LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123604.D
Acq On : 16 Apr 2021 21:50
Operator : JU/CG
Sample : M2050-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

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: BF123604.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	11	23	28	rVB	1887953	2767991	32.33%	3.883%
2	5.116	511	515	524	rVB	102234	136568	1.60%	0.192%
3	5.504	577	581	585	rBV	8398966	8202333	95.80%	11.507%
4	6.510	747	752	755	rBV	8270234	8540064	99.75%	11.980%
5	6.704	780	785	788	rBV2	90750	110263	1.29%	0.155%
6	6.869	809	813	816	rBV	2339071	1880199	21.96%	2.638%
7	7.433	901	909	912	rBV	5716832	5768770	67.38%	8.093%
8	8.151	1026	1031	1034	rBV	2761010	2506892	29.28%	3.517%
9	9.233	1209	1215	1218	rBV	9293141	8561858	100.00%	12.011%
10	9.316	1225	1229	1231	rBV	99271	97708	1.14%	0.137%
11	9.622	1279	1281	1285	rBV	234757	222640	2.60%	0.312%
12	9.769	1303	1306	1311	rVB	110544	99035	1.16%	0.139%
13	9.916	1324	1331	1334	rBV	2779569	2558220	29.88%	3.589%
14	10.116	1362	1365	1368	rBV	122388	103372	1.21%	0.145%
15	10.704	1459	1465	1468	rBV	5830592	5578771	65.16%	7.826%
16	10.821	1482	1485	1490	rBV2	131603	139315	1.63%	0.195%
17	11.204	1547	1550	1554	rVB	119148	110266	1.29%	0.155%
18	11.269	1554	1561	1564	rVV5	108265	176308	2.06%	0.247%
19	11.298	1564	1566	1571	rVB2	104938	101163	1.18%	0.142%
20	11.404	1580	1584	1586	rBV	2791567	2338228	27.31%	3.280%
21	11.427	1586	1588	1591	rVV	1144492	857179	10.01%	1.202%
22	11.474	1594	1596	1599	rVB	237318	189389	2.21%	0.266%
23	11.633	1617	1623	1625	rBV2	103765	142144	1.66%	0.199%
24	11.698	1631	1634	1637	rBV	114393	90171	1.05%	0.126%
25	11.904	1666	1669	1671	rBV	181538	141351	1.65%	0.198%
26	11.933	1671	1674	1678	rVV	857839	696839	8.14%	0.978%
27	12.016	1685	1688	1690	rBV2	248417	246892	2.88%	0.346%
28	12.039	1690	1692	1696	rVB	161039	136175	1.59%	0.191%
29	12.110	1701	1704	1707	rBV	127171	106706	1.25%	0.150%
30	12.204	1717	1720	1721	rBV	118391	108999	1.27%	0.153%
31	12.221	1721	1723	1728	rVB	143104	111966	1.31%	0.157%
32	12.457	1760	1763	1766	rBV	164686	157110	1.83%	0.220%
33	12.498	1766	1770	1775	rVB2	163000	200358	2.34%	0.281%
34	12.539	1775	1777	1782	rBV2	116611	121562	1.42%	0.171%
35	12.621	1787	1791	1794	rBV	1546259	1371826	16.02%	1.924%
36	12.721	1804	1808	1810	rBV2	160756	180509	2.11%	0.253%

LSC Area Percent Report

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Acq On : 16 Apr 2021 21:50
Operator : JU/CG
Sample : M2050-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

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

37	12.851	1824	1830	1832	rBV	1251644	1307099	15.27%	1.834%
38	12.874	1832	1834	1842	rVB3	332992	469464	5.48%	0.659%
39	12.998	1851	1855	1858	rVB	6623770	5810875	67.87%	8.152%
40	13.068	1863	1867	1870	rBV3	115344	162262	1.90%	0.228%
41	13.174	1883	1885	1889	rVB	185603	173943	2.03%	0.244%
42	13.227	1891	1894	1900	rVV4	108847	208665	2.44%	0.293%
43	13.280	1900	1903	1906	rVV2	148895	145734	1.70%	0.204%
44	13.404	1922	1924	1928	rBV2	100661	101561	1.19%	0.142%
45	13.686	1970	1972	1986	rVB3	289609	579909	6.77%	0.814%
46	13.827	1994	1996	1998	rBV	106627	89251	1.04%	0.125%
47	13.910	2005	2010	2016	rBV2	473409	678478	7.92%	0.952%
48	14.051	2029	2034	2037	rBV2	1738104	2089518	24.40%	2.931%
49	14.074	2037	2038	2044	rVB	647306	492208	5.75%	0.690%
50	14.527	2113	2115	2118	rBV2	135701	139439	1.63%	0.196%
51	15.104	2209	2213	2220	rBV	502564	1007895	11.77%	1.414%
52	15.415	2262	2266	2271	rVB	318689	429907	5.02%	0.603%
53	15.474	2272	2276	2281	rBV	424296	517259	6.04%	0.726%
54	15.545	2283	2288	2291	rBV	938333	1216506	14.21%	1.707%
55	17.027	2537	2540	2548	rVB2	233225	430560	5.03%	0.604%
56	17.480	2613	2617	2627	rVB	189523	373801	4.37%	0.524%

