LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119463.D
Acq On : 20 Mar 2020 3:13
Operator : CG/JU
Sample : L1913-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

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-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	499	506	512	rVB	89470	121124	1.86%	0.198%
2	5.463	568	574	577	rBV	6676251	6495298	100.00%	10.611%
3	6.469	740	745	748	rBV	5677986	6286301	96.78%	10.270%
4	6.669	777	779	785	rBV	86275	89238	1.37%	0.146%
5	6.851	806	810	813	rBV	2337618	1840046	28.33%	3.006%
6	7.010	832	837	840	rBV	5726784	5141272	79.15%	8.399%
7	7.410	900	905	908	rBV	4287905	4082775	62.86%	6.670%
8	8.134	1024	1028	1031	rBV	2644666	2239642	34.48%	3.659%
9	9.216	1207	1212	1215	rBV	6790107	5985892	92.16%	9.779%
10	9.298	1222	1226	1235	rBV2	100626	156062	2.40%	0.255%
11	9.604	1275	1278	1283	rBV	737236	610221	9.39%	0.997%
12	9.751	1300	1303	1307	rBV	163233	139403	2.15%	0.228%
13	9.892	1321	1327	1331	rBV	2450866	2076266	31.97%	3.392%
14	10.092	1358	1361	1364	rBV2	74694	72790	1.12%	0.119%
15	10.439	1417	1420	1426	rVB2	61530	72215	1.11%	0.118%
16	10.680	1457	1461	1464	rBV	3701562	3207008	49.37%	5.239%
17	10.804	1479	1482	1490	rVB3	137459	189347	2.92%	0.309%
18	11.280	1561	1563	1568	rVB2	87198	94565	1.46%	0.154%
19	11.380	1576	1580	1583	rBV	2238988	1956089	30.12%	3.196%
20	11.404	1583	1584	1587	rVV	519695	299389	4.61%	0.489%
21	11.457	1587	1593	1595	rVV	186332	186994	2.88%	0.305%
22	11.680	1629	1631	1635	rBV	96147	77388	1.19%	0.126%
23	11.886	1663	1666	1667	rBV	97460	82842	1.28%	0.135%
24	11.910	1667	1670	1676	rVV	998555	882488	13.59%	1.442%
25	11.992	1681	1684	1687	rBV2	198152	230282	3.55%	0.376%
26	12.092	1698	1701	1703	rBV	87253	78832	1.21%	0.129%
27	12.180	1713	1716	1718	rBV	81856	81684	1.26%	0.133%
28	12.433	1756	1759	1762	rBV	169081	162047	2.49%	0.265%
