LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123655.D
Acq On : 20 Apr 2021 21:55
Operator : JU/CG
Sample : M2076-18
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-14.5-15.0

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-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123655.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	498	506	512	rVB	64374	78062	1.28%	0.149%
2	5.475	571	576	579	rBV	6260077	5938465	97.00%	11.370%
3	6.486	743	748	754	rBV	6309846	6122382	100.00%	11.722%
4	6.851	806	810	813	rBV	1751453	1543880	25.22%	2.956%
5	6.910	817	820	828	rBV3	39343	68265	1.12%	0.131%
6	7.028	837	840	844	rBV	186648	165412	2.70%	0.317%
7	7.410	897	905	908	rBV	4509101	4060987	66.33%	7.775%
8	8.133	1023	1028	1030	rBV	2506955	1996684	32.61%	3.823%
9	8.151	1030	1031	1035	rVB	285283	223010	3.64%	0.427%
10	8.845	1146	1149	1153	rVB	276361	220630	3.60%	0.422%
11	8.945	1162	1166	1170	rVB	196115	153928	2.51%	0.295%
12	9.210	1207	1211	1215	rBV	6533679	5880053	96.04%	11.258%
13	9.292	1222	1225	1227	rBV	72797	72125	1.18%	0.138%
14	9.480	1252	1257	1260	rBV3	55365	76894	1.26%	0.147%
