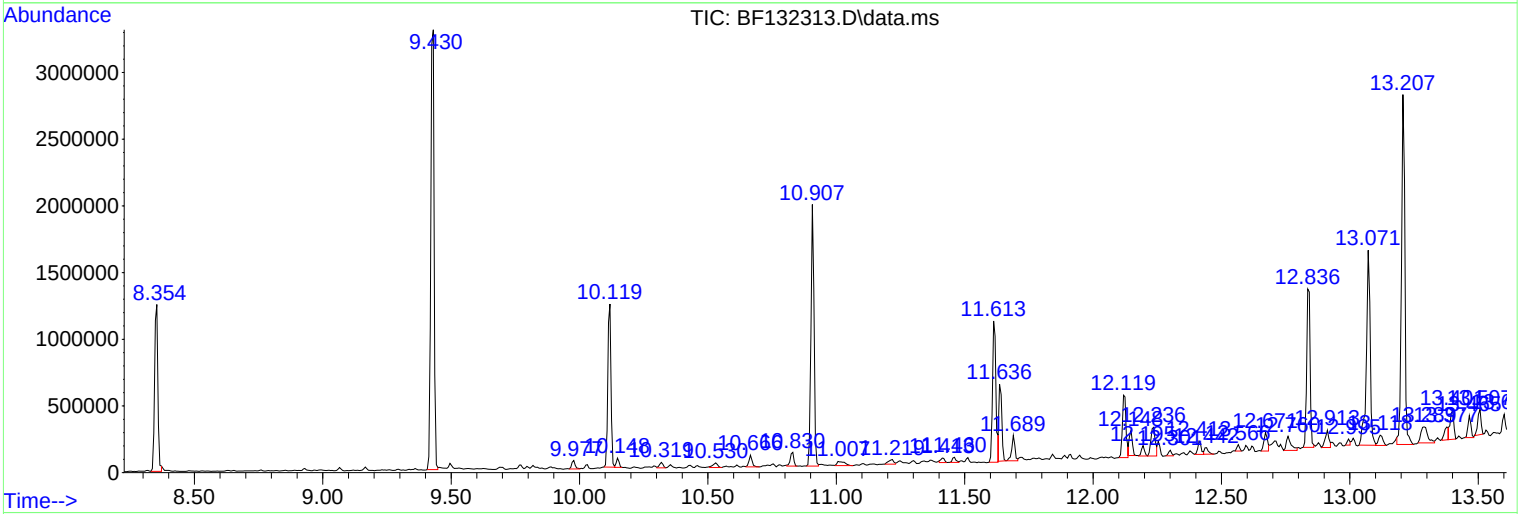
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

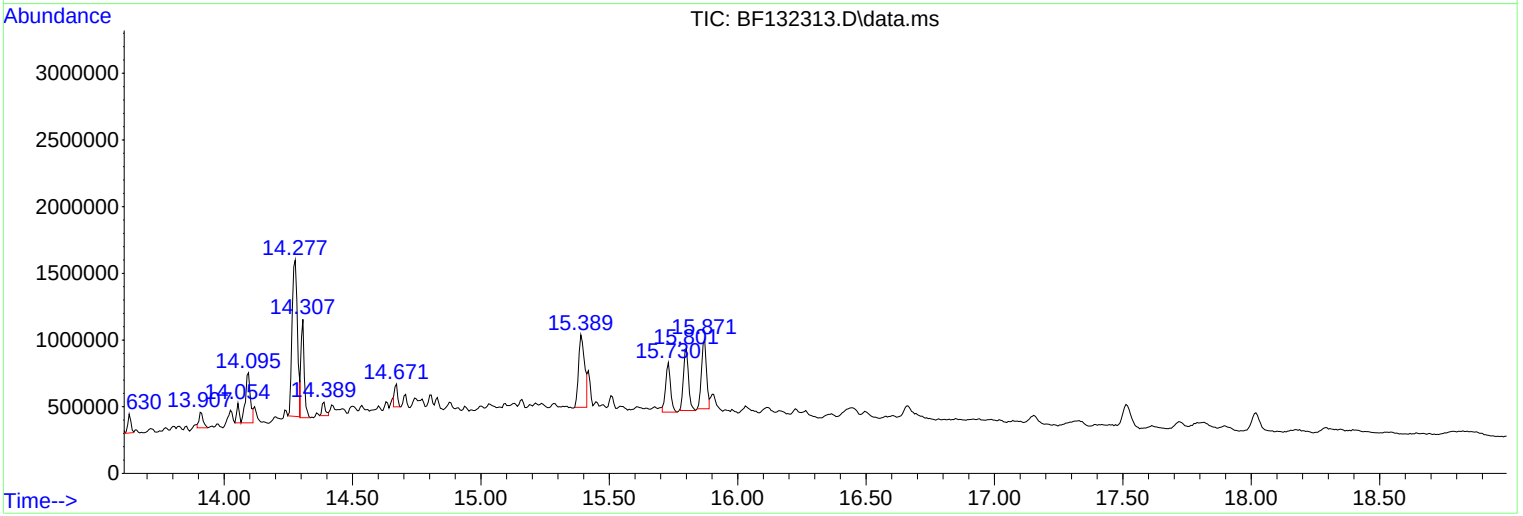
Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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\BF020223\
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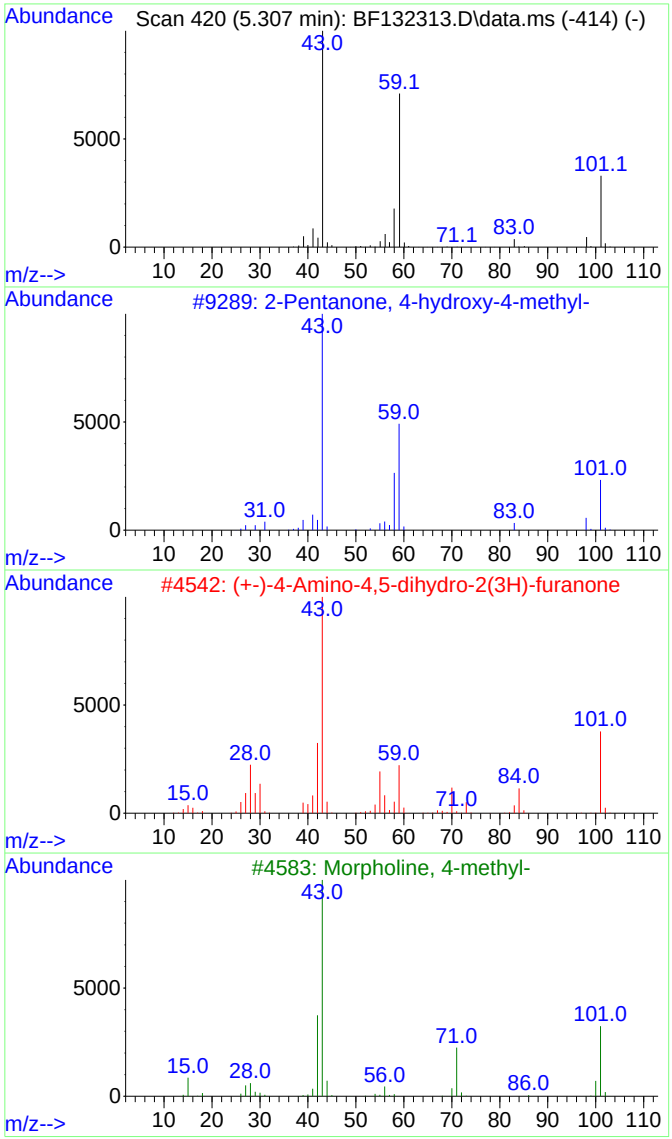
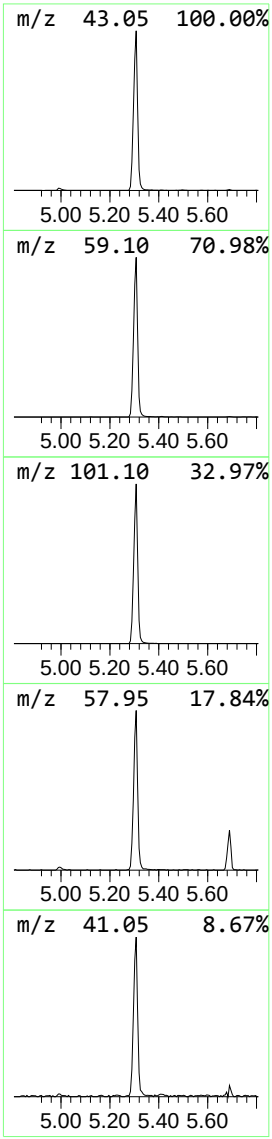
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.307	23.80 ng	1067070	1,4-Dichlorobenzene-d4	7.066