Sum of corrected areas: 71283474

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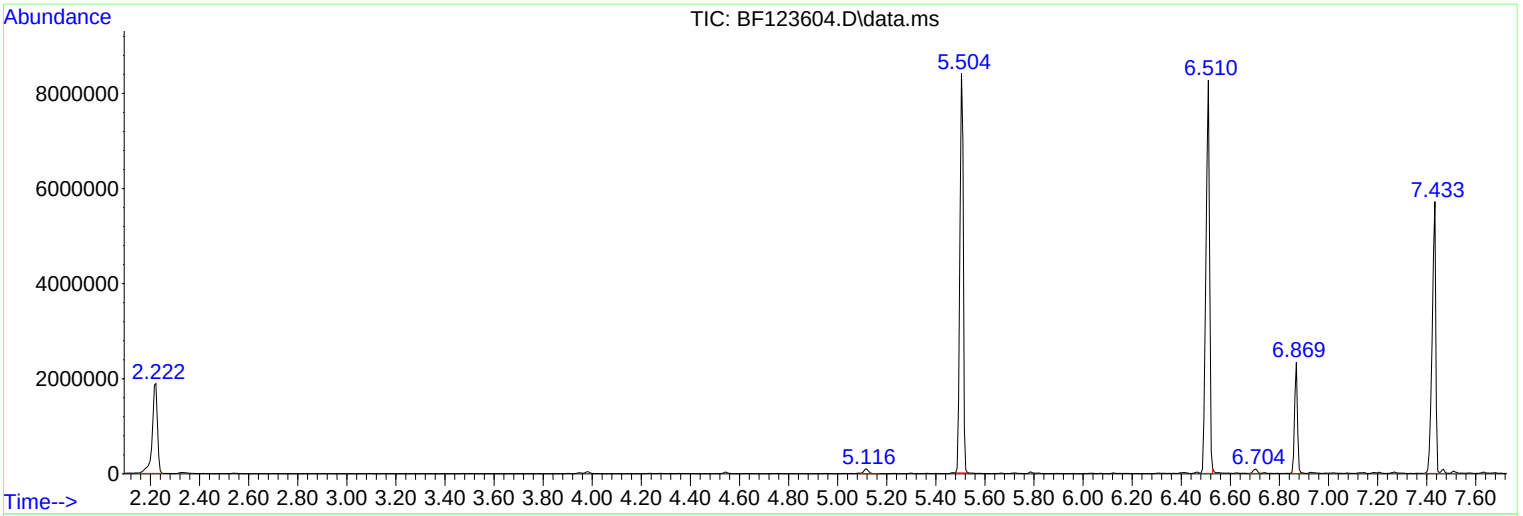
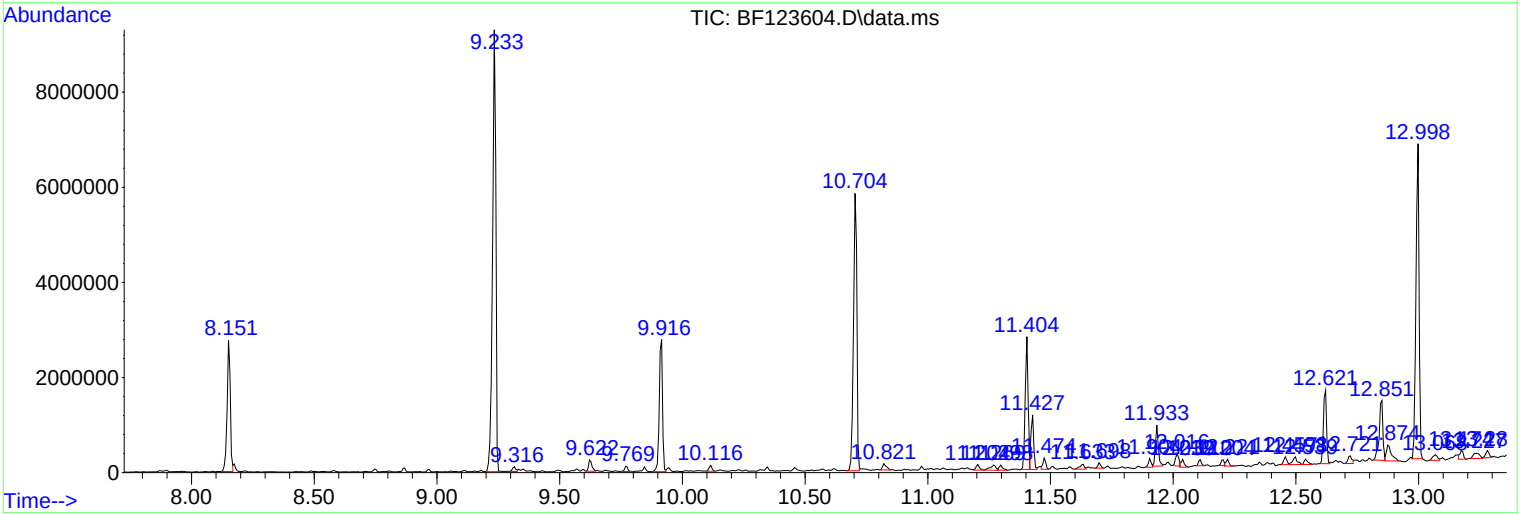
Sample : M2050-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