15	9.604	1275	1278	1282	rBV	254353	221376	3.62%	0.424%
16	9.892	1321	1327	1330	rBV	2584590	2105459	34.39%	4.031%
17	9.922	1330	1332	1336	rVB	330473	250291	4.09%	0.479%
18	10.092	1358	1361	1364	rBV	211857	189961	3.10%	0.364%
19	10.327	1398	1401	1403	rVB2	71648	65270	1.07%	0.125%
20	10.439	1416	1420	1423	rBV	319099	260850	4.26%	0.499%
21	10.680	1457	1461	1465	rBV	4707168	4065630	66.41%	7.784%
22	10.804	1479	1482	1486	rBV3	92000	135017	2.21%	0.259%
23	11.251	1550	1558	1560	rBV5	95557	164299	2.68%	0.315%
24	11.274	1560	1562	1568	rVB2	120358	129800	2.12%	0.249%
25	11.380	1576	1580	1582	rBV	2463907	1993565	32.56%	3.817%
26	11.404	1582	1584	1587	rVV	1272410	939968	15.35%	1.800%
27	11.451	1587	1592	1595	rVB	264954	279326	4.56%	0.535%
28	11.610	1613	1619	1621	rBV2	133694	163477	2.67%	0.313%
29	11.674	1628	1630	1633	rBV	82038	72694	1.19%	0.139%
30	11.886	1663	1666	1668	rBV	87393	75629	1.24%	0.145%
31	11.910	1668	1670	1674	rBV	395791	357711	5.84%	0.685%
32	11.998	1681	1685	1687	rBV	214134	212015	3.46%	0.406%
33	12.086	1697	1700	1702	rBV2	90299	66108	1.08%	0.127%
34	12.363	1744	1747	1750	rBV3	68202	75120	1.23%	0.144%
