LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
Data File : BF135824.D
Acq On : 17 Oct 2023 21:32
Operator : CG\JU
Sample : 04878-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11995

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: BF135824.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	485	489	500	rBV	212441	299787	16.28%	1.269%
2	5.375	556	559	575	rBV	1561929	1826366	99.18%	7.728%
3	6.393	729	732	760	rBV	1860872	1841478	100.00%	7.792%
4	6.740	787	791	802	rBV	469931	455451	24.73%	1.927%
5	7.304	884	887	900	rBV	1157675	1036589	56.29%	4.386%
6	8.016	1005	1008	1015	rBV	688210	578079	31.39%	2.446%
7	9.092	1188	1191	1195	rBV	2199096	1784093	96.88%	7.550%
8	9.210	1207	1211	1215	rBV	44044	45018	2.44%	0.190%
9	9.775	1303	1307	1311	rBV	732056	621840	33.77%	2.631%
10	9.992	1341	1344	1346	rBV3	26127	26414	1.43%	0.112%
11	10.175	1373	1375	1377	rBV3	20927	22830	1.24%	0.097%
12	10.569	1439	1442	1447	rBV	887112	912323	49.54%	3.861%
13	11.275	1559	1562	1564	rBV	578223	546056	29.65%	2.311%
14	11.298	1564	1566	1569	rVB	700050	538877	29.26%	2.280%
15	11.810	1650	1653	1657	rVB	372747	321488	17.46%	1.360%
16	12.316	1736	1739	1745	rVB2	274851	285056	15.48%	1.206%
17	12.498	1767	1770	1774	rBV	1621370	1412626	76.71%	5.978%
18	12.727	1803	1809	1813	rVB	1228189	1287153	69.90%	5.447%
19	12.869	1829	1833	1836	rVB	1400472	1271015	69.02%	5.378%
20	13.063	1863	1866	1869	rVB	153278	155768	8.46%	0.659%
21	13.127	1874	1877	1879	rVV	94363	80947	4.40%	0.343%
22	13.163	1881	1883	1888	rVB3	98861	140308	7.62%	0.594%
23	13.257	1897	1899	1902	rBV	77816	74569	4.05%	0.316%
24	13.586	1952	1955	1957	rVB	133780	116254	6.31%	0.492%
25	13.686	1969	1972	1974	rBV2	189828	194060	10.54%	0.821%
26	13.739	1978	1981	1983	rVV	116215	135524	7.36%	0.573%
27	13.798	1987	1991	1996	rVB	242858	304409	16.53%	1.288%
28	13.933	2007	2014	2017	rBV2	831927	1420187	77.12%	6.010%
29	13.963	2017	2019	2023	rVB	812686	740569	40.22%	3.134%
30	14.045	2030	2033	2037	rVB	132171	122374	6.65%	0.518%
31	14.157	2048	2052	2054	rBV2	60866	86812	4.71%	0.367%
32	14.180	2054	2056	2060	rVB	90694	70610	3.83%	0.299%
33	14.316	2076	2079	2080	rBV2	58810	59024	3.21%	0.250%
34	14.363	2085	2087	2089	rVB2	52675	40101	2.18%	0.170%
35	14.392	2089	2092	2096	rBV3	98649	133030	7.22%	0.563%
36	14.427	2096	2098	2100	rBV3	47889	41410	2.25%	0.175%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
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Operator : CG\JU
Sample : 04878-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

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	14.663	2136	2138	2143	rVB2	61994	68500	3.72%	0.290%
38	14.833	2164	2167	2172	rVB	97265	111384	6.05%	0.471%
39	14.986	2189	2193	2196	rBV	885295	1231408	66.87%	5.211%
40	15.098	2209	2212	2219	rBV	126656	155175	8.43%	0.657%
41	15.186	2224	2227	2228	rBV2	47879	49933	2.71%	0.211%
42	15.286	2240	2244	2250	rVV	487179	576014	31.28%	2.437%
43	15.357	2252	2256	2261	rBV	538061	662443	35.97%	2.803%
44	15.416	2262	2266	2269	rVV	443409	523781	28.44%	2.216%
45	15.451	2269	2272	2279	rVB2	141625	210602	11.44%	0.891%
46	15.851	2336	2340	2348	rVB3	67456	105549	5.73%	0.447%
47	16.921	2516	2522	2532	rVB	239154	535478	29.08%	2.266%
48	17.374	2594	2599	2609	rBV	168336	372848	20.25%	1.578%