29	12.474	1763	1766	1771	rVV5	121164	194578	3.00%	0.318%
30	12.516	1771	1773	1778	rVB3	101849	127426	1.96%	0.208%
31	12.598	1783	1787	1789	rBV	1353330	1212767	18.67%	1.981%
32	12.698	1800	1804	1806	rBV2	323675	320294	4.93%	0.523%
33	12.827	1820	1826	1828	rBV	1465051	1470504	22.64%	2.402%
34	12.974	1847	1851	1854	rBV	5474540	5013530	77.19%	8.190%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119463.D
Acq On : 20 Mar 2020 3:13
Operator : CG/JU
Sample : L1913-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

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-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.045	1860	1863	1866	rVB	86518	101374	1.56%	0.166%
36	13.133	1875	1878	1879	rBV2	91988	103359	1.59%	0.169%
37	13.157	1879	1882	1884	rVB	222370	216755	3.34%	0.354%
38	13.216	1889	1892	1895	rVB2	171877	212330	3.27%	0.347%
39	13.257	1896	1899	1902	rBV2	210212	196799	3.03%	0.321%
40	13.351	1913	1915	1918	rVB	133504	99765	1.54%	0.163%
41	13.380	1918	1920	1923	rBV	140284	116150	1.79%	0.190%
42	13.551	1947	1949	1952	rBV3	136817	119634	1.84%	0.195%
43	13.804	1990	1992	1993	rBV	128965	86552	1.33%	0.141%
44	13.868	2000	2003	2013	rVB2	1121531	1263684	19.46%	2.064%
45	14.027	2025	2030	2032	rBV2	2001945	2611232	40.20%	4.266%
46	14.051	2032	2034	2036	rVB	665091	507657	7.82%	0.829%
47	14.198	2057	2059	2063	rVB3	239635	234931	3.62%	0.384%
48	14.504	2109	2111	2114	rBV2	385435	330803	5.09%	0.540%
49	14.815	2161	2164	2167	rBV	292848	274658	4.23%	0.449%
50	15.068	2203	2207	2210	rBV	547927	875722	13.48%	1.431%
51	15.157	2220	2222	2231	rVB2	342545	532220	8.19%	0.869%
52	15.368	2256	2258	2264	rVB	360906	436181	6.72%	0.713%
53	15.433	2266	2269	2273	rVB	454848	484278	7.46%	0.791%
54	15.498	2276	2280	2283	rBV	1026418	1132178	17.43%	1.850%

Sum of corrected areas: 61212861