35	12.439	1757	1760	1762	rBV2	67056	69429	1.13%	0.133%
36	12.474	1764	1766	1771	rVB2	123697	110654	1.81%	0.212%

LSC Area Percent Report

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Operator : JU/CG
Sample : M2076-18
Misc :
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Instrument : BNA_F
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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
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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.598	1784	1787	1790	rBV	1206635	926142	15.13%	1.773%
38	12.639	1792	1794	1800	rVB4	112323	102719	1.68%	0.197%
39	12.827	1820	1826	1828	rBV	800860	882637	14.42%	1.690%
40	12.851	1828	1830	1842	rVB4	207092	317336	5.18%	0.608%
41	12.974	1847	1851	1854	rVV	4703311	4504001	73.57%	8.623%
42	13.157	1879	1882	1885	rVB	167493	168975	2.76%	0.324%
43	13.204	1888	1890	1891	rBV	99522	72287	1.18%	0.138%
44	13.257	1897	1899	1902	rVB	98461	89035	1.45%	0.170%
45	13.351	1913	1915	1918	rVB	79192	64732	1.06%	0.124%
46	13.380	1918	1920	1923	rBV3	79218	76413	1.25%	0.146%
47	13.551	1947	1949	1952	rBV2	95976	70827	1.16%	0.136%
48	13.886	2002	2006	2020	rVB2	412312	818551	13.37%	1.567%
49	14.027	2025	2030	2033	rVV2	1677321	1912281	31.23%	3.661%
50	14.051	2033	2034	2041	rVB	436291	295512	4.83%	0.566%
51	14.198	2056	2059	2061	rBV2	99010	106159	1.73%	0.203%
52	14.504	2108	2111	2114	rBV2	141298	139527	2.28%	0.267%
53	15.074	2204	2208	2216	rVB	328611	674404	11.02%	1.291%
54	15.157	2219	2222	2224	rBV2	144750	155856	2.55%	0.298%
55	15.380	2257	2260	2266	rVB	241691	294885	4.82%	0.565%
56	15.439	2267	2270	2274	rVB	286310	297233	4.85%	0.569%
57	15.504	2277	2281	2285	rBV	1021358	1291960	21.10%	2.474%
58	16.233	2401	2405	2412	rVB9	102340	210161	3.43%	0.402%
59	17.427	2603	2608	2613	rVB2	92816	154149	2.52%	0.295%

Sum of corrected areas: 52230208

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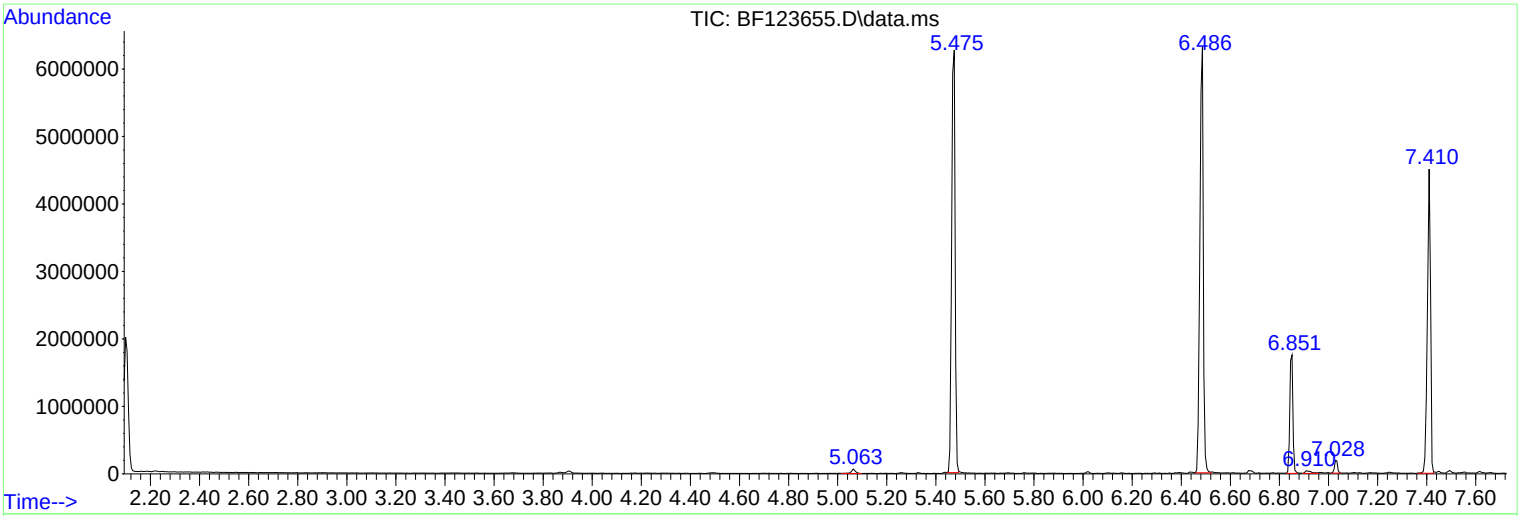
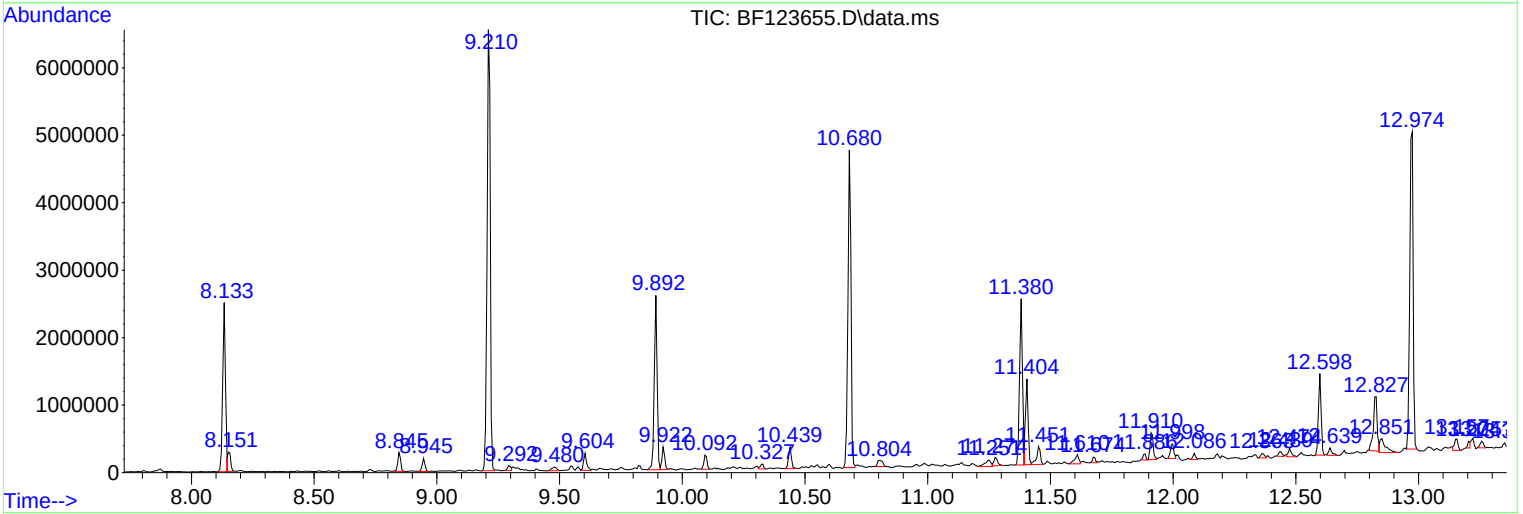
Misc :
ALS Vial : 19 Sample Multiplier: 1

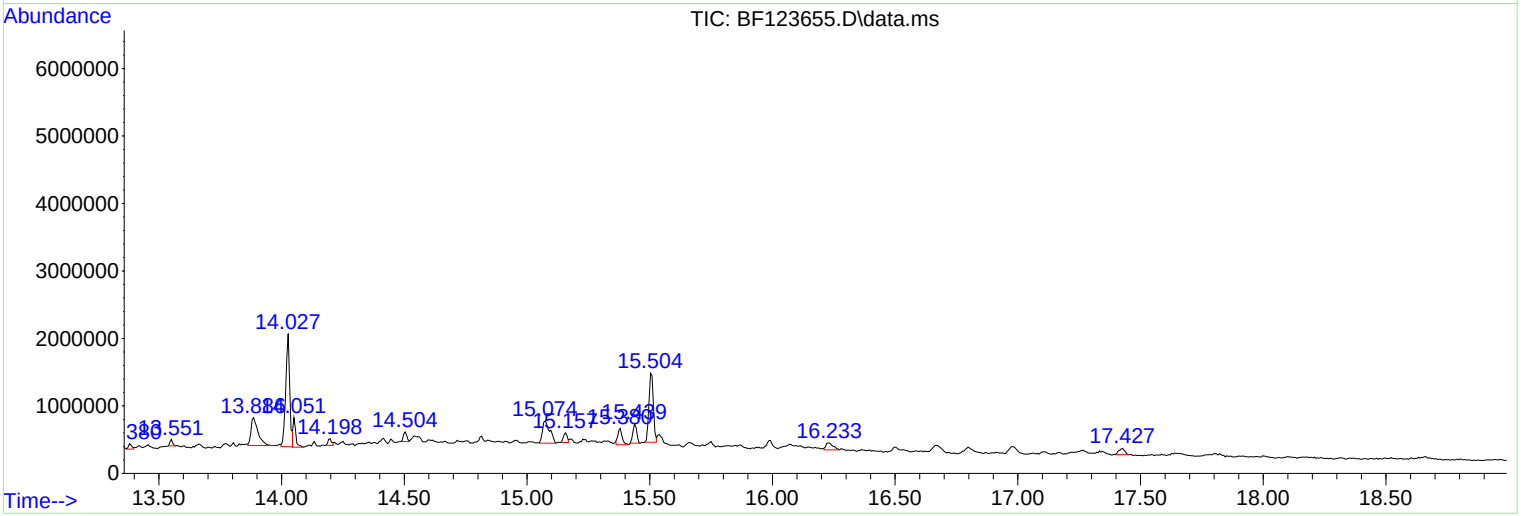
Instrument :
BNA_F
ClientSampleId :
SB-18-14.5-15.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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TIC Library : C:\DATABASE\NIST11.L