Sum of corrected areas: 23631610

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Instrument :
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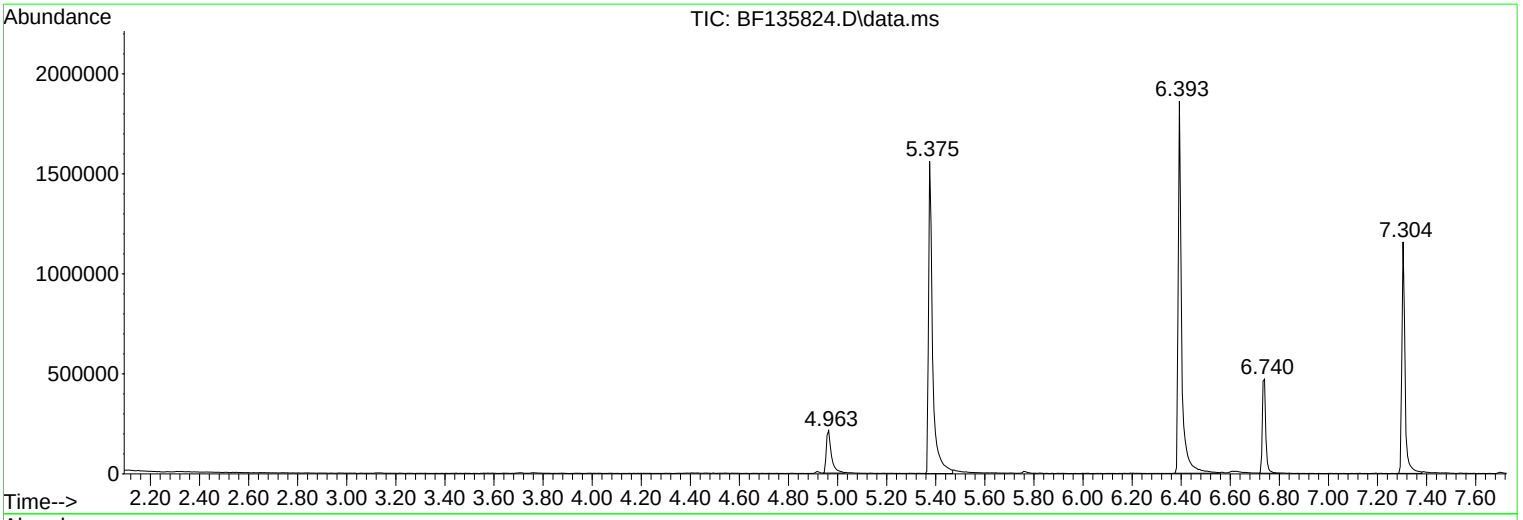
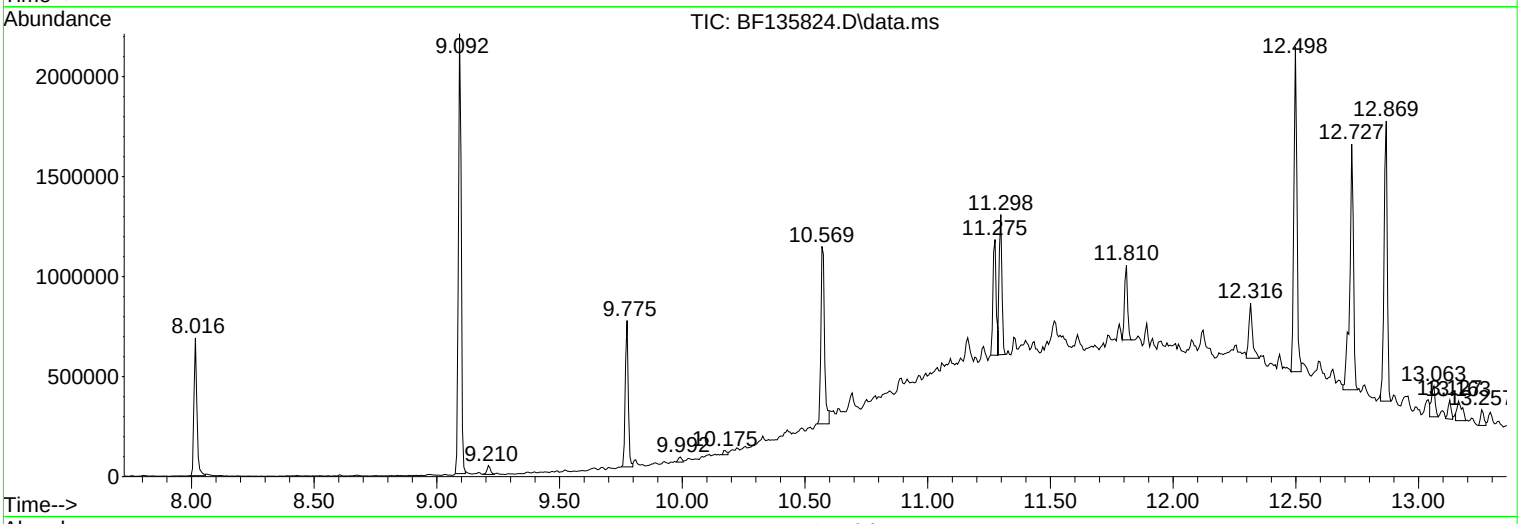
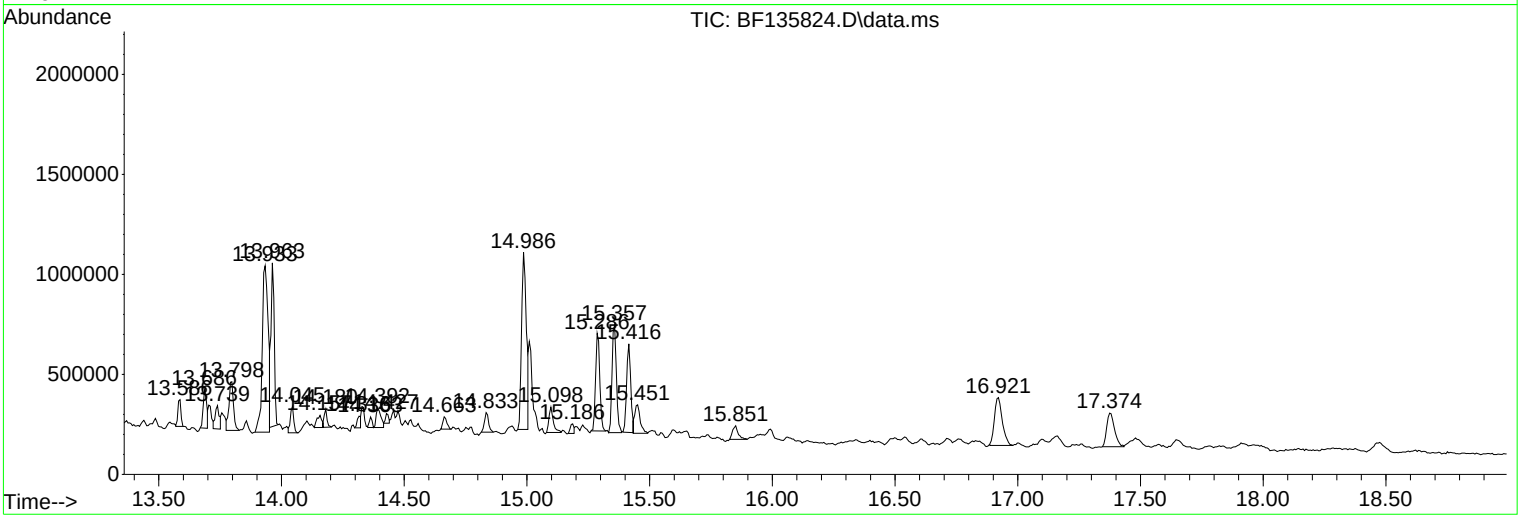
ClientSampleId :
72-11995