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Operator : CG/JU
Sample : L1913-15
Misc :
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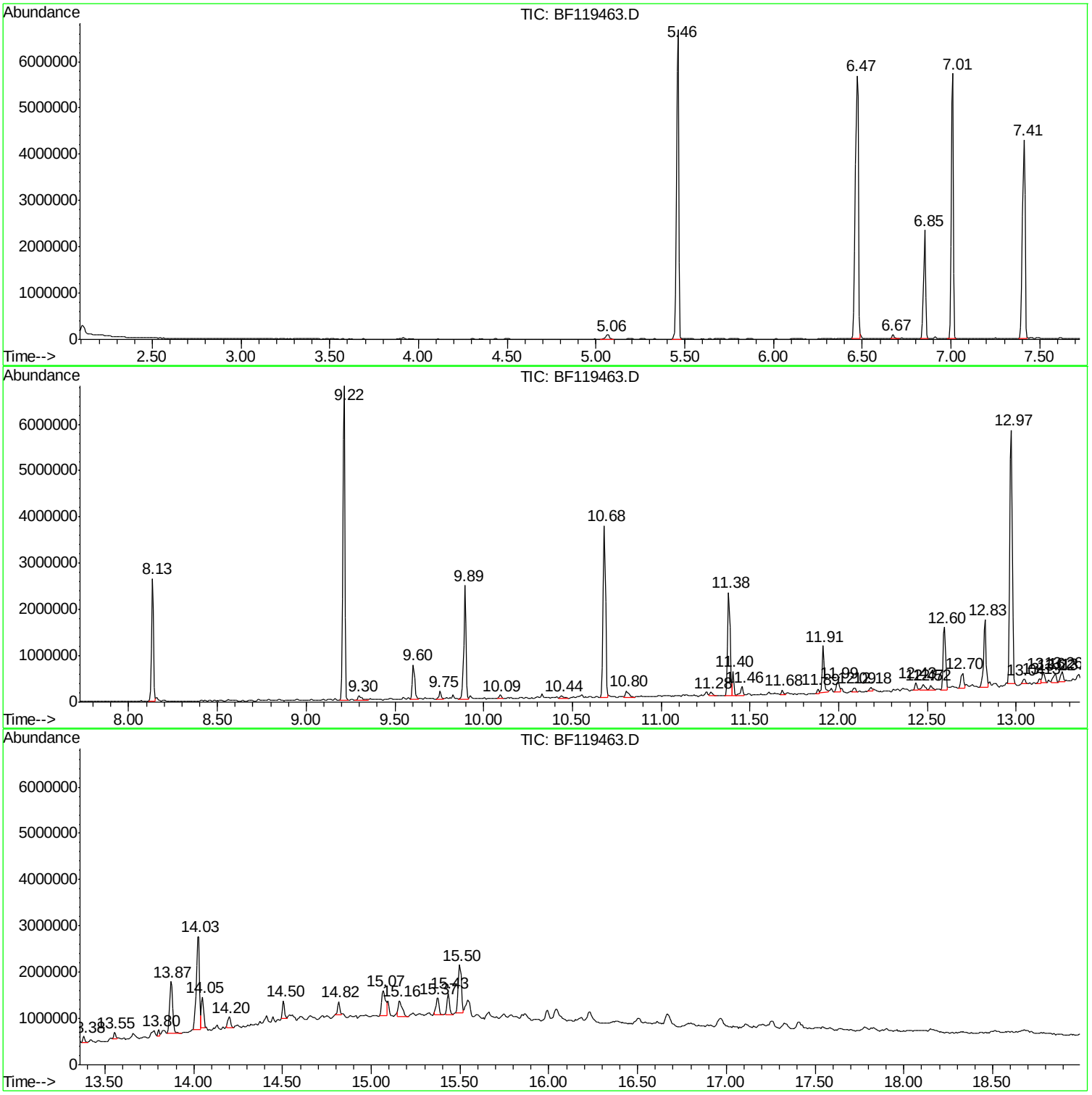
Instrument :
BNA_F
ClientSampleId :
MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119463.D
Acq On : 20 Mar 2020 3:13
Operator : CG/JU
Sample : L1913-15
Misc :
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Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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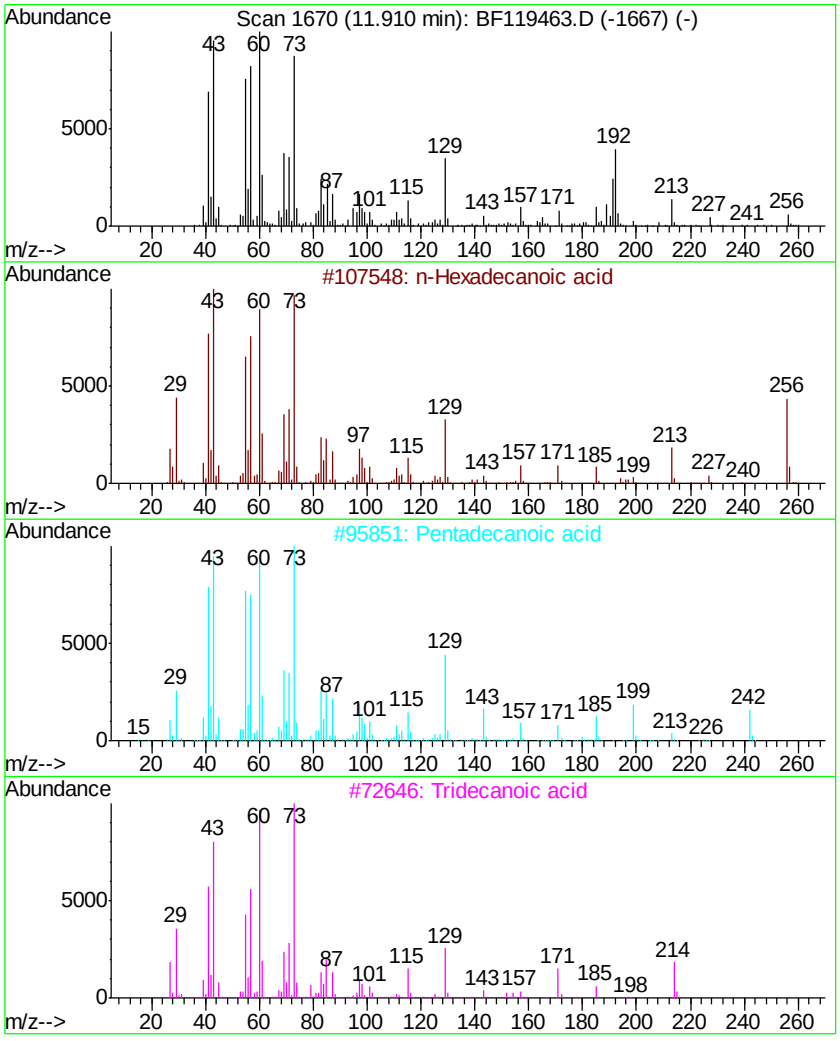
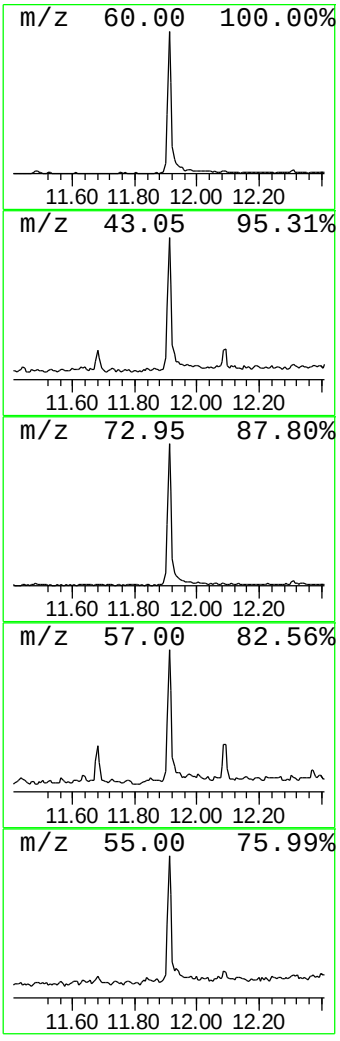
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	9.02 ng	882488	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
3	Tridecanoic acid	214	C13H26O2	000638-53-9	49
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119463.D
Acq On : 20 Mar 2020 3:13
Operator : CG/JU