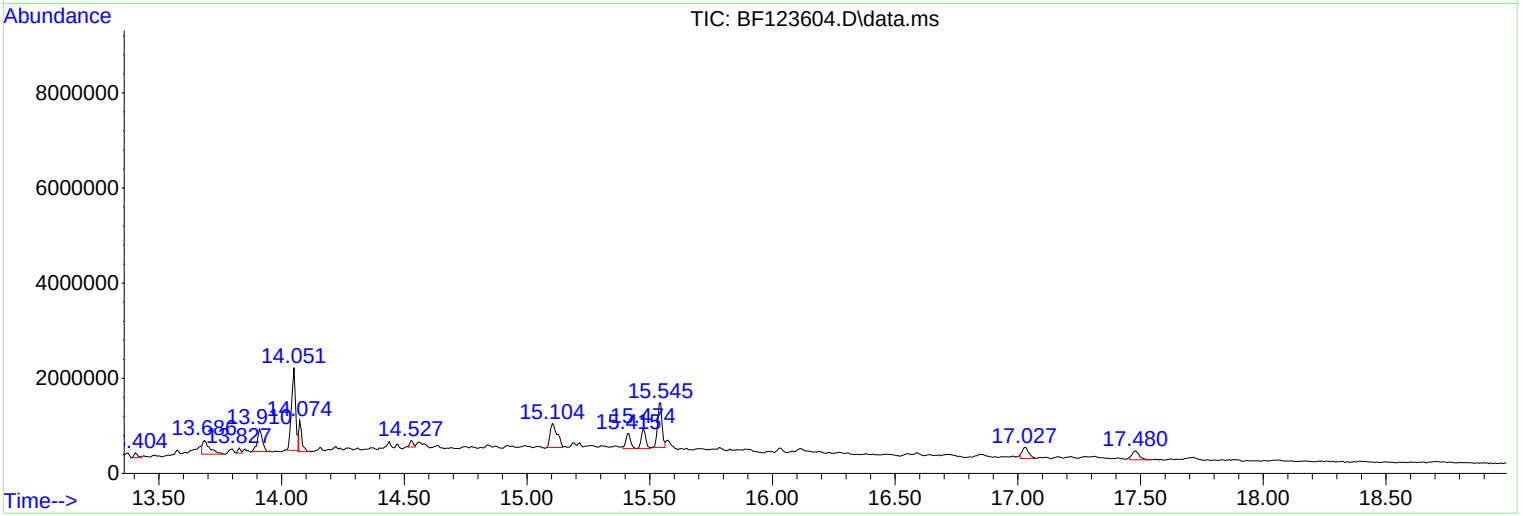
Instrument :
BNA_F
ClientSampleId :
TP-6