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	47
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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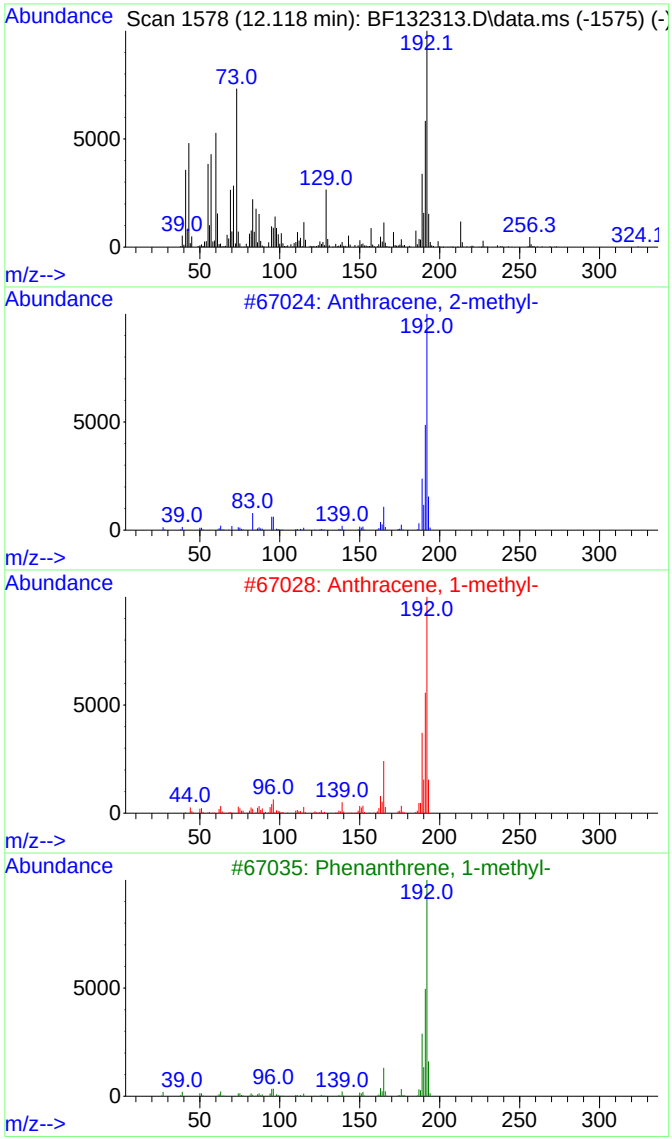
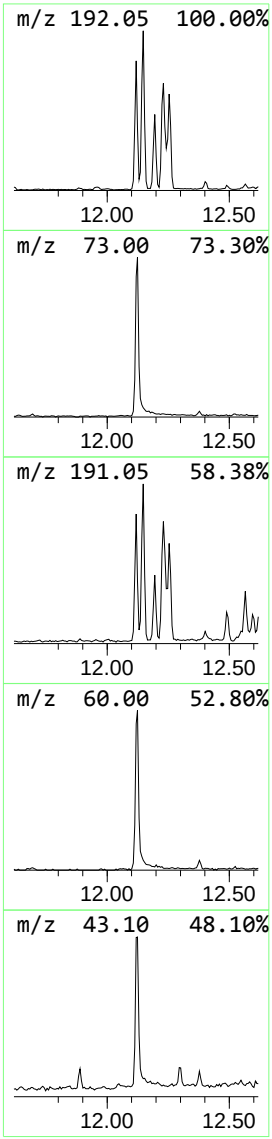
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.118	9.50 ng	473314	Phenanthrene-d10	11.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90