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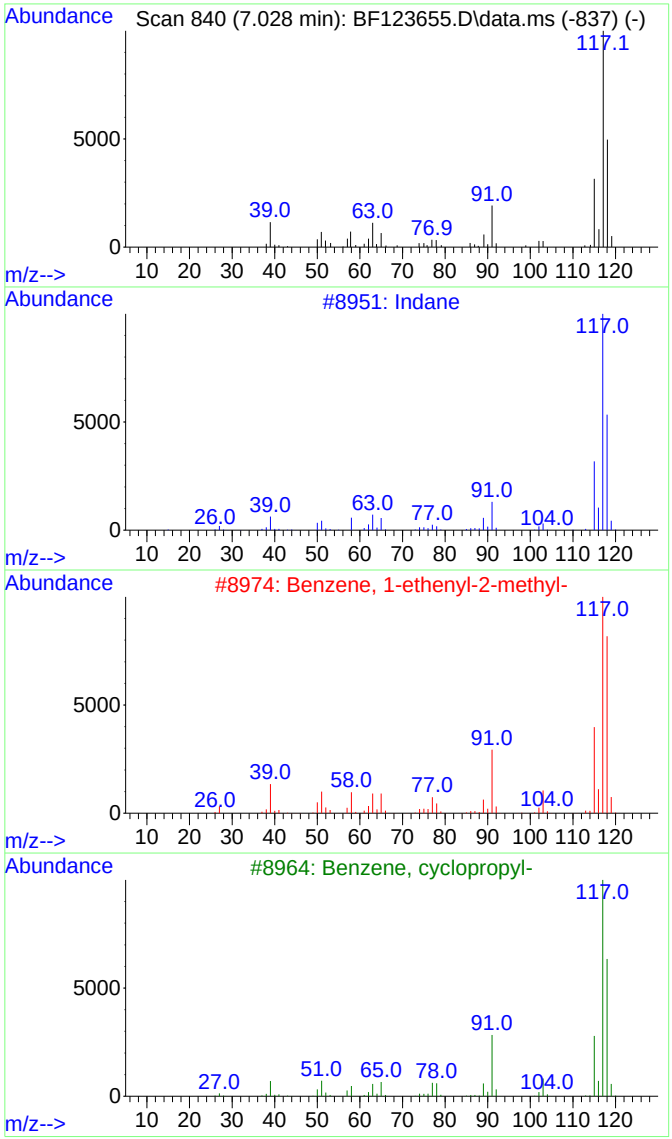
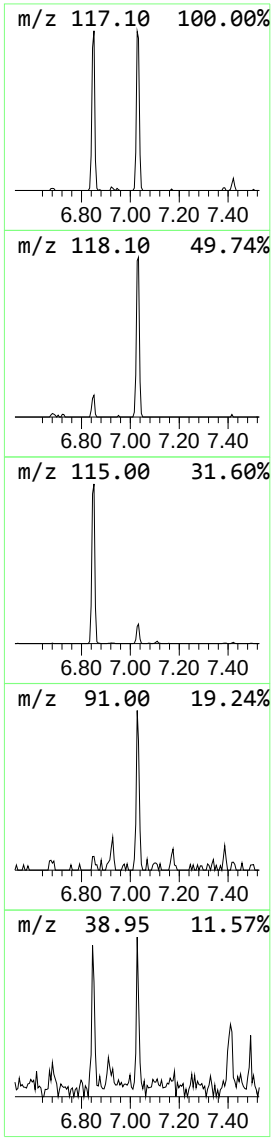
****

Peak Number 1 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.028	2.14 ng	165412	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	78
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
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Acq On : 20 Apr 2021 21:55
Operator : JU/CG
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-18-14.5-15.0

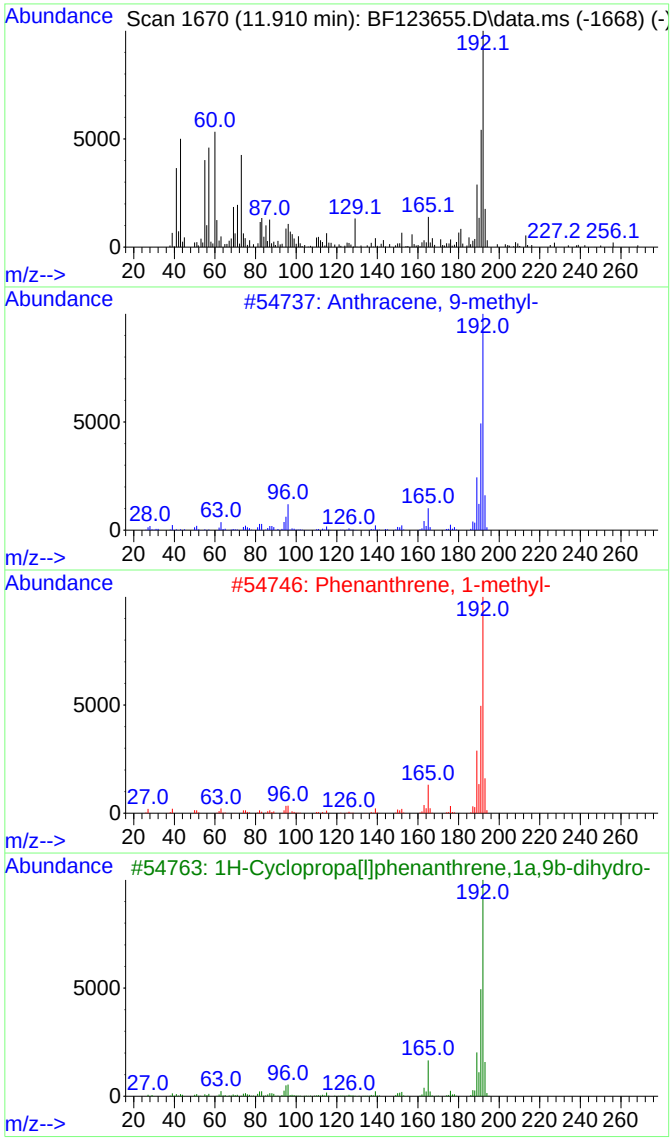
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

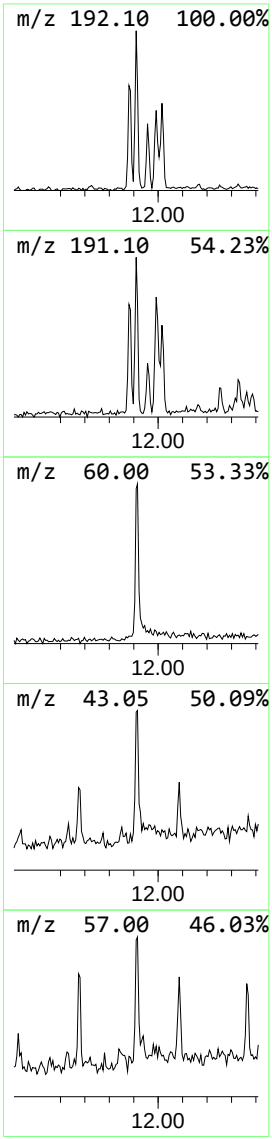
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Anthracene, 9-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.59 ng	357711	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	96
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123655.D
Acq On : 20 Apr 2021 21:55
Operator : JU/CG
Sample : M2076-18
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-14.5-15.0