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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Data File : BF123604.D
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Instrument : BNA_F
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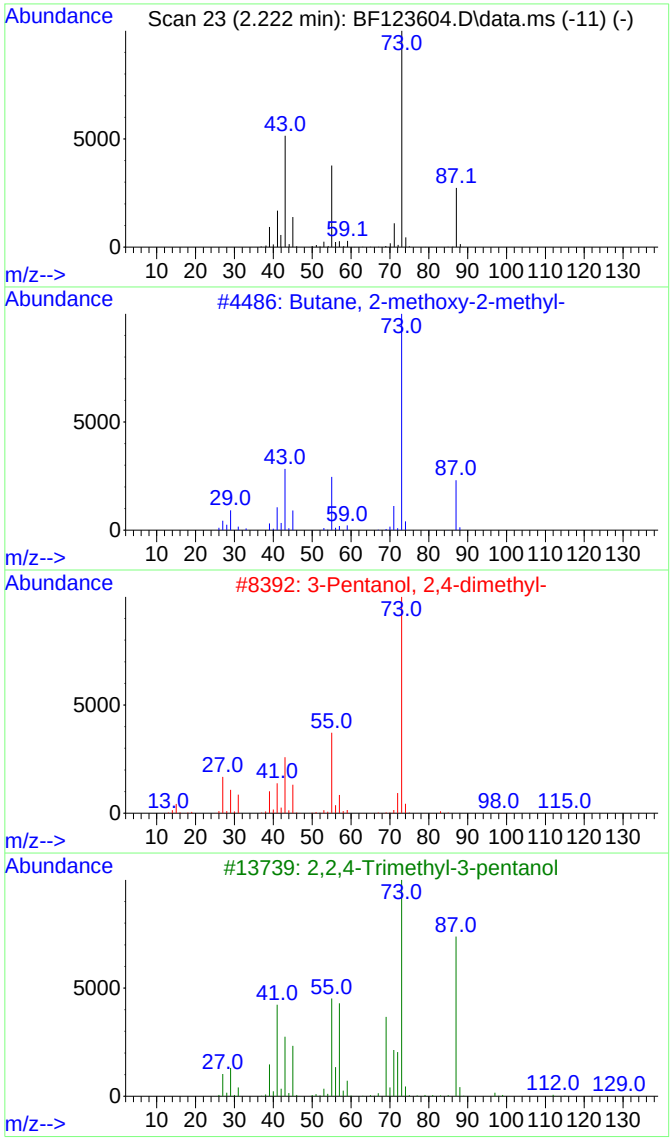
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

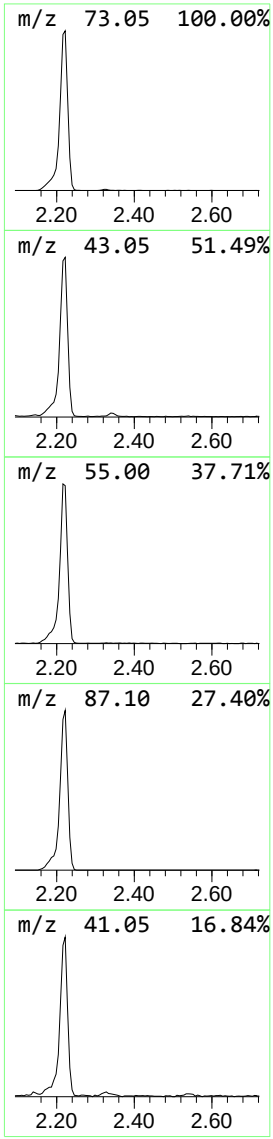
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	29.44 ng	2767990	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123604.D
Acq On : 16 Apr 2021 21:50
Operator : JU/CG
Sample : M2050-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