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Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

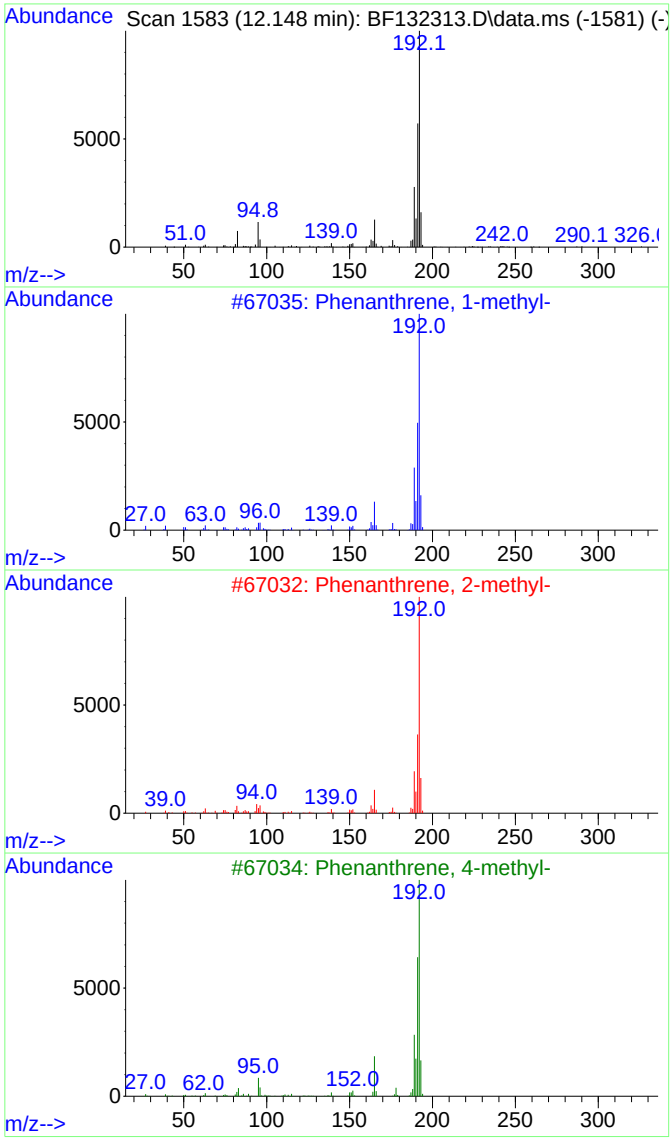
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

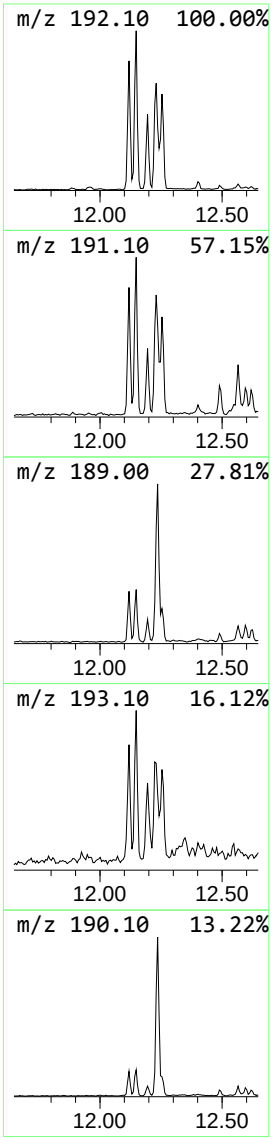
****

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.148	2.96 ng	147744	Phenanthrene-d10	11.613

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	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020223\
Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

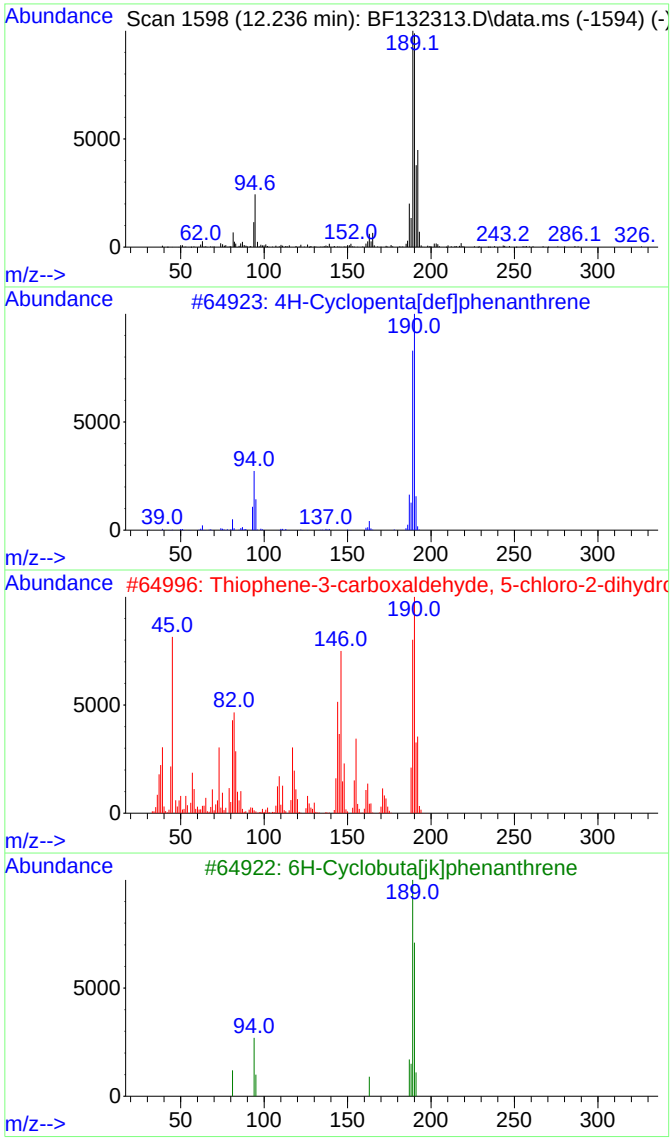
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