Sample : L1913-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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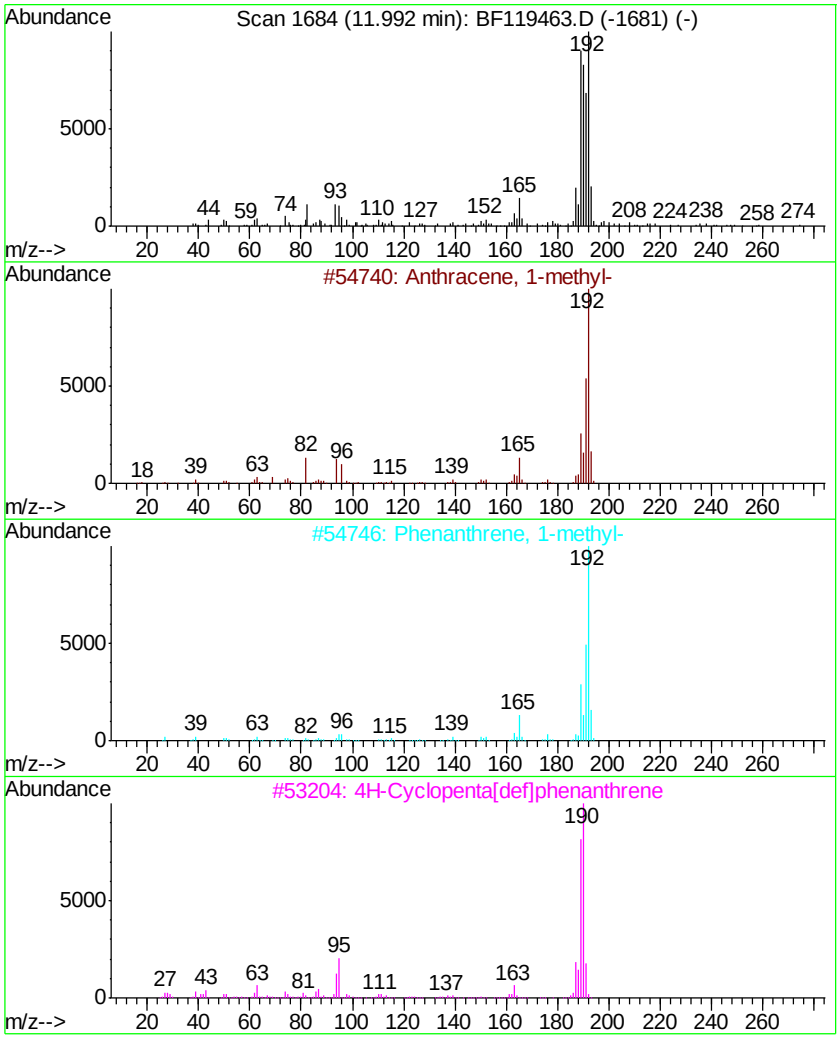
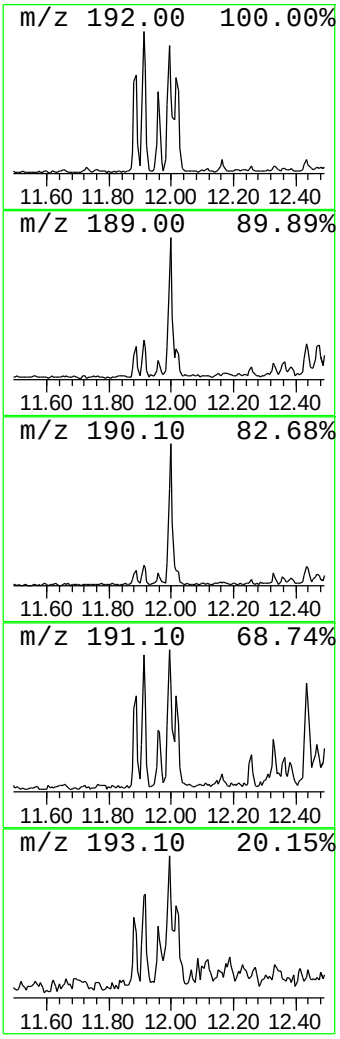
Peak Number 3 Anthracene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.35 ng	230282	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	60
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	60
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	46
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	46





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119463.D
Acq On : 20 Mar 2020 3:13
Operator : CG/JU
Sample : L1913-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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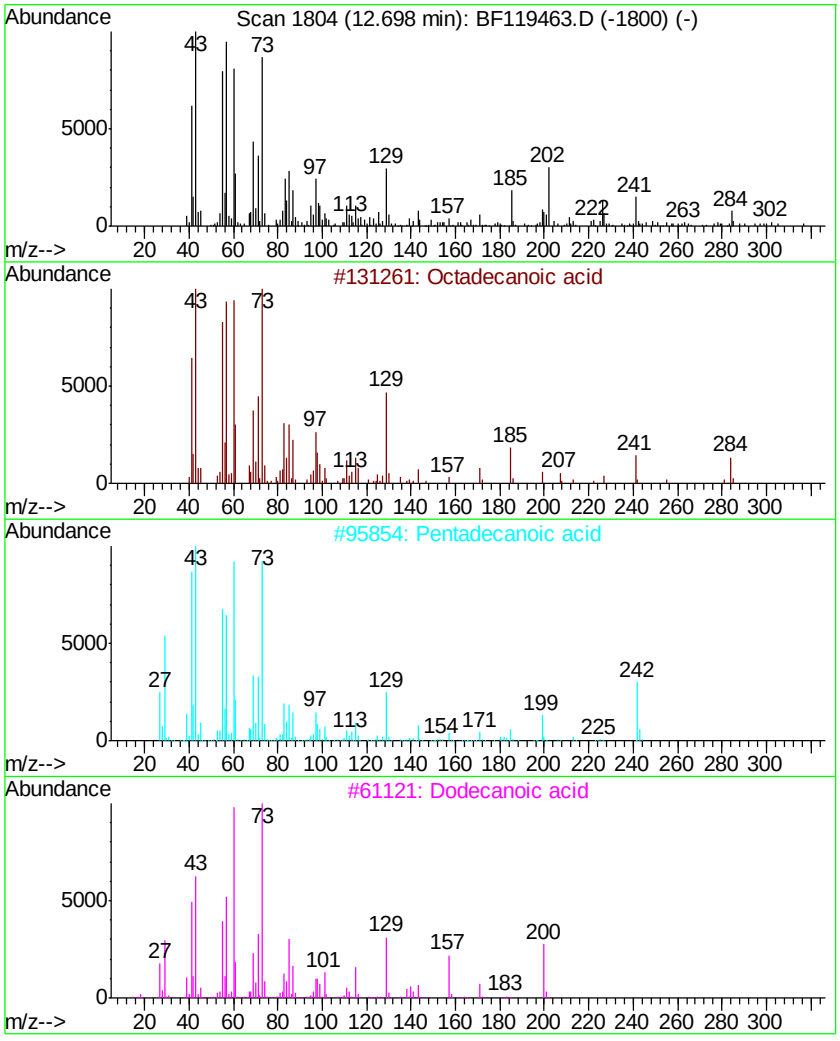
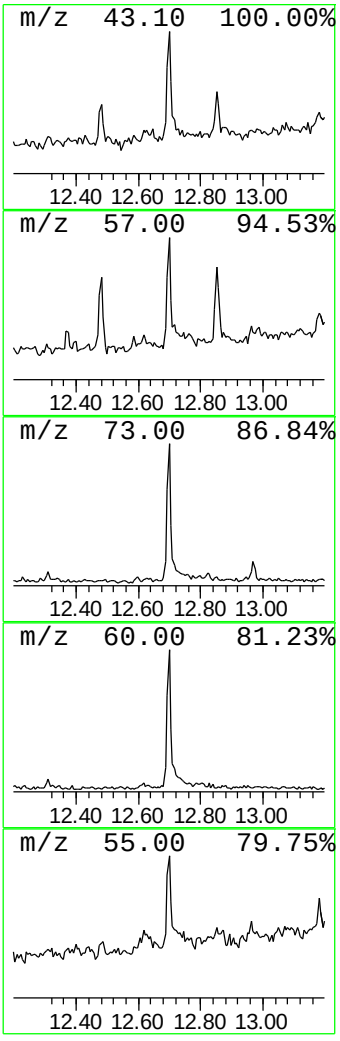
Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.27 ng	320294	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119463.D
Acq On : 20 Mar 2020 3:13