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

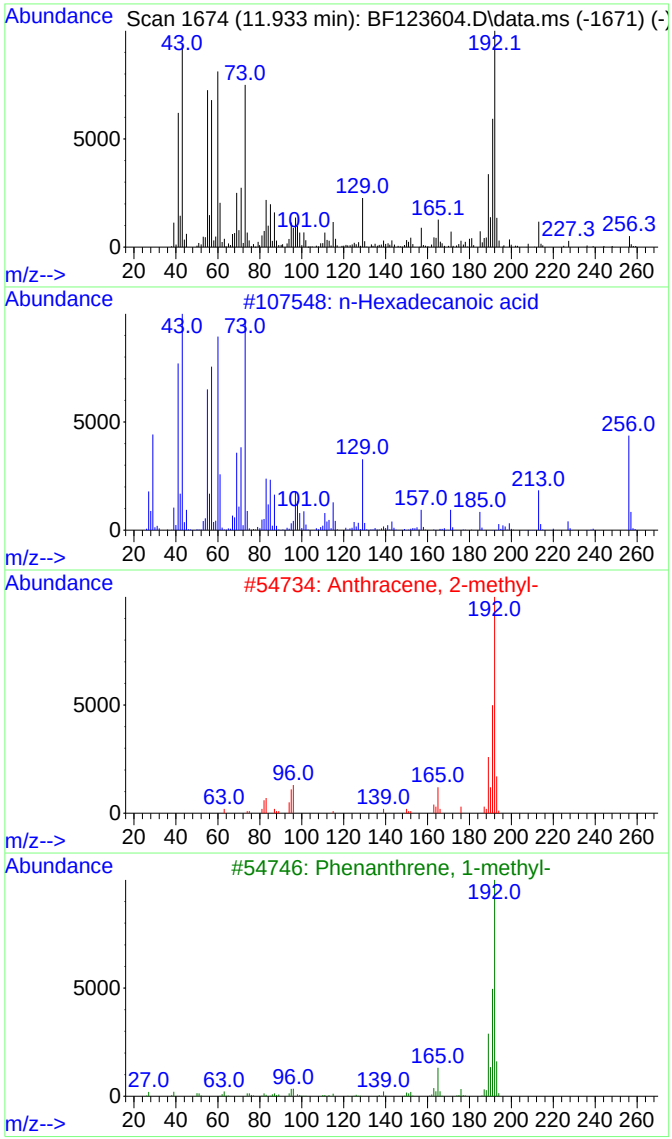
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

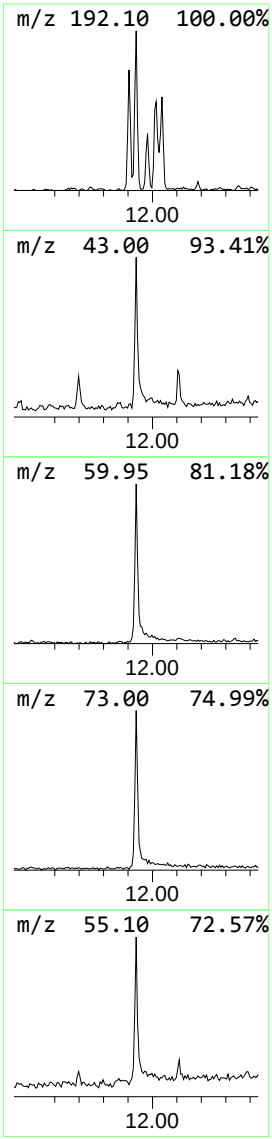
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	5.96 ng	696839	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	83
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	83
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123604.D
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Operator : JU/CG
Sample : M2050-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

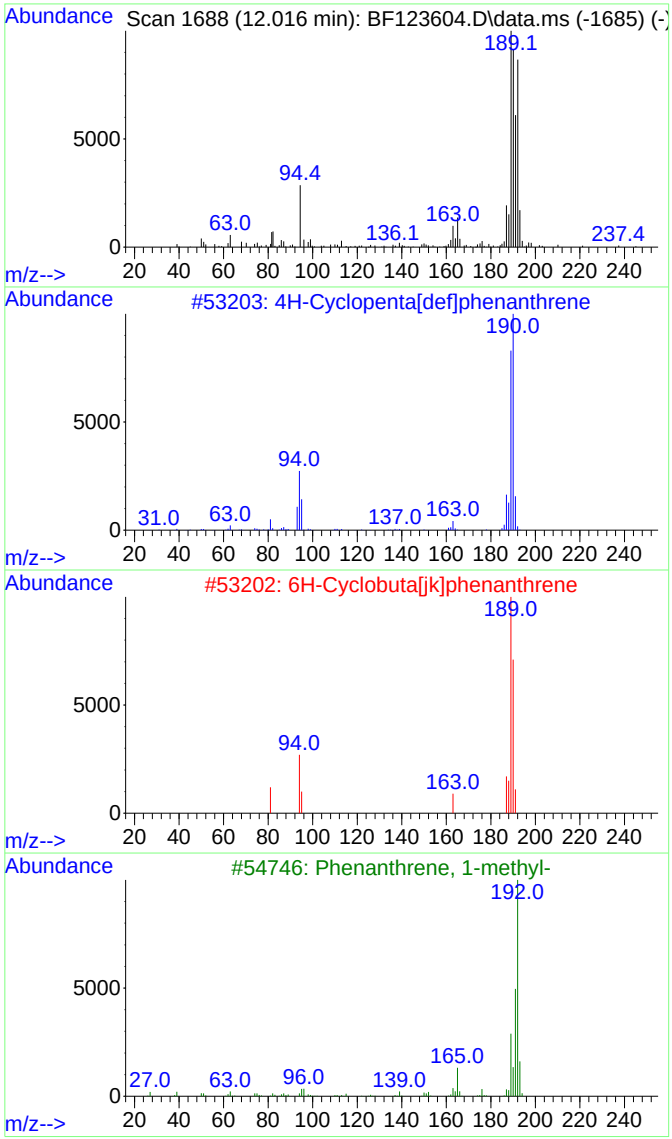
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