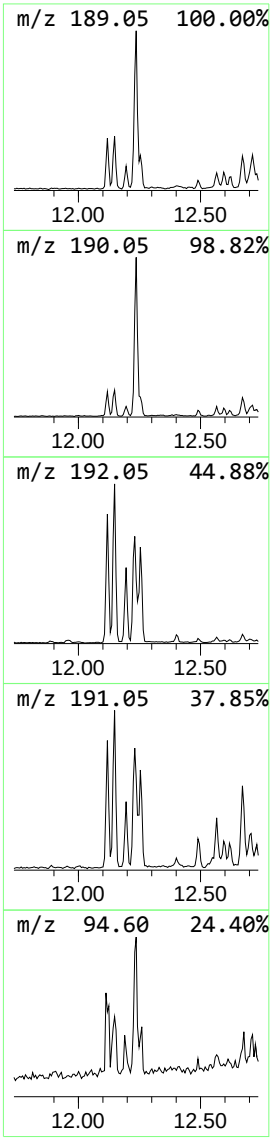
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.236	5.25 ng	261388	Phenanthrene-d10	11.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020223\
Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

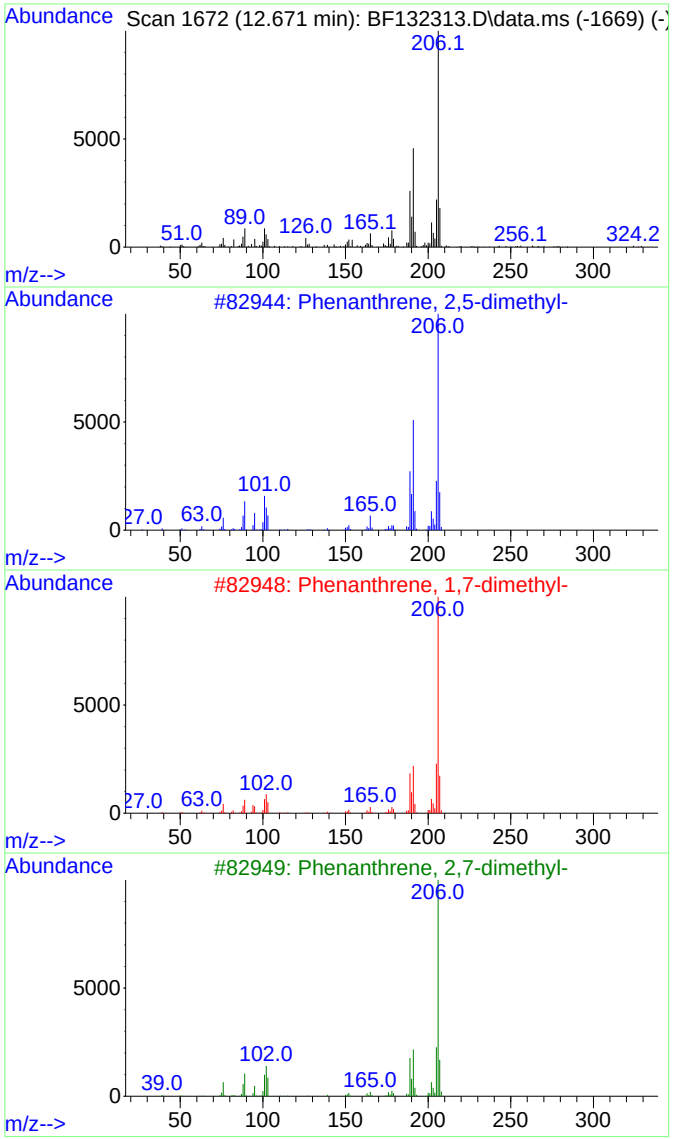
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

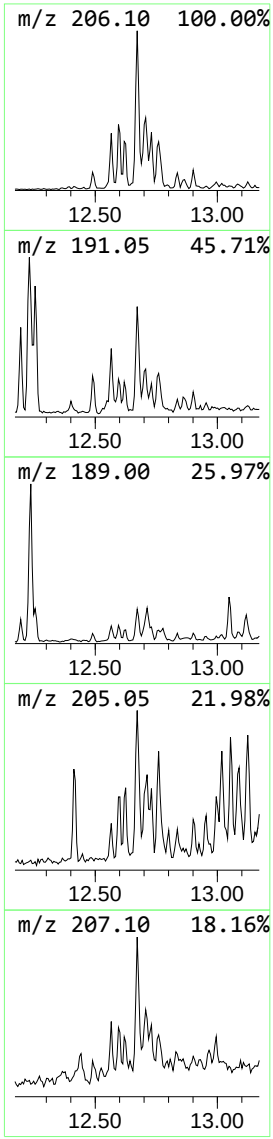
****

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.671	2.74 ng	136525	Phenanthrene-d10	11.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	94
2	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	91
3	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	90
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