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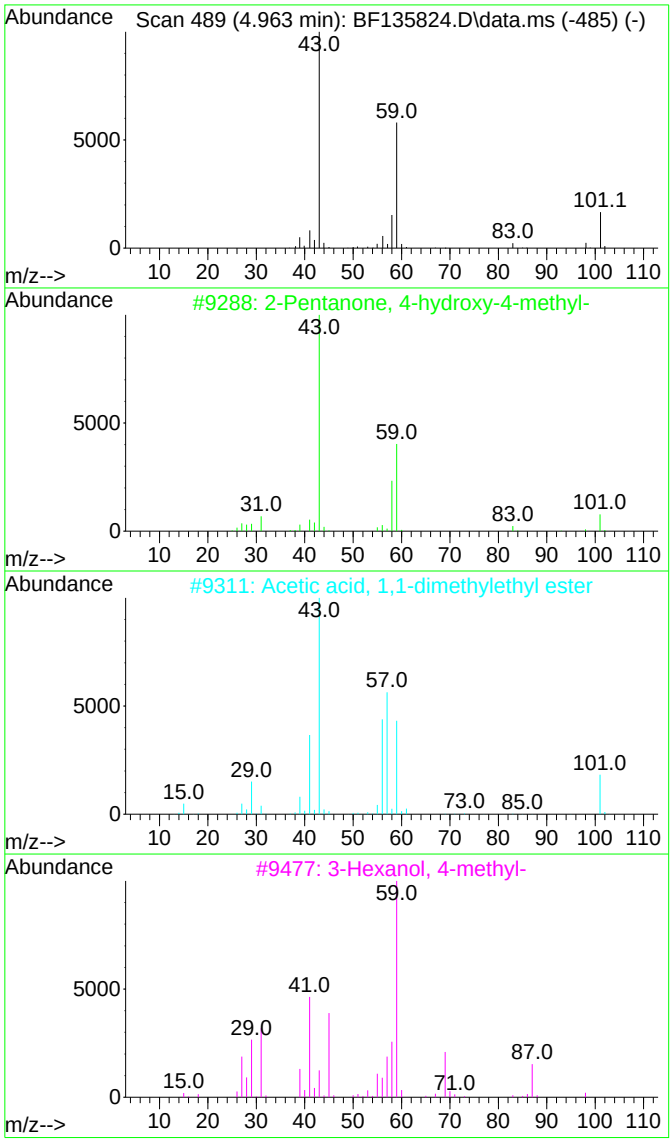
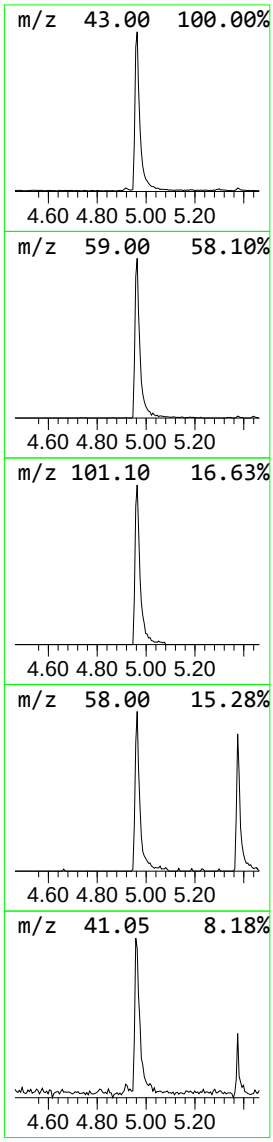
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	13.16 ng	299787	1,4-Dichlorobenzene-d4	6.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Operator : CG\JU
Sample : 04878-01
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ALS Vial : 11 Sample Multiplier: 1

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

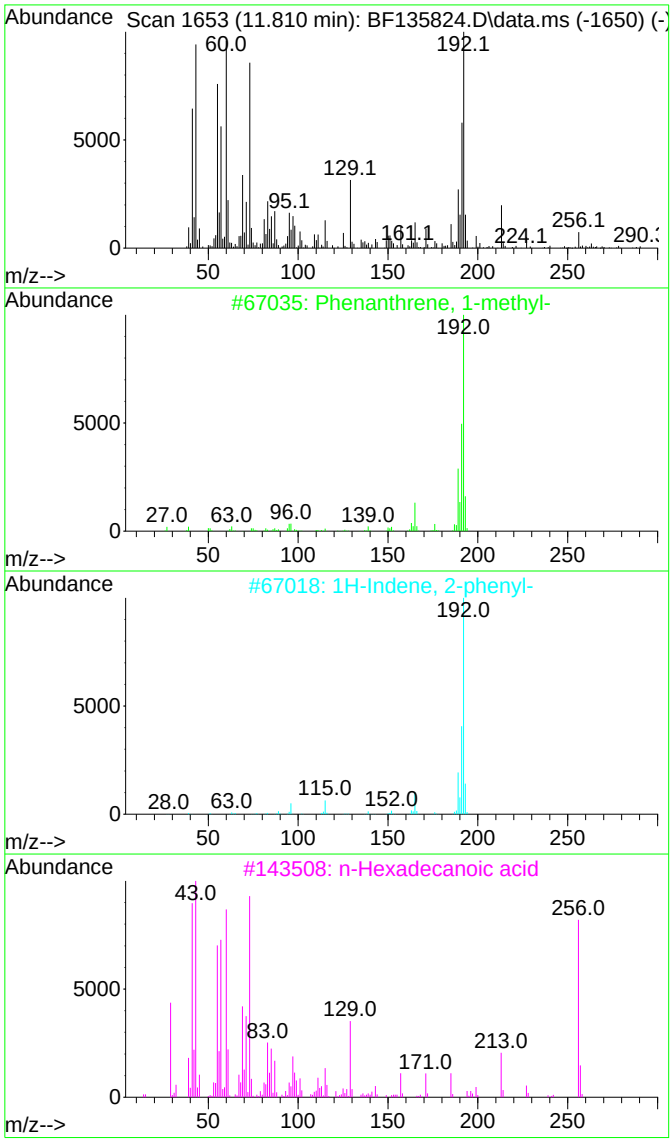
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

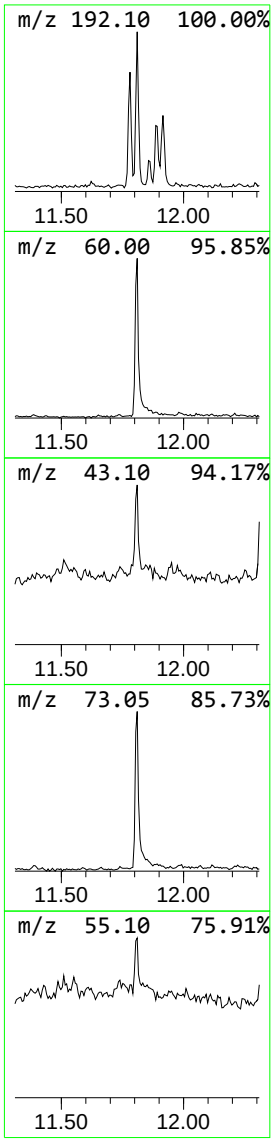
****

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	11.77 ng	321488	Phenanthrene-d10	11.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	80
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	80
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	56