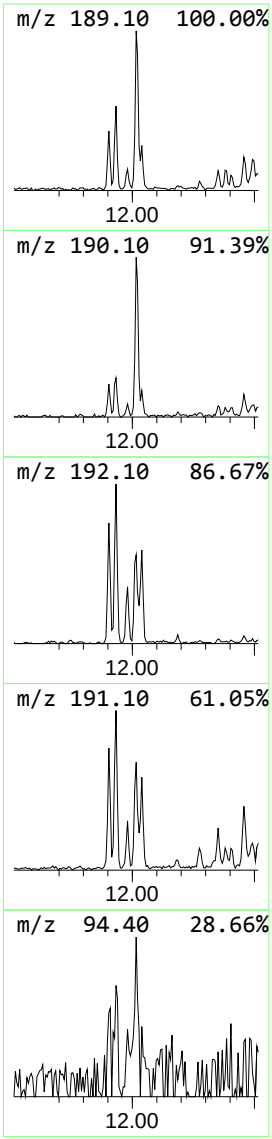
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.015	2.11 ng	246892	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123604.D
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Sample : M2050-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-6

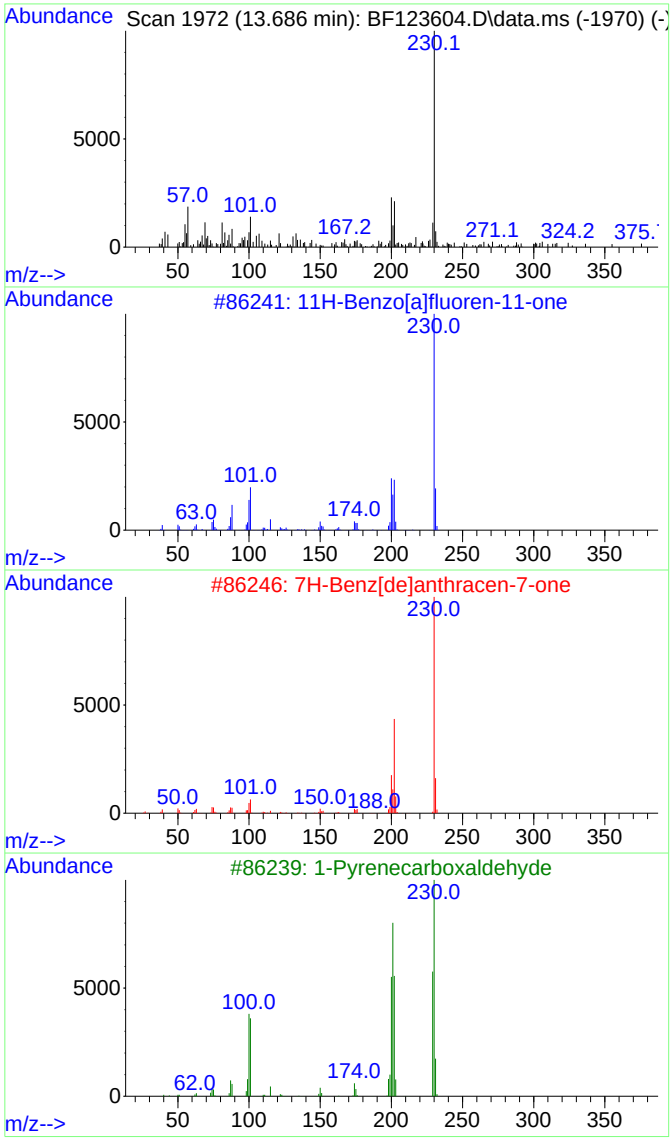
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