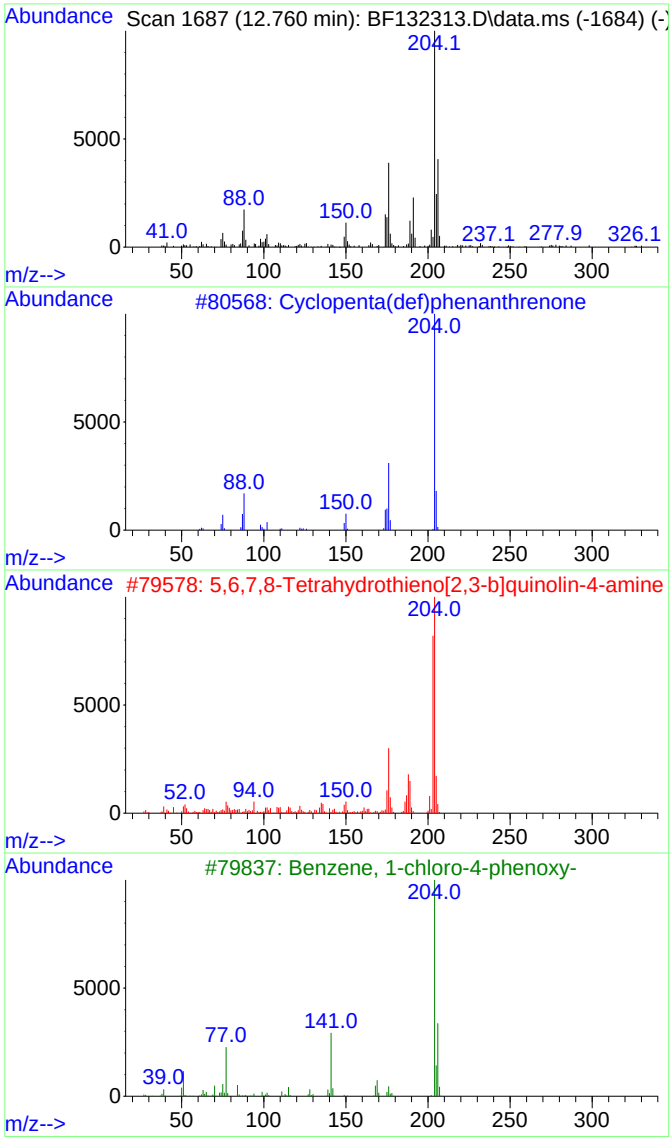
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

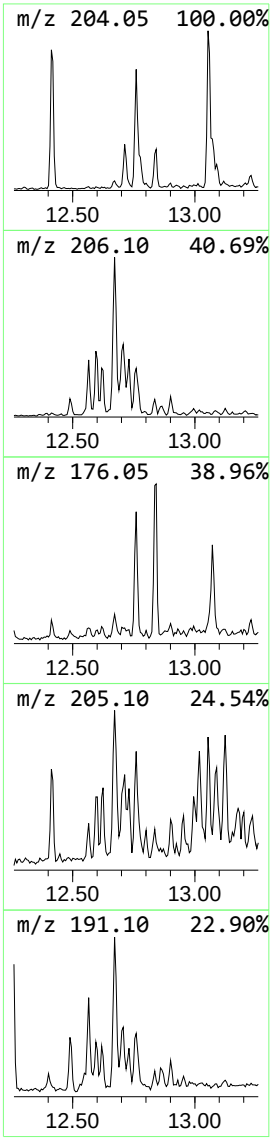
****

Peak Number 6 Cyclopenta(def)phenanthrenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.760	2.75 ng	137259	Phenanthrene-d10	11.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	96
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	50
3	Benzene, 1-chloro-4-phenoxy-	204	C12H9ClO	007005-72-3	46
4	[1,1'-Biphenyl]-4-ol, 4'-chloro-	204	C12H9ClO	028034-99-3	46
5	[1,1'-Biphenyl]-2-ol, 5-chloro-	204	C12H9ClO	000607-12-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020223\
Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

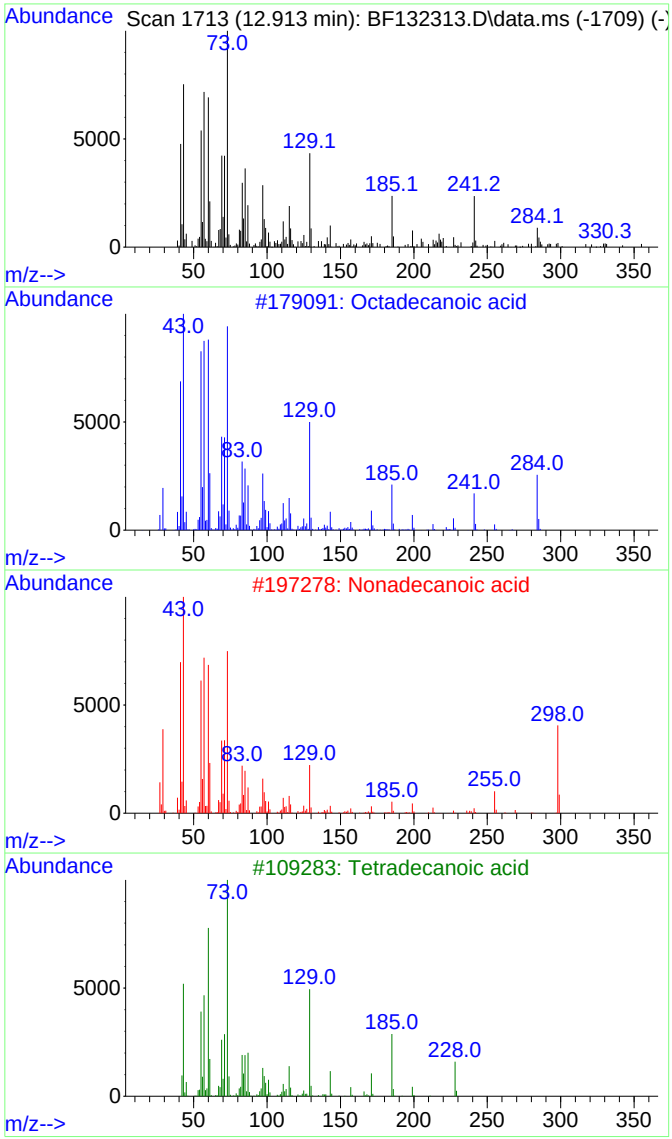
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