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Acq On : 17 Oct 2023 21:32
Operator : CG\JU
Sample : 04878-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

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

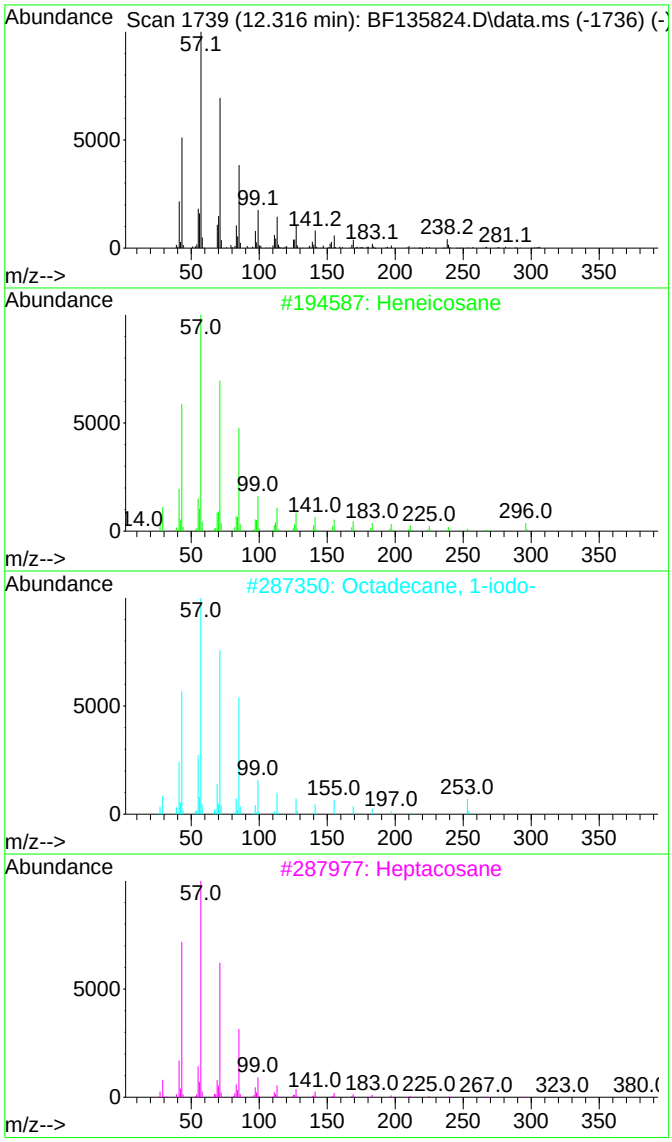
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

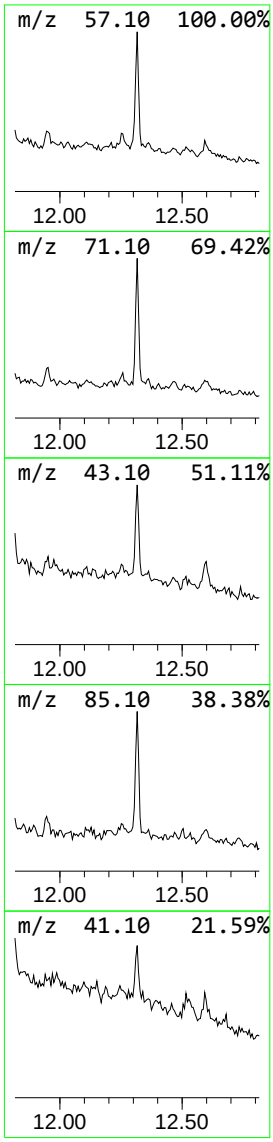
****

Peak Number 3 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.316	10.44 ng	285056	Phenanthrene-d10	11.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
3	Heptacosane	380	C27H56	000593-49-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

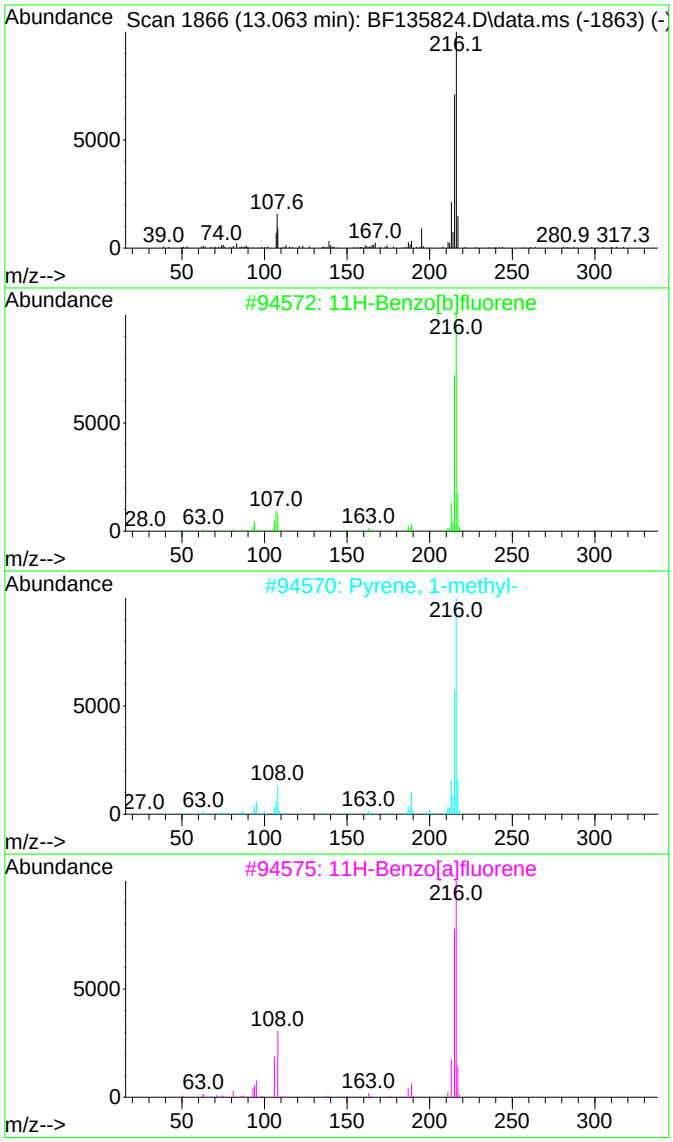
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