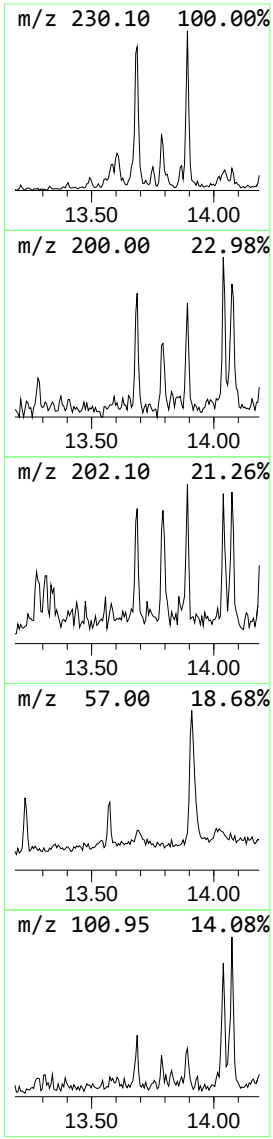
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 11H-Benzo[a]fluoren-11-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.686	5.55 ng	579909	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	81
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	70
3	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	50
4	Naphthacene, 5,12-dihydro-	230	C18H14	000959-02-4	47
5	8-Chlorobenzo[h][1,6]-naphthyrid...	230	C12H7ClN2O	025100-26-9	43





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

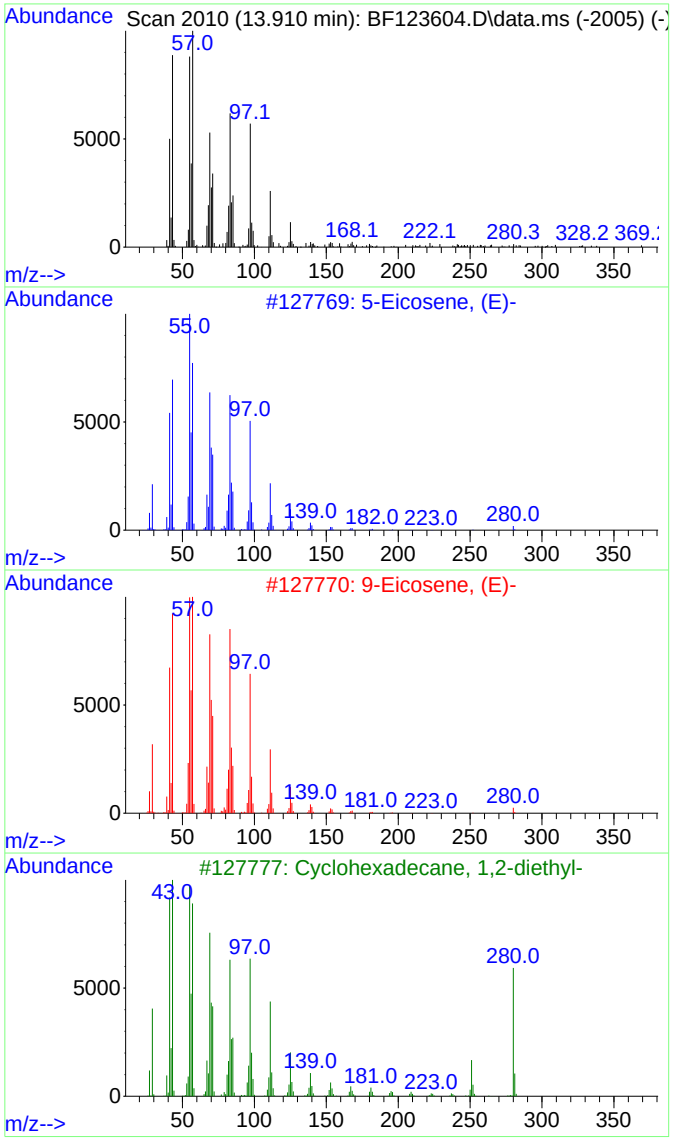
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

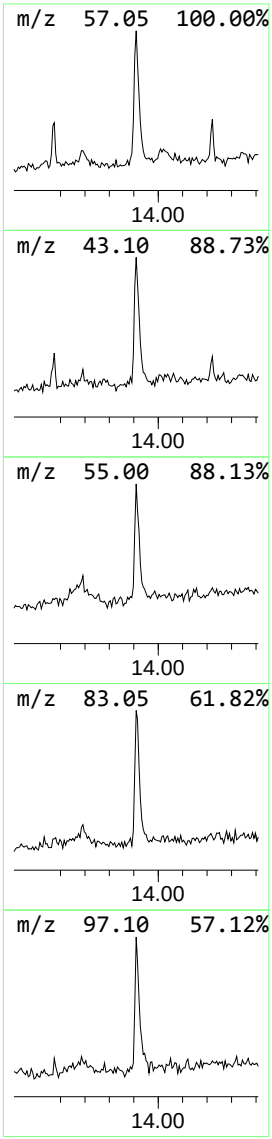
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	6.49 ng	678478	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	92
4	Cyclotetracosane	336	C24H48	000297-03-0	91
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