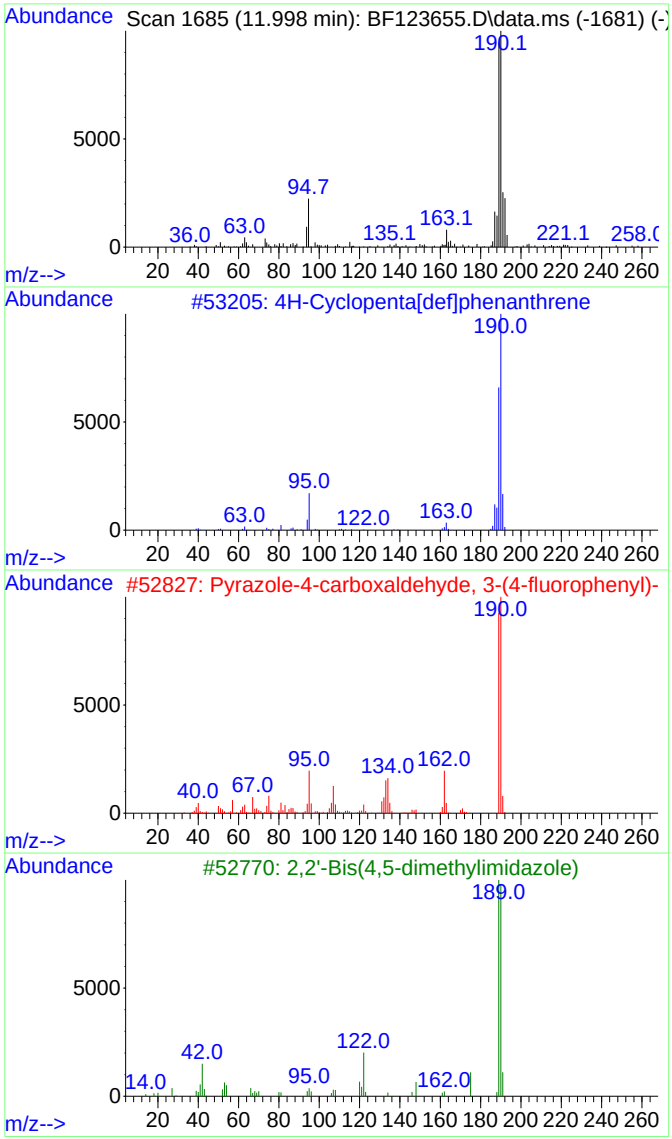
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

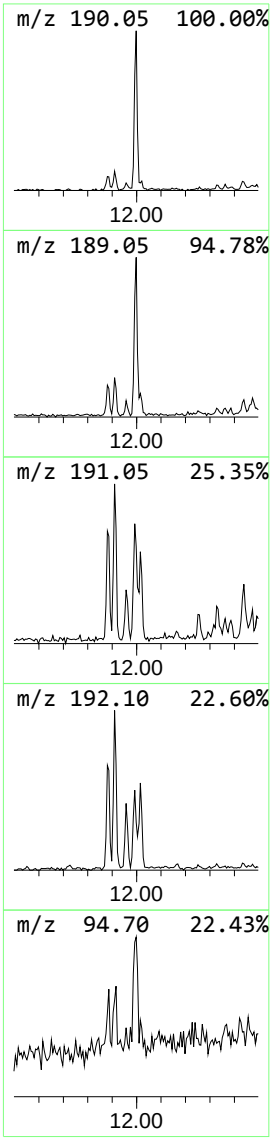
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.998	2.13 ng	212015	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	53
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	Pyrimidine, 6-oxo-4-(4-fluorophe...	190	C10H7FN2O	085979-57-3	23
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
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Instrument : BNA_F
ClientSampleId : SB-18-14.5-15.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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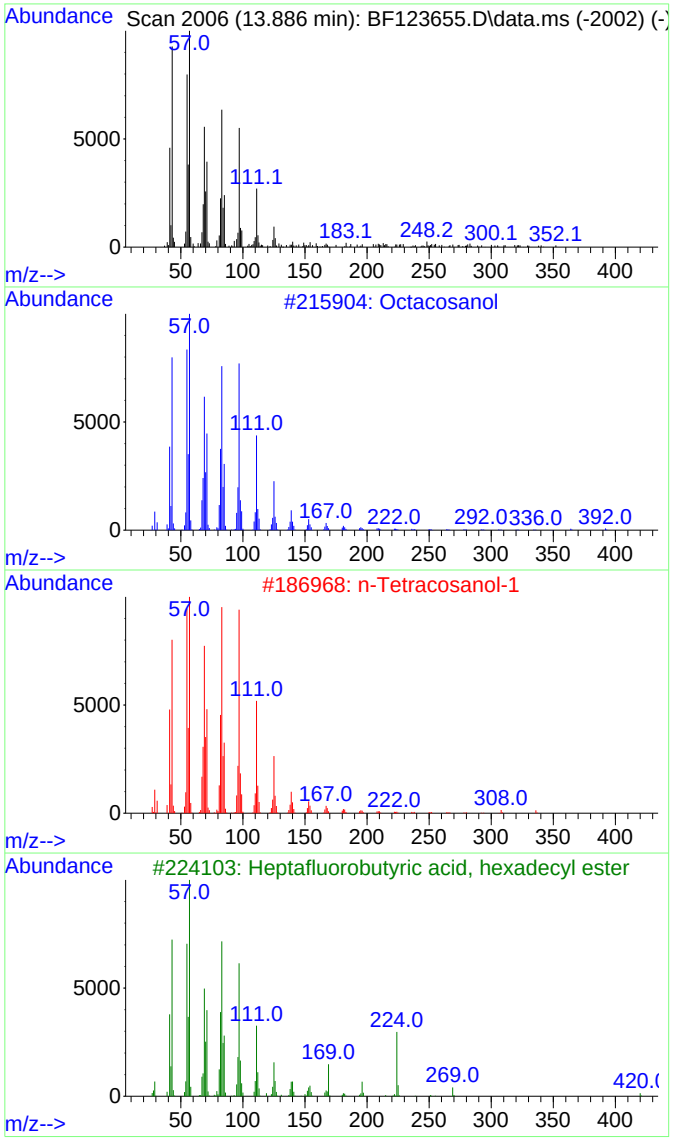
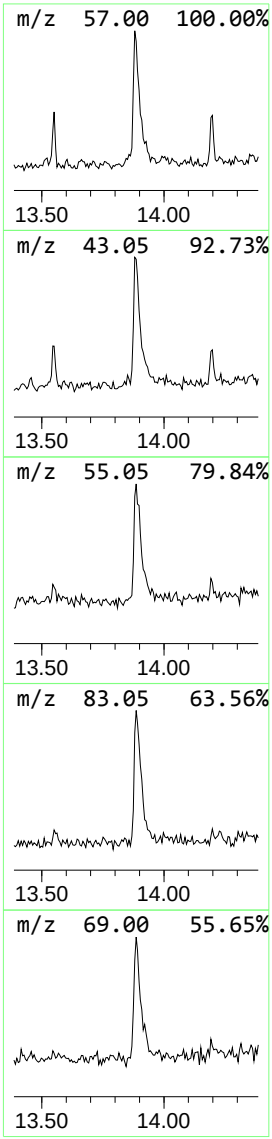
Peak Number 4 Octacosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	8.56 ng	818551	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	86
4	17-Pentatriacontene	491	C35H70	006971-40-0	83
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	72





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Instrument : BNA_F