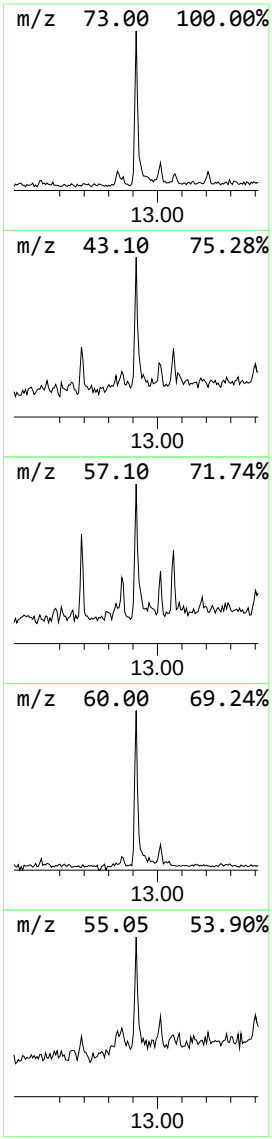
****

Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.913	2.69 ng	134300	Phenanthrene-d10	11.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Nonadecanoic acid	298	C19H38O2	000646-30-0	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	30





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Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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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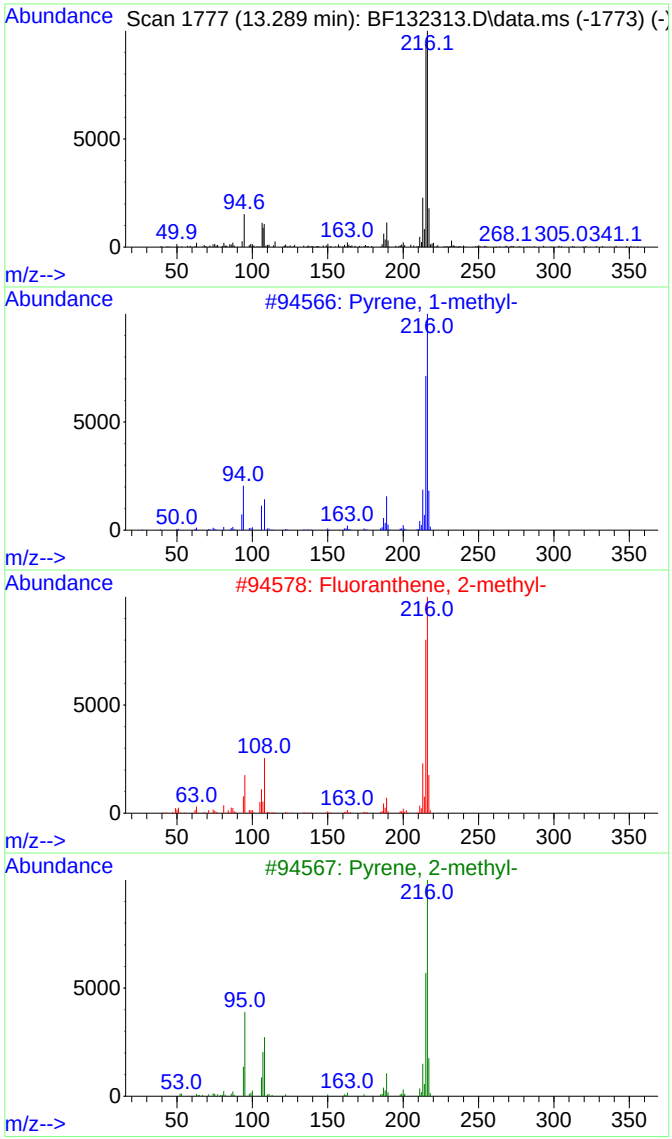
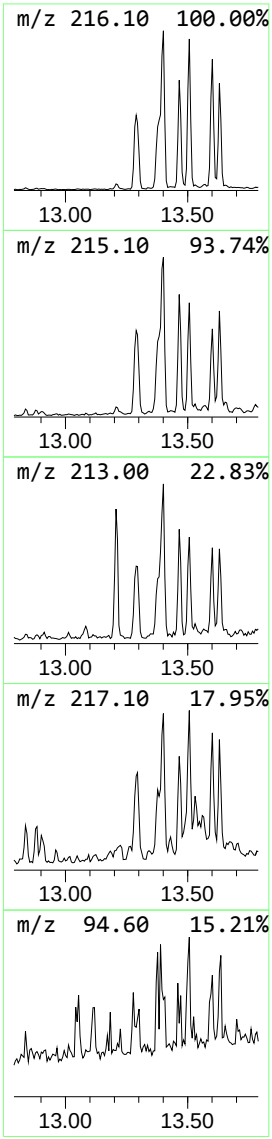
Peak Number 8 Pyrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.289	2.56 ng	222937	Chrysene-d12	14.277

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	98
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	89
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	83