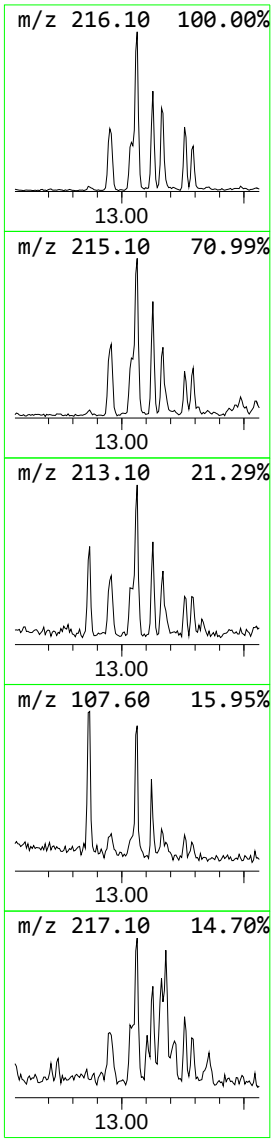
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.063	2.19 ng	155768	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	74
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	72
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	64
5	Pyrene, 4-methyl-	216	C17H12	003353-12-6	58





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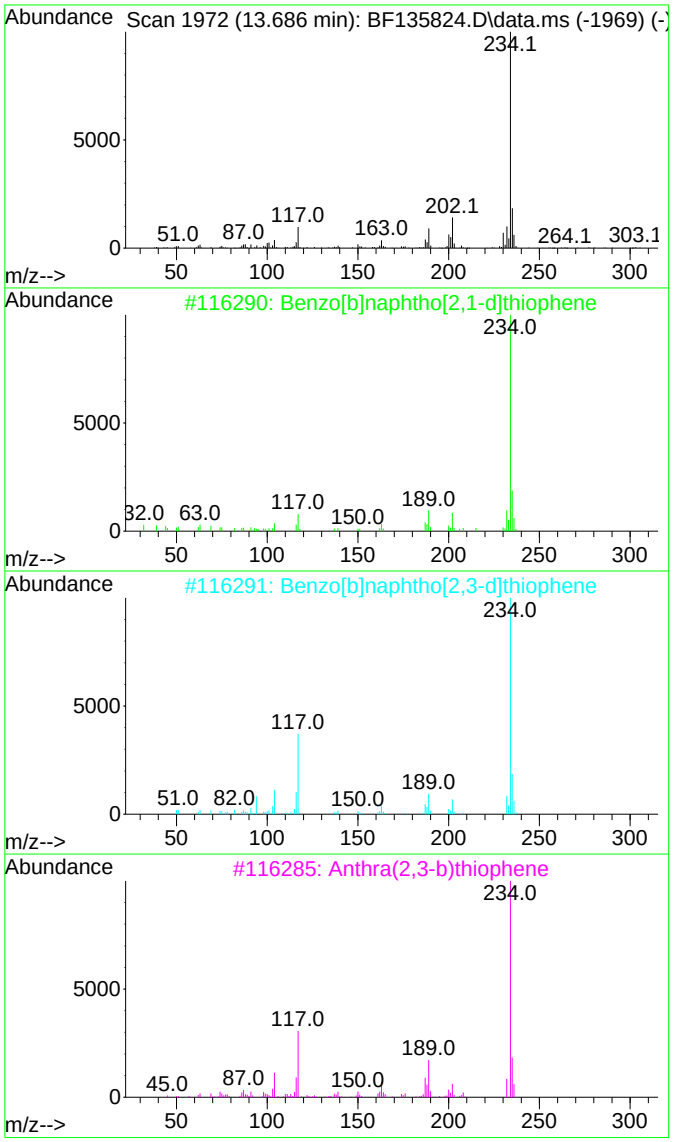
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

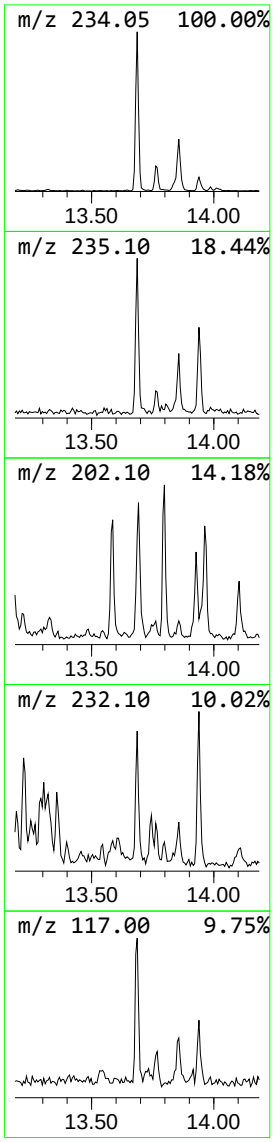
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.686	2.73 ng	194060	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	94
2	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	90
3	Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	80
4	Phenanthro(2,1-b)thiophene	234	C16H10S	000219-25-0	74
5	Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	64