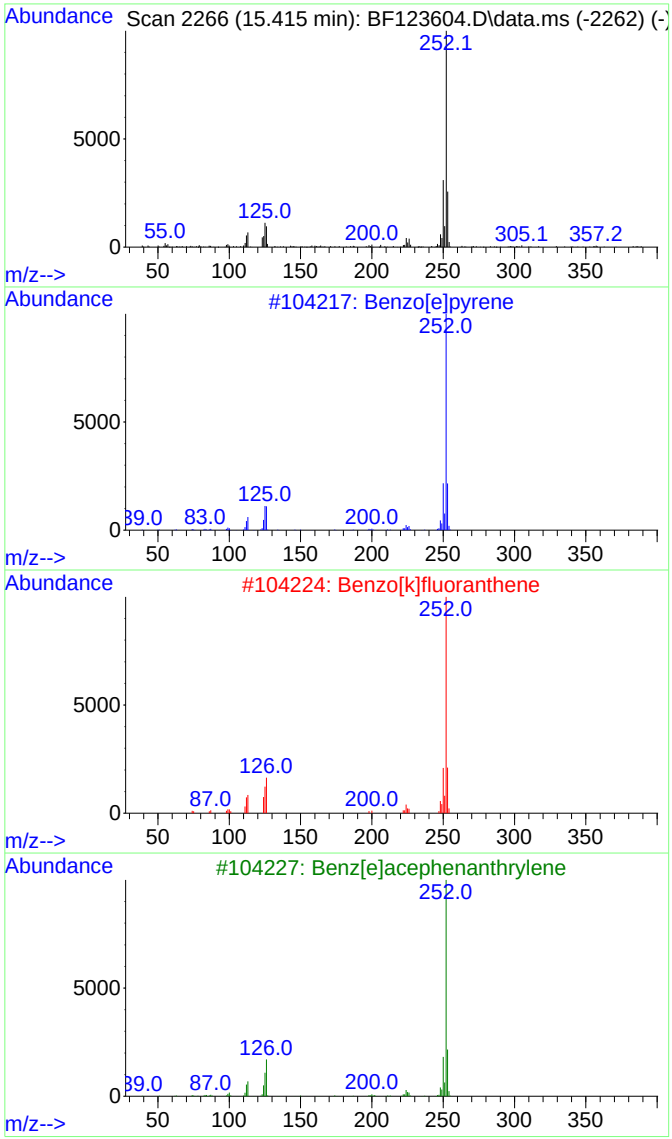
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

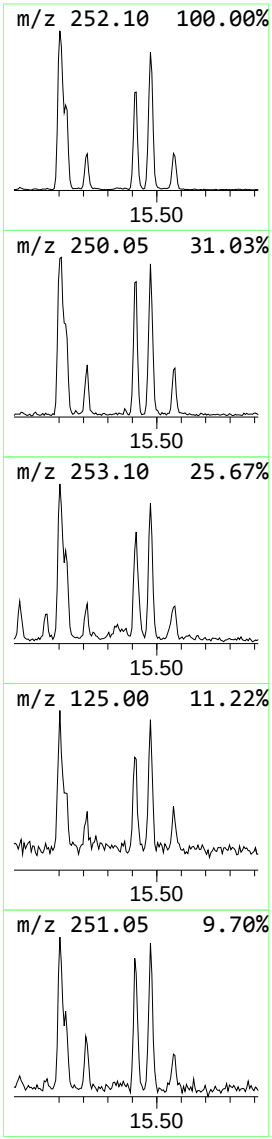
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.415	7.07 ng	429907	Perylene-d12	15.545

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	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123604.D
Acq On : 16 Apr 2021 21:50
Operator : JU/CG
Sample : M2050-17
Misc :
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Instrument : BNA_F
ClientSampleId : TP-6

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
Butane, 2-metho...	2.222	29.4	ng	2767990	1	6.869	1880200	20.0
n-Hexadecanoic ...	11.933	6.0	ng	696839	4	11.404	2338230	20.0
4H-Cyclopenta[d...	12.015	2.1	ng	246892	4	11.404	2338230	20.0
11H-Benzo[a]flu...	13.686	5.5	ng	579909	5	14.051	2089520	20.0
5-Eicosene, (E)-	13.910	6.5	ng	678478	5	14.051	2089520	20.0
Benzo[e]pyrene	15.415	7.1	ng	429907	6	15.545	1216510	20.0