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Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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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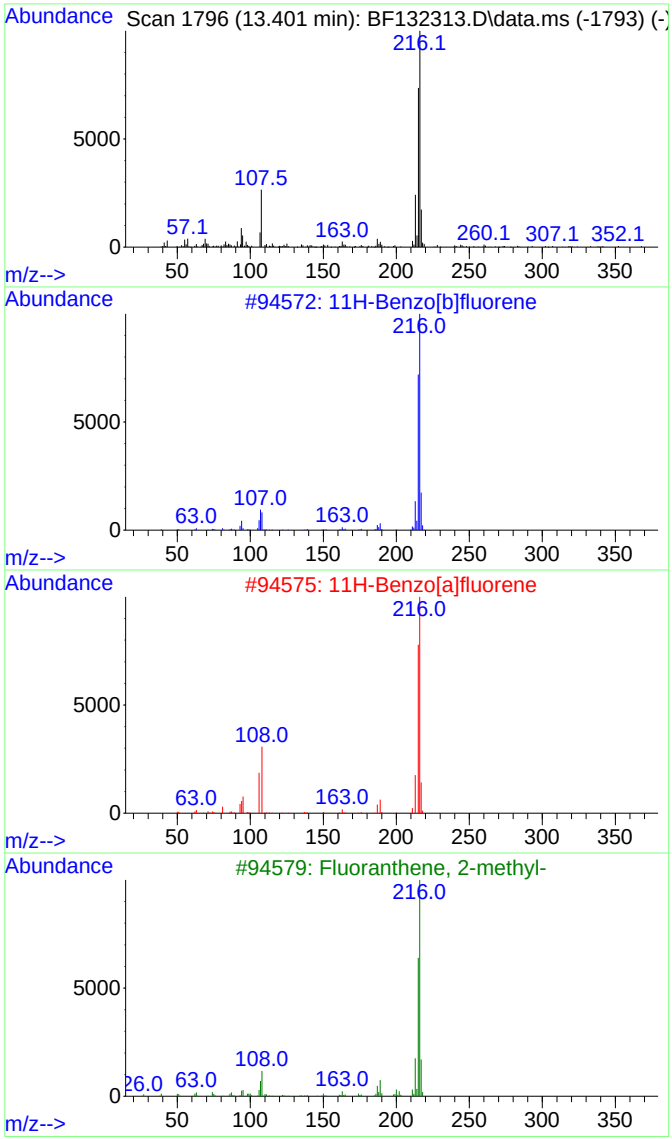
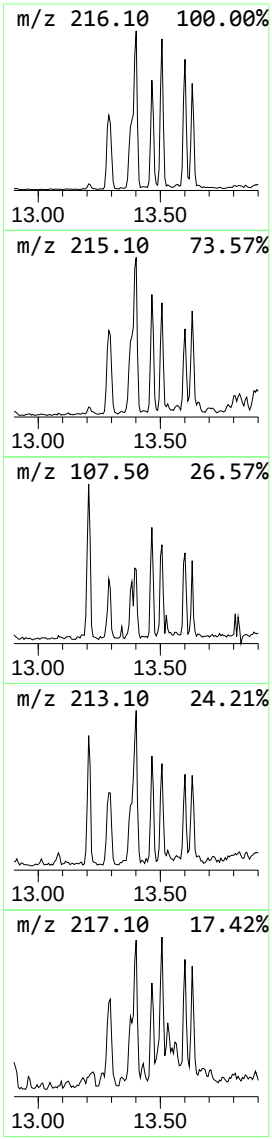
Peak Number 9 11H-Benzo[b]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.401	2.42 ng	210669	Chrysene-d12	14.277

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
4	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	64
5	Benzoic acid, 3-(3,5-dimethyl-1-...	216	C12H12N2O2	312531-88-7	59





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Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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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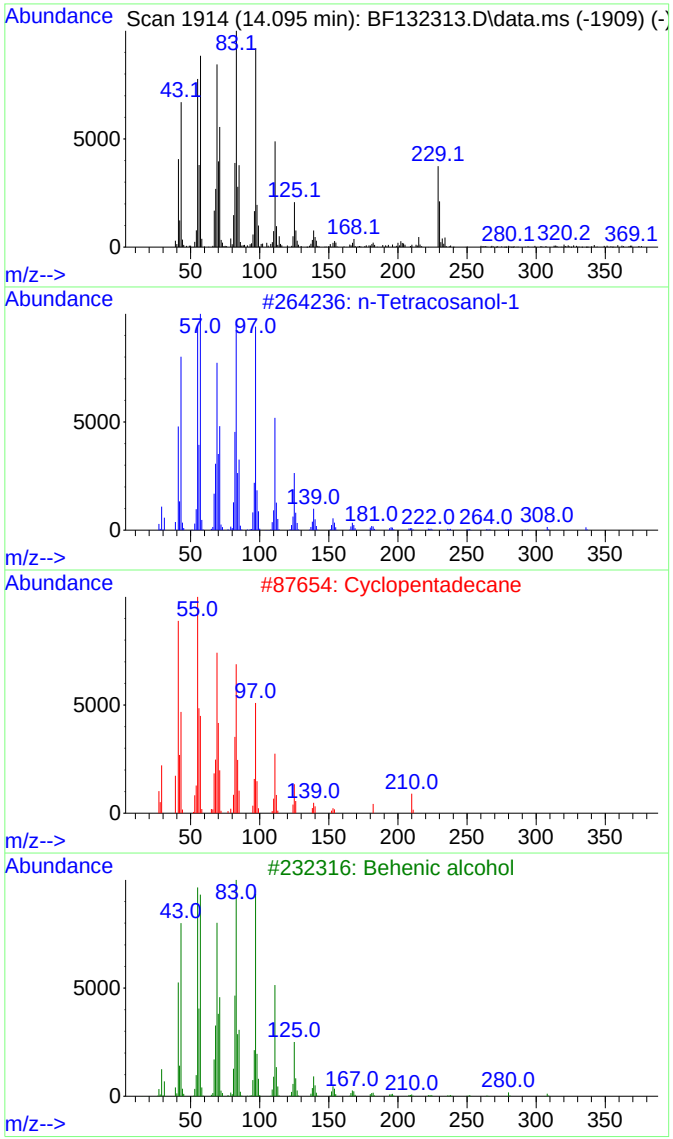
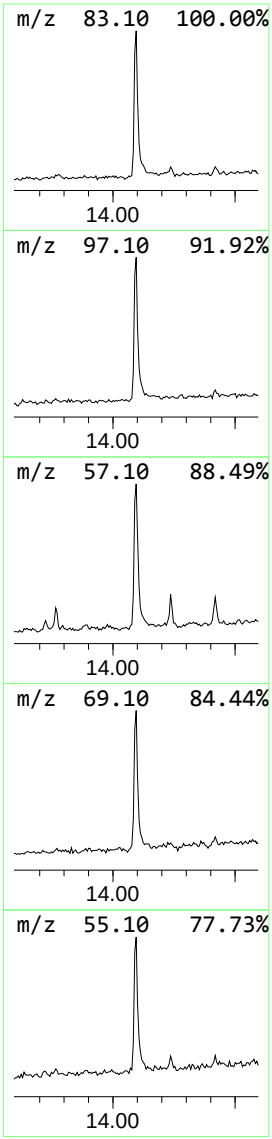
Peak Number 10 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.095	5.97 ng	519552	Chrysene-d12	14.277