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

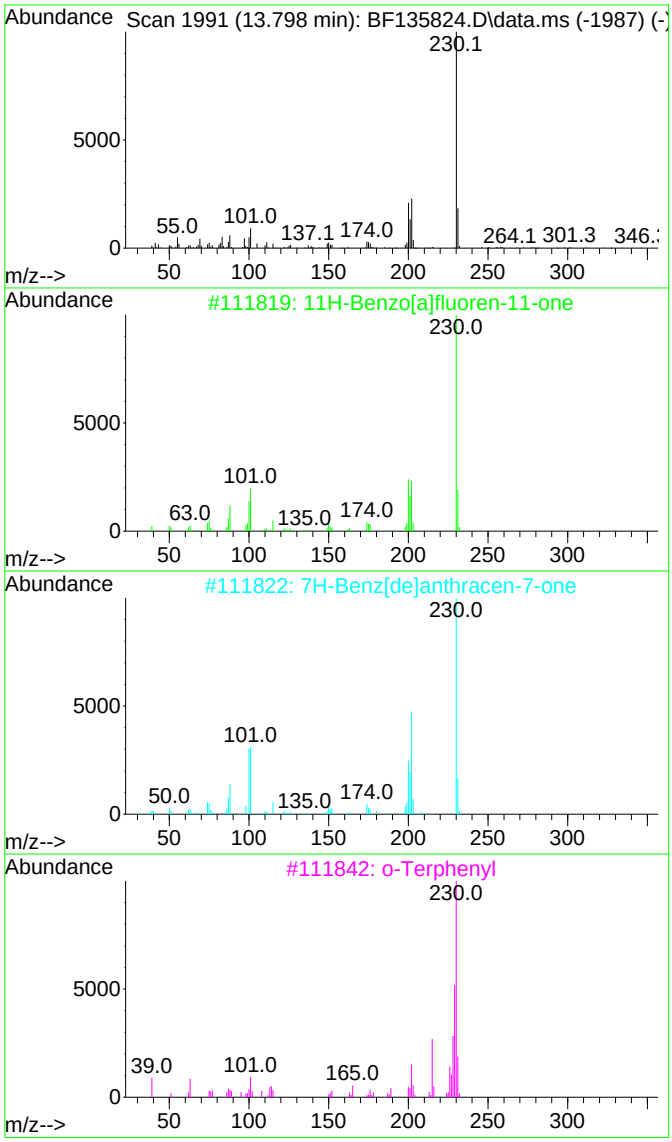
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

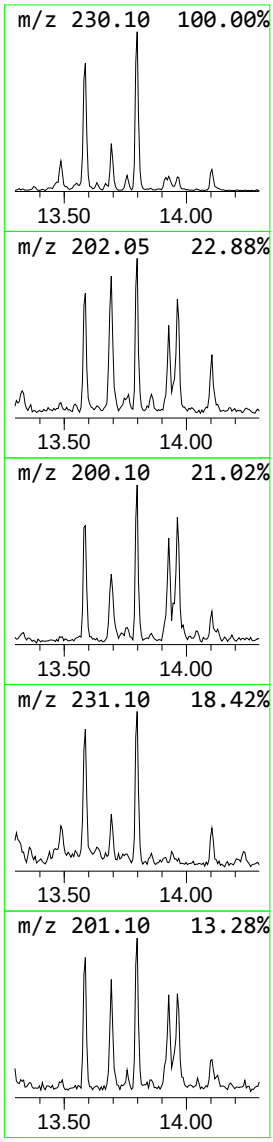
****

Peak Number 6 11H-Benzo[a]fluoren-11-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	4.29 ng	304409	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	94
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	86
3	o-Terphenyl	230	C18H14	000084-15-1	53
4	5-Amino-7-imino-4,8-diazatricycl...	230	C12H14N4O	1000388-35-6	52
5	Benzo(b)phenazine	230	C16H10N2	000257-97-6	47





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ALS Vial : 11 Sample Multiplier: 1

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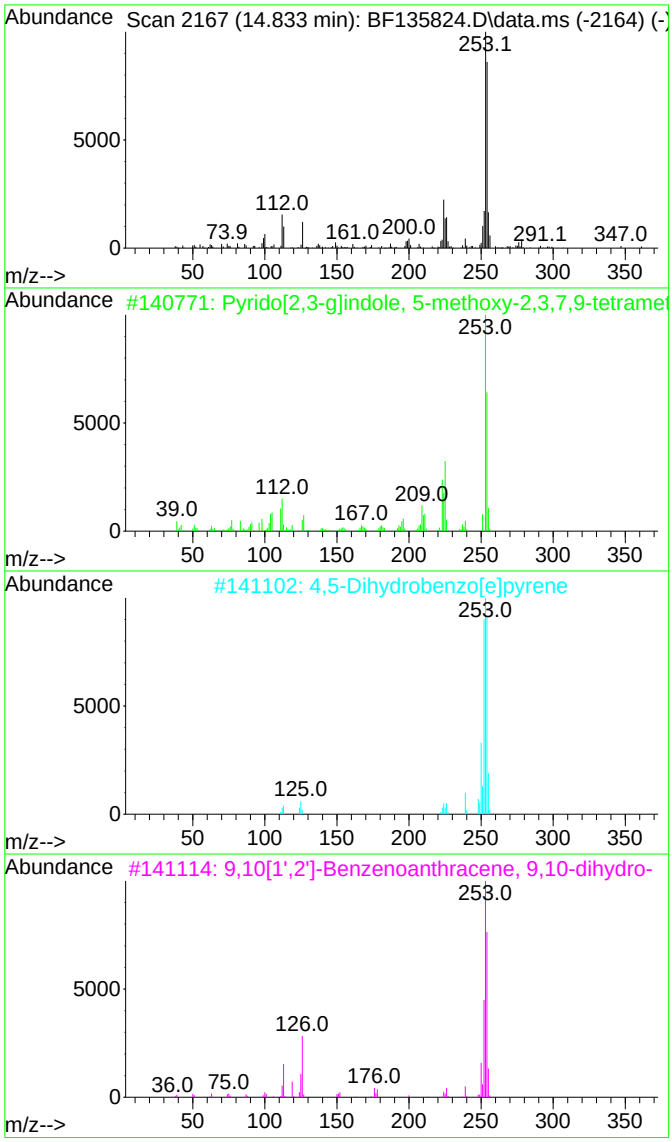
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