ClientSampleId : SB-18-14.5-15.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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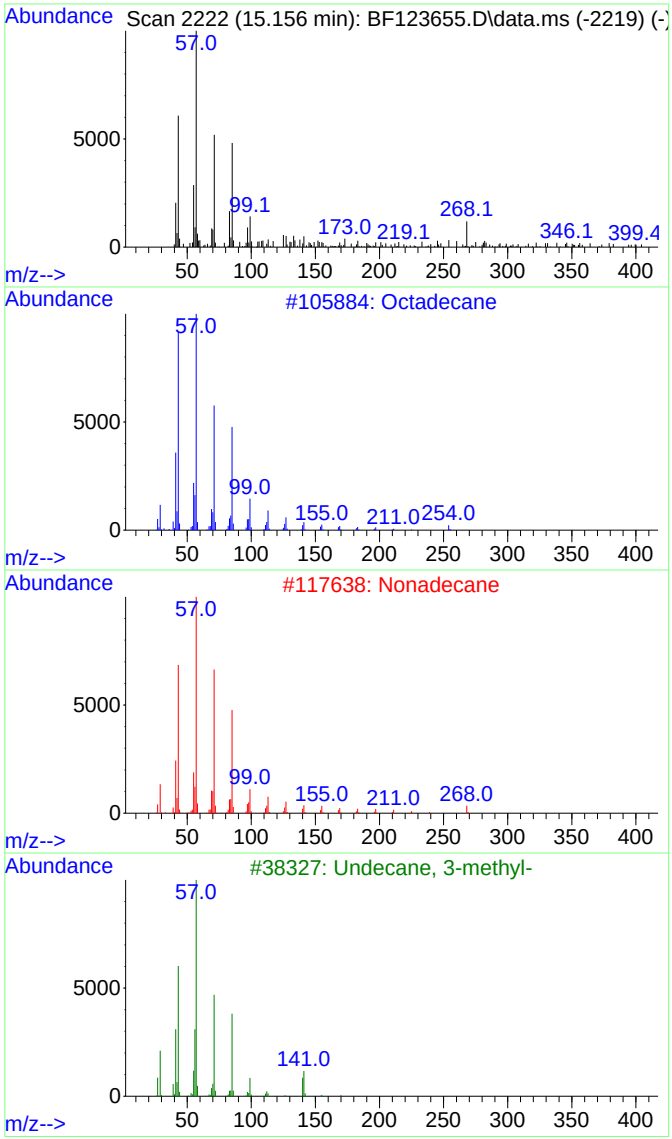
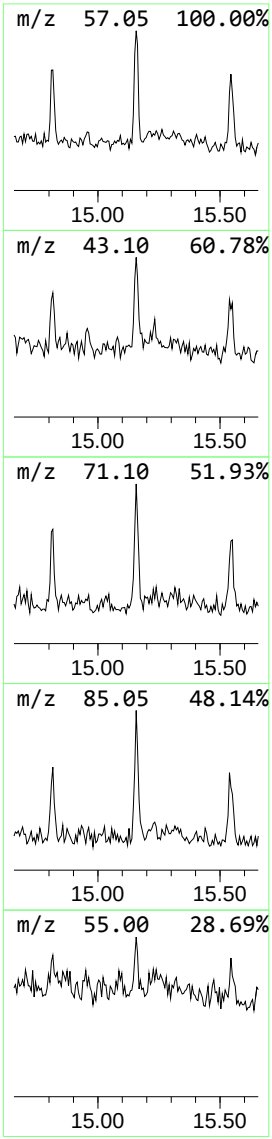
Peak Number 5 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.156	2.41 ng	155856	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	87
2	Nonadecane	268	C19H40	000629-92-5	80
3	Undecane, 3-methyl-	170	C12H26	001002-43-3	72
4	Tetracosane	338	C24H50	000646-31-1	70
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	68





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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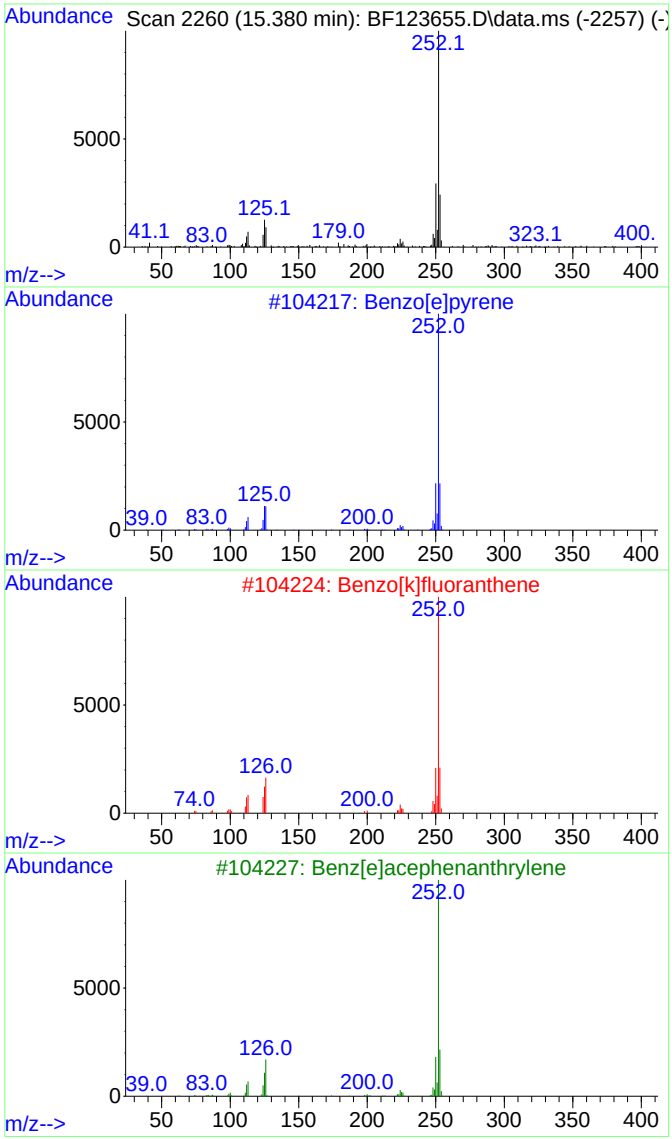
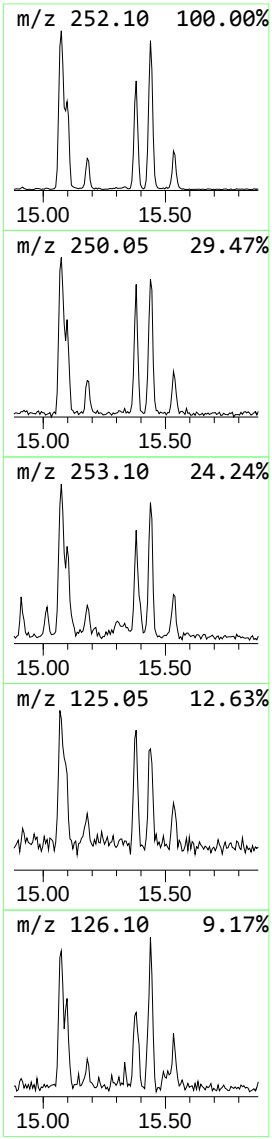
Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	4.56 ng	294885	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





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Data File : BF123655.D
Acq On : 20 Apr 2021 21:55
Operator : JU/CG
Sample : M2076-18
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-14.5-15.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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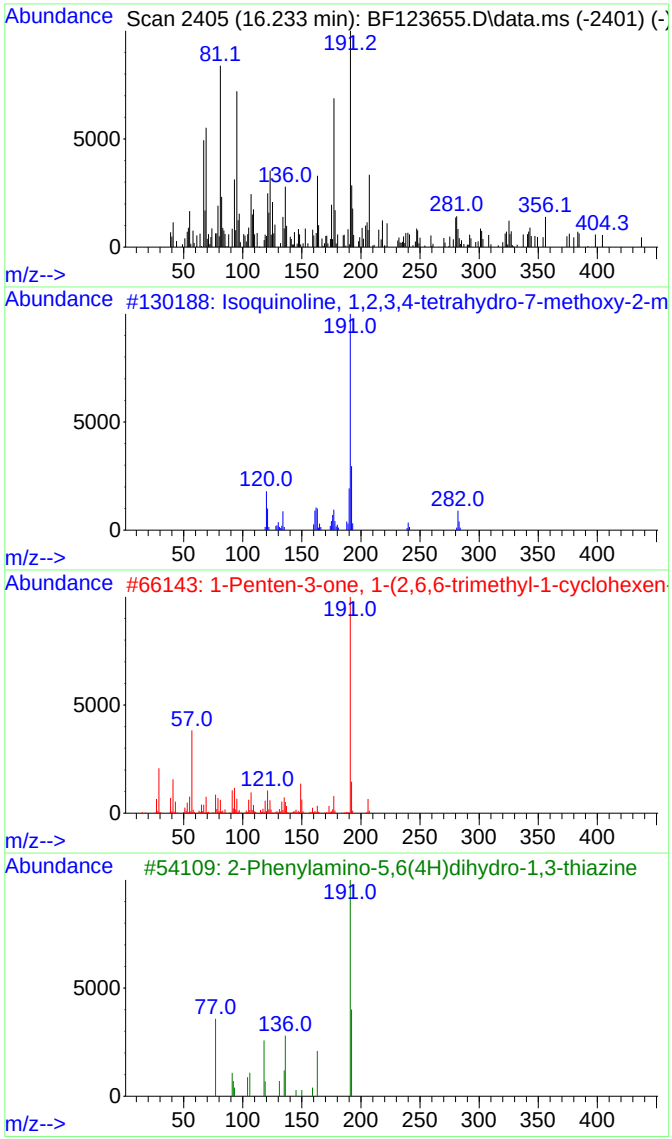