Operator : CG/JU
Sample : L1913-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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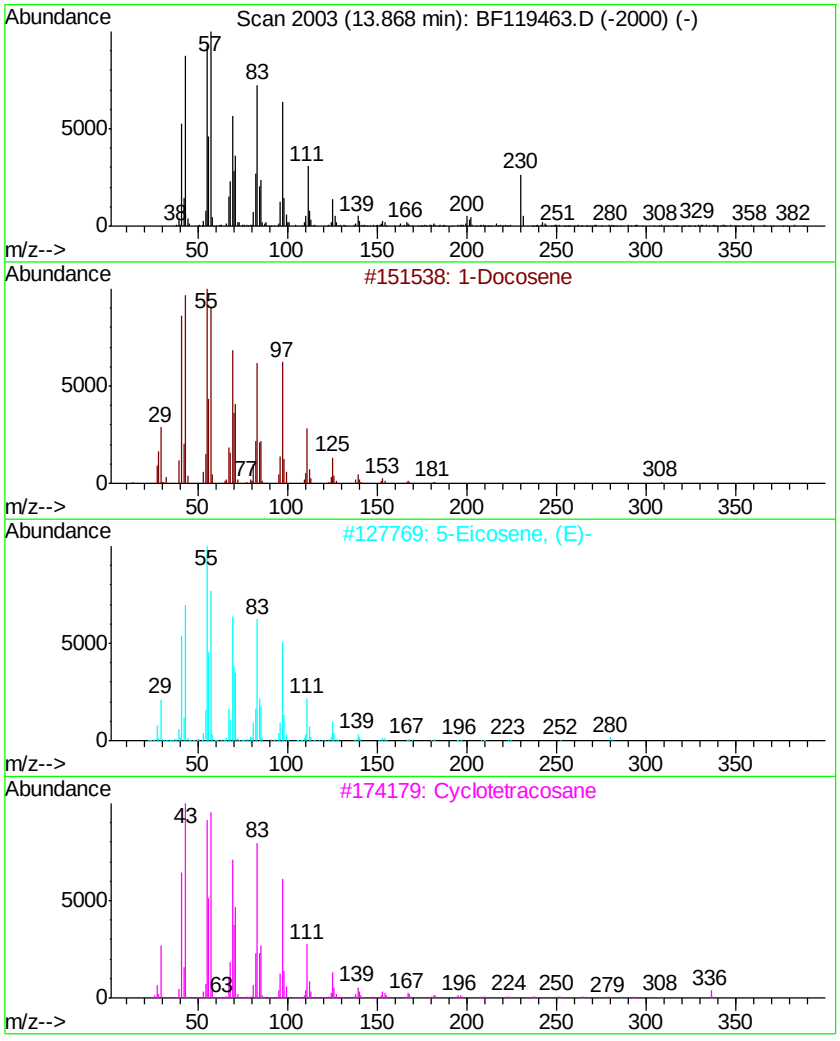
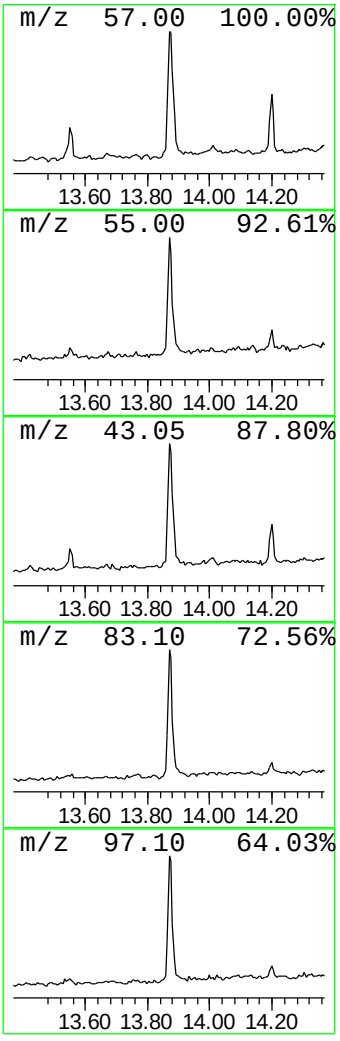
Peak Number 5 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	9.68 ng	1263680	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	93
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
3	Cyclotetracosane	336	C24H48	000297-03-0	90
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





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Misc :
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Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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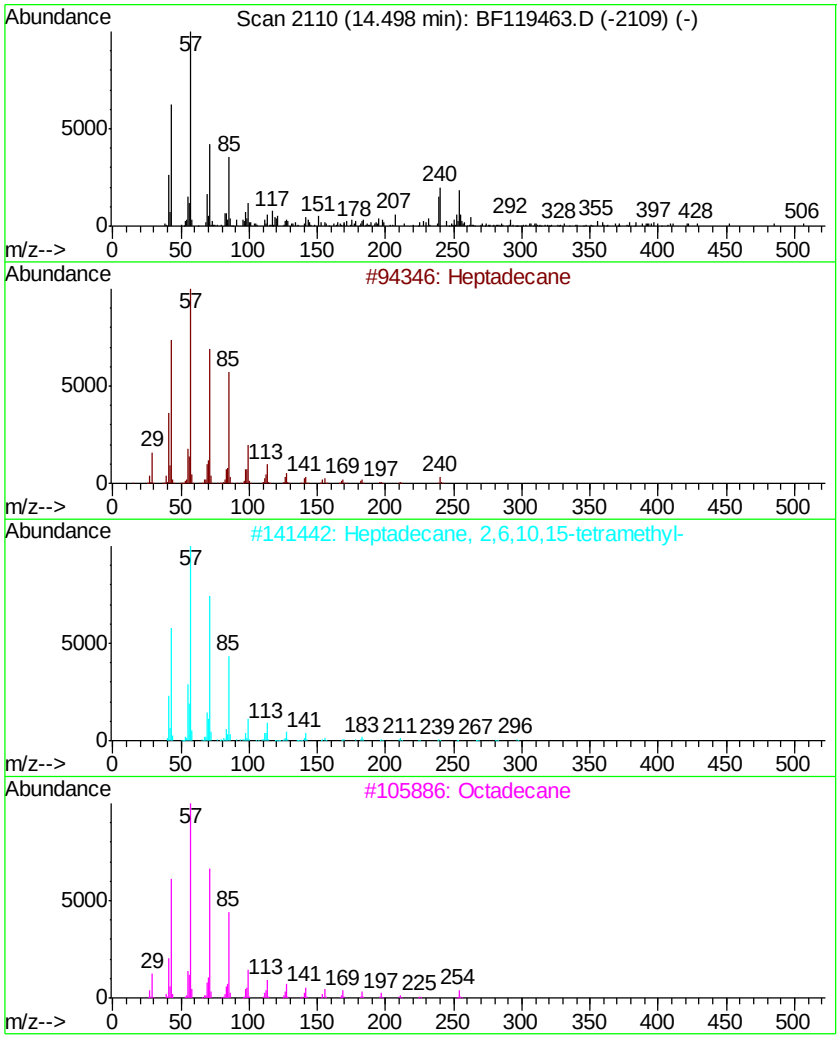
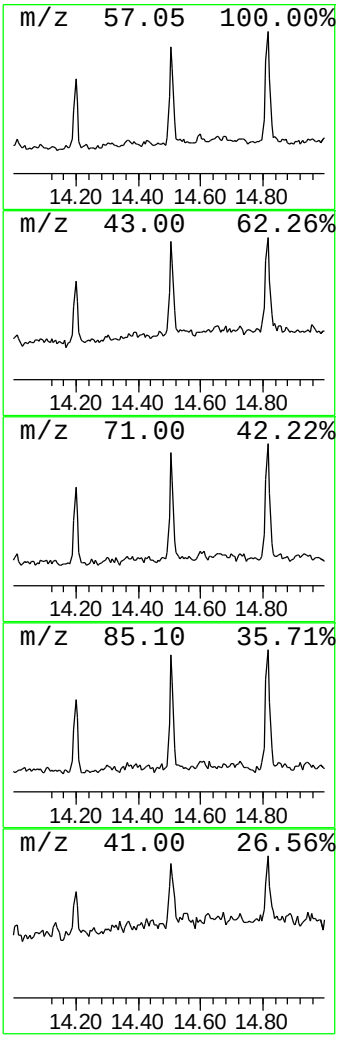
Peak Number 6 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.53 ng	330803	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3	Octadecane	254	C18H38	000593-45-3	83
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	68
5	Tetradecane	198	C14H30	000629-59-4	64





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Sample : L1913-15
Misc :
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Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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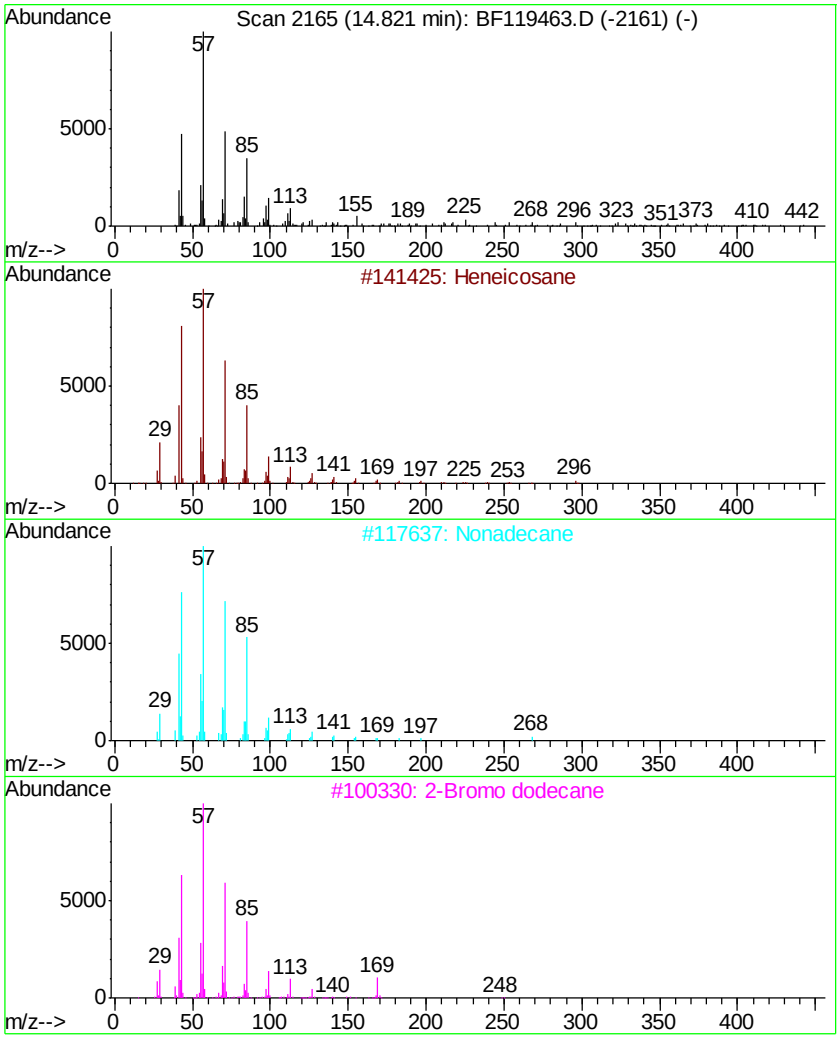
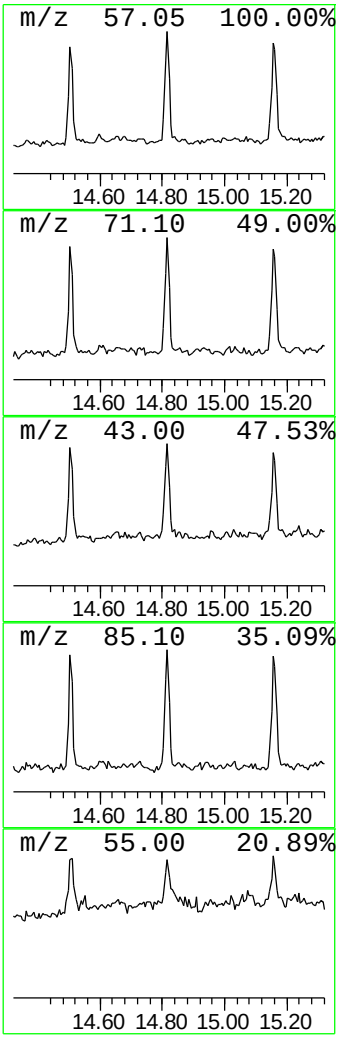
Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	4.85 ng	274658	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	Nonadecane	268	C19H40	000629-92-5	91
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	89
5	Heptacosane	380	C27H56	000593-49-7	87





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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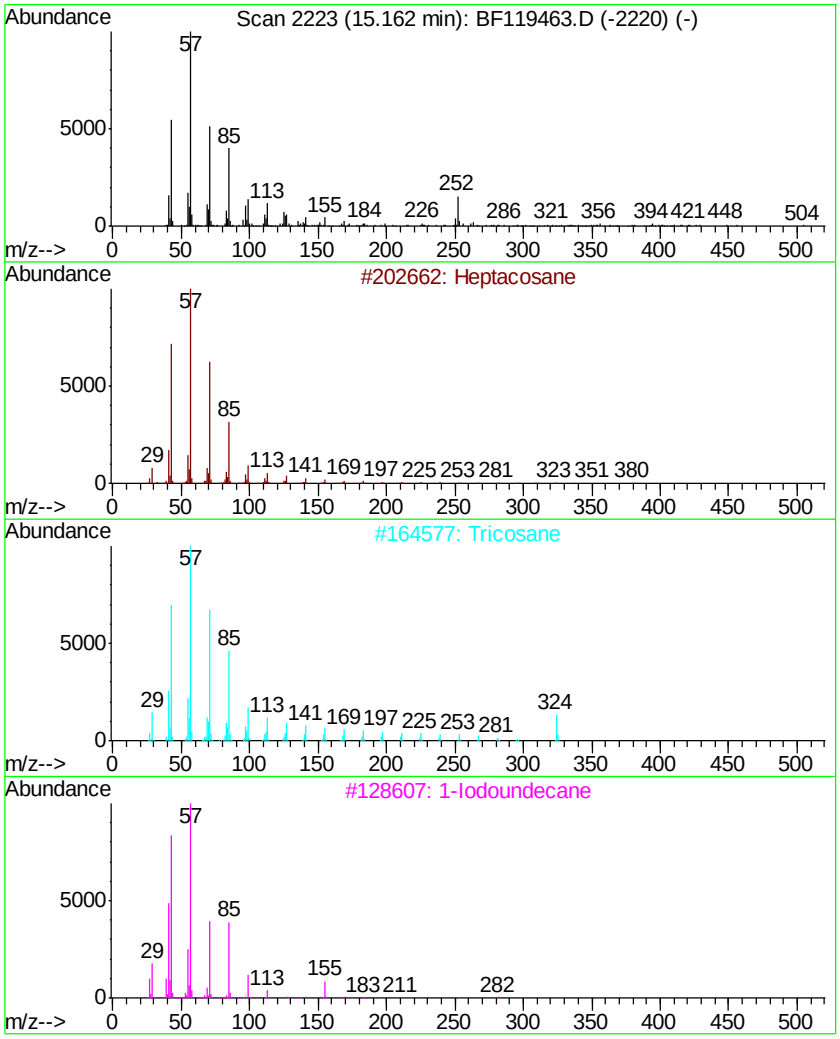