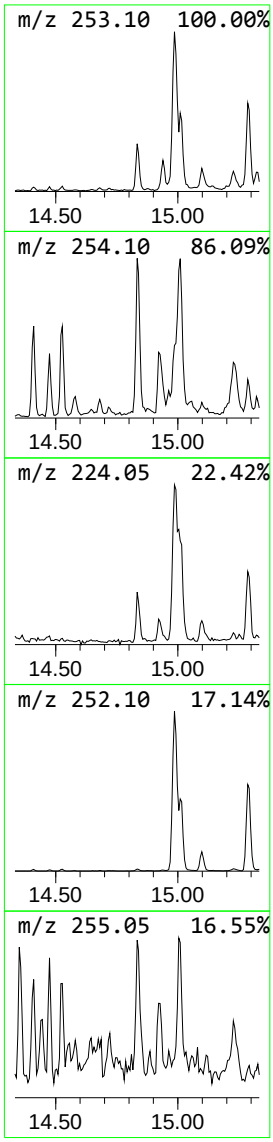
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pyrido[2,3-g]indole, 5-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	4.25 ng	111384	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrido[2,3-g]indole, 5-methoxy-2...	254	C16H18N2O	201991-45-9	64
2	4,5-Dihydrobenzo[e]pyrene	254	C20H14	095676-42-9	64
3	9,10[1',2']-Benzenoanthracene, 9...	254	C20H14	000477-75-8	64
4	Phenanthrene, 1-phenyl-	254	C20H14	004325-76-2	59
5	Benzofuran-6-ol-3-one, 2-[4-hydr...	254	C15H10O4	1000128-64-9	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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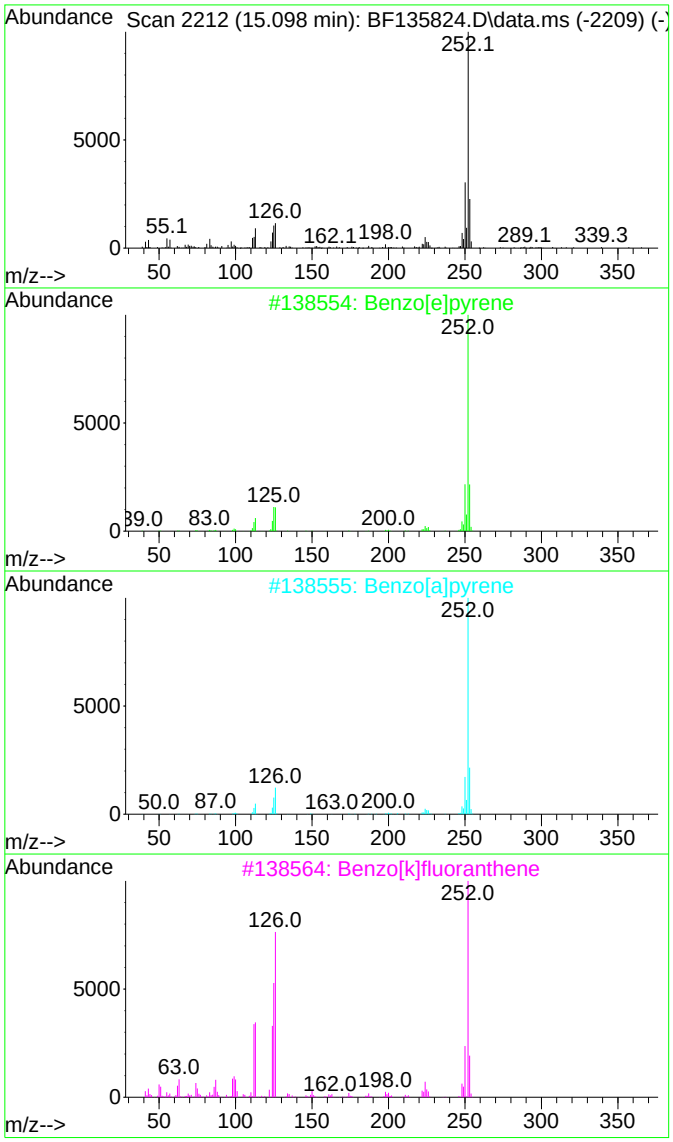
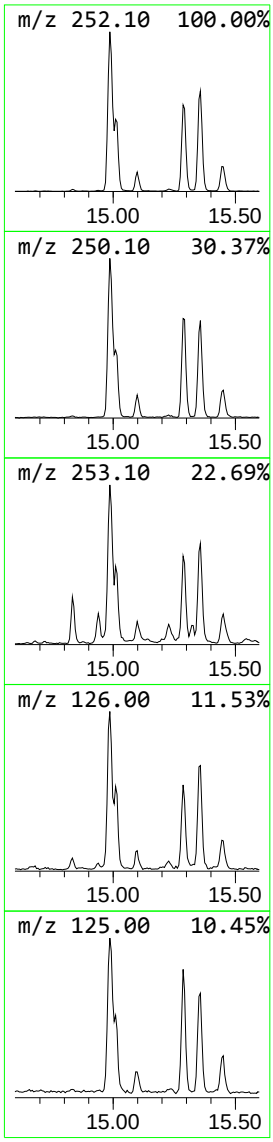
Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	5.93 ng	155175	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
Data File : BF135824.D
Acq On : 17 Oct 2023 21:32
Operator : CG\JU
Sample : 04878-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

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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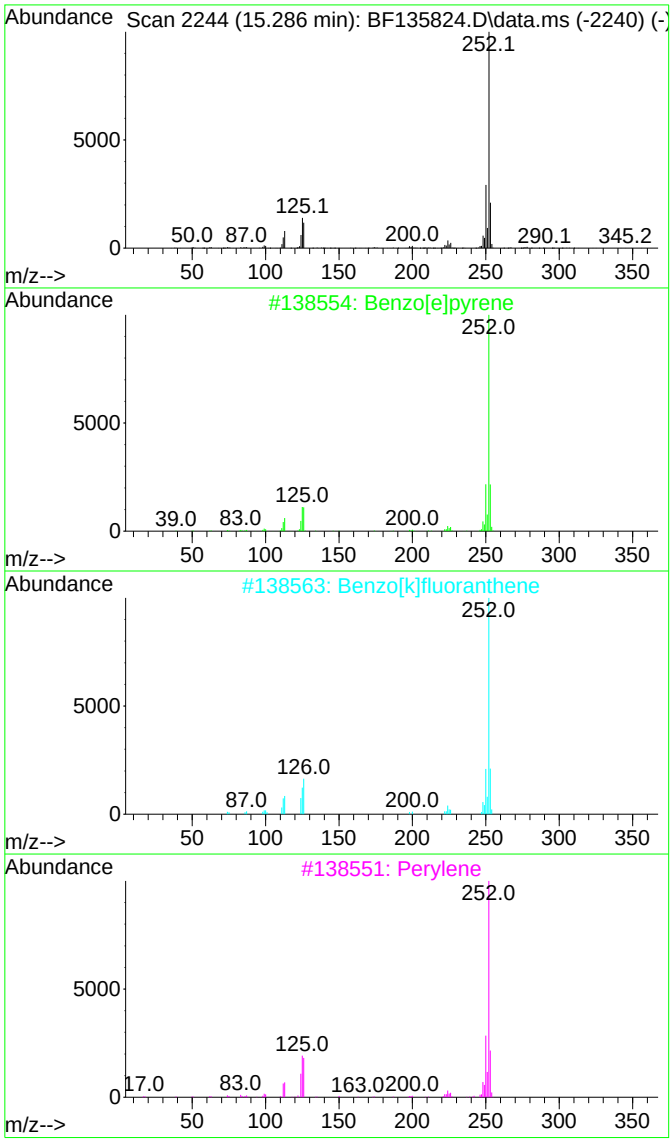
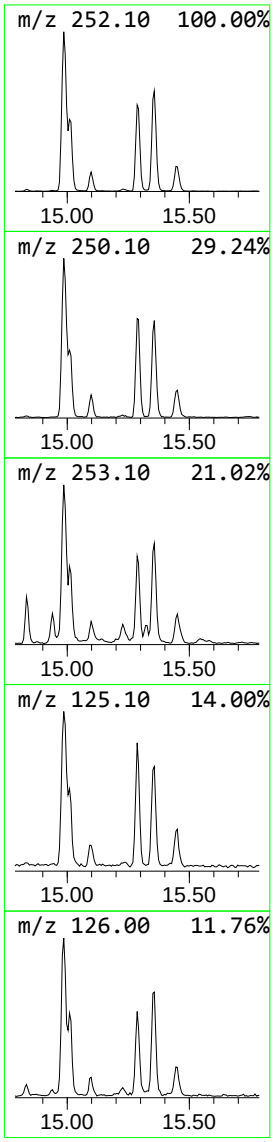
Peak Number 9 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	21.99 ng	576014	Perylene-d12	15.416