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	1-Nonadecene	266	C19H38	018435-45-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020223\
Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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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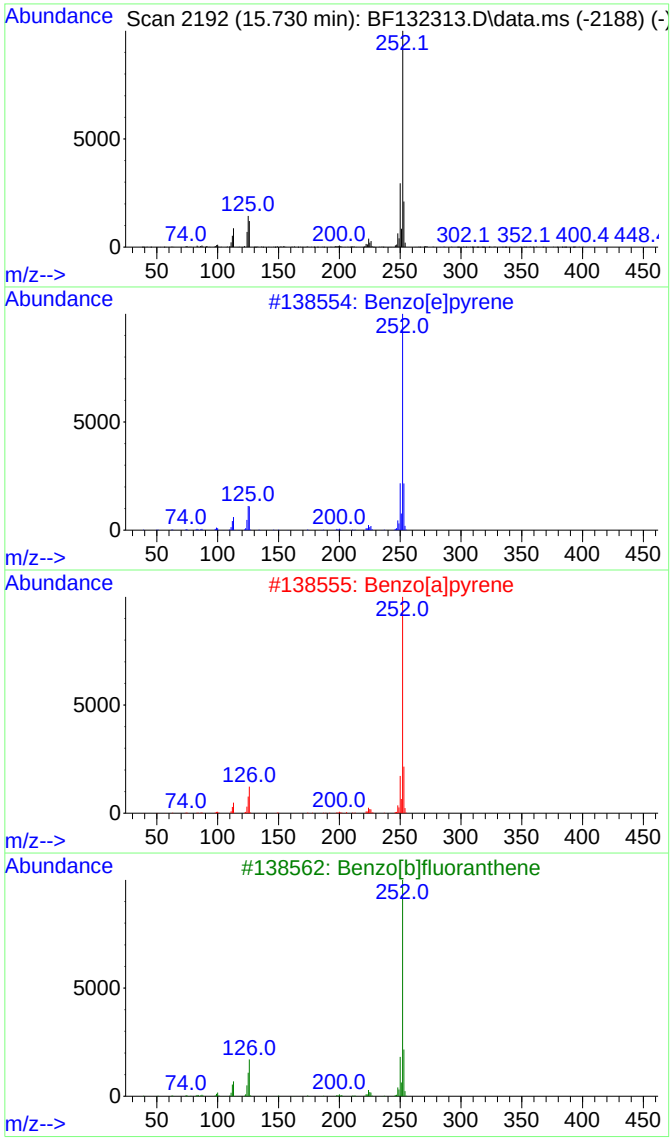
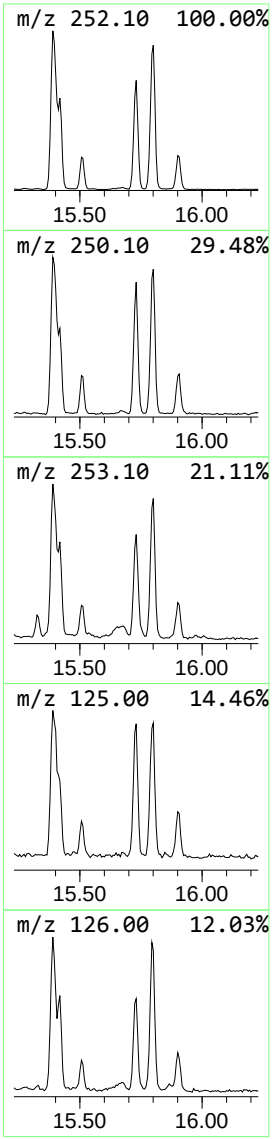
Peak Number 11 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.730	13.59 ng	482485	Perylene-d12	15.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Perylene	252	C20H12	000198-55-0	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020223\
Data File : BF132313.D
Acq On : 03 Feb 2023 02:35
Operator : CG\JU
Sample : 01390-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCKPILE-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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-...	5.307	23.8	ng	1067070	1	7.066	896791	20.0
Anthracene, 2-m...	12.118	9.5	ng	473314	4	11.613	996697	20.0
Phenanthrene, 1...	12.148	3.0	ng	147744	4	11.613	996697	20.0
4H-Cyclopenta[d...	12.236	5.3	ng	261388	4	11.613	996697	20.0
Phenanthrene, 2...	12.671	2.7	ng	136525	4	11.613	996697	20.0
Cyclopenta(def)...	12.760	2.8	ng	137259	4	11.613	996697	20.0
Octadecanoic acid	12.913	2.7	ng	134300	4	11.613	996697	20.0
Pyrene, 1-methyl-	13.289	2.6	ng	222937	5	14.277	1740260	20.0
11H-Benzo[b]flu...	13.401	2.4	ng	210669	5	14.277	1740260	20.0
n-Tetracosanol-1	14.095	6.0	ng	519552	5	14.277	1740260	20.0
Benzo[e]pyrene	15.730	13.6	ng	482485	6	15.871	710252	20.0