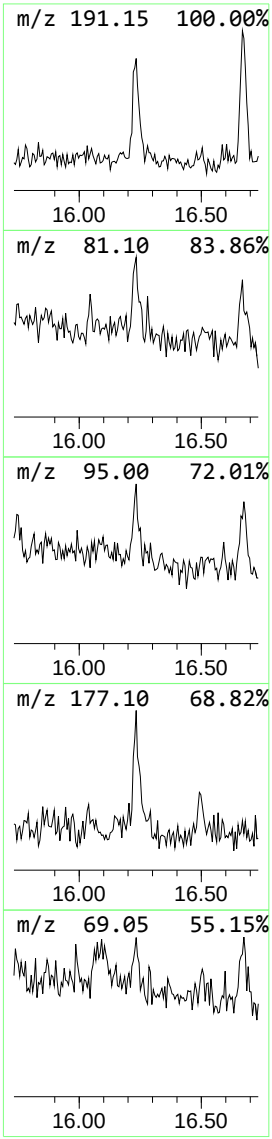
Peak Number 7 unknown16.233 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.233	3.25 ng	210161	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	49
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	22
3	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	22
4	1,2-Diheptylcyclopropene	236	C17H32	035365-53-8	22
5	2-Chloro-4,6-dimethylquinoline	191	C11H10ClN	003913-18-6	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123655.D
Acq On : 20 Apr 2021 21:55
Operator : JU/CG
Sample : M2076-18
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-14.5-15.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Indane	7.028	2.1	ng	165412	1	6.851	1543880	20.0
Anthracene, 9-m...	11.910	3.6	ng	357711	4	11.380	1993570	20.0
4H-Cyclopenta[d...	11.998	2.1	ng	212015	4	11.380	1993570	20.0
Octacosanol	13.886	8.6	ng	818551	5	14.027	1912280	20.0
Octadecane	15.156	2.4	ng	155856	6	15.504	1291960	20.0
Benzo[e]pyrene	15.380	4.6	ng	294885	6	15.504	1291960	20.0
unknown16.233	16.233	3.3	ng	210161	6	15.504	1291960	20.0