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





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
Data File : BF135824.D
Acq On : 17 Oct 2023 21:32
Operator : CG\JU
Sample : 04878-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

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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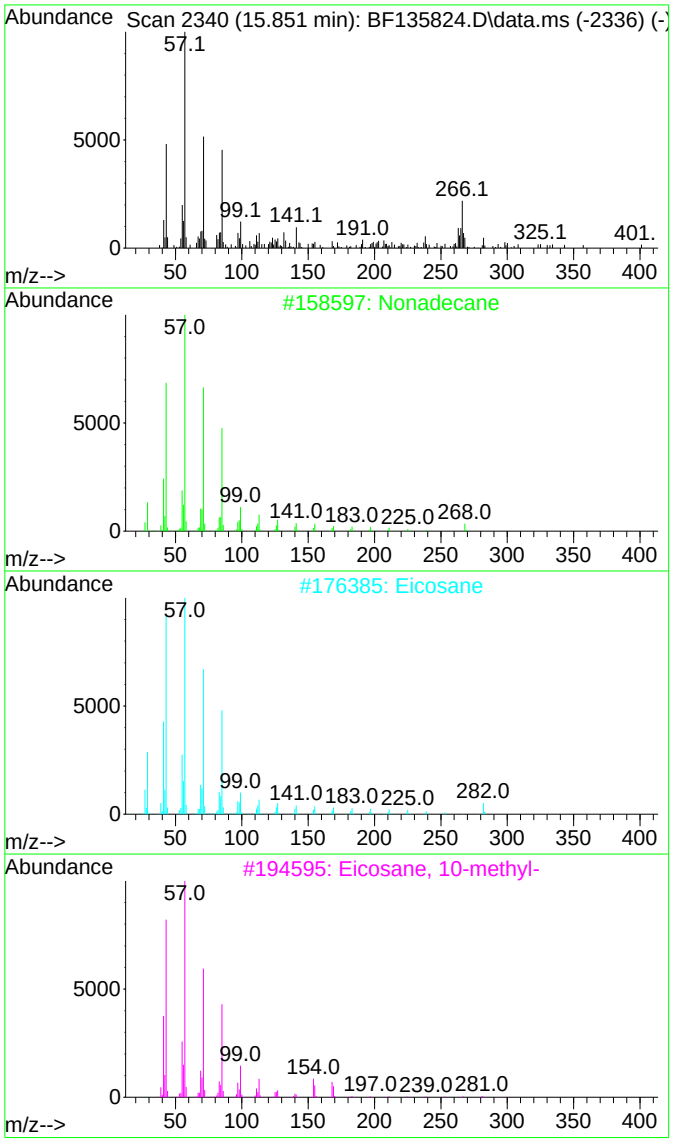
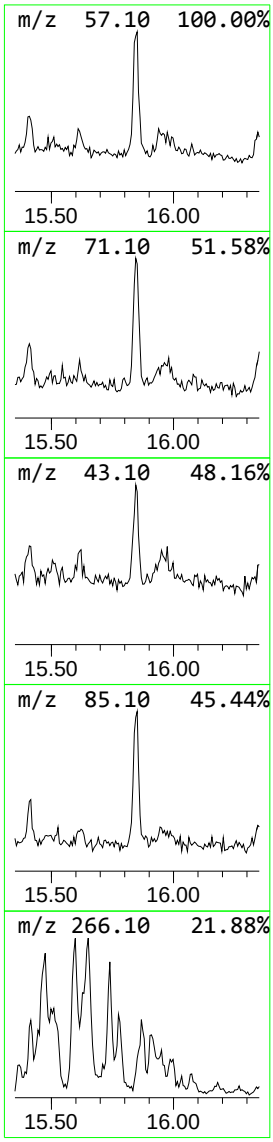
Peak Number 10 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.851	4.03 ng	105549	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Eicosane	282	C20H42	000112-95-8	78
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	55
4	Tetradecane	198	C14H30	000629-59-4	55
5	Docosane	310	C22H46	000629-97-0	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
Data File : BF135824.D
Acq On : 17 Oct 2023 21:32
Operator : CG\JU
Sample : 04878-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

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	13.2	ng	299787	1	6.740	455451	20.0
Phenanthrene, 1...	11.810	11.8	ng	321488	4	11.275	546056	20.0
Heneicosane	12.316	10.4	ng	285056	4	11.275	546056	20.0
11H-Benzo[b]flu...	13.063	2.2	ng	155768	5	13.939	1420190	20.0
Benzo[b]naphtho...	13.686	2.7	ng	194060	5	13.939	1420190	20.0
11H-Benzo[a]flu...	13.798	4.3	ng	304409	5	13.939	1420190	20.0
Pyrido[2,3-g]in...	14.833	4.3	ng	111384	6	15.416	523781	20.0
Benzo[e]pyrene	15.098	5.9	ng	155175	6	15.416	523781	20.0
Perylene	15.286	22.0	ng	576014	6	15.416	523781	20.0
Nonadecane	15.851	4.0	ng	105549	6	15.416	523781	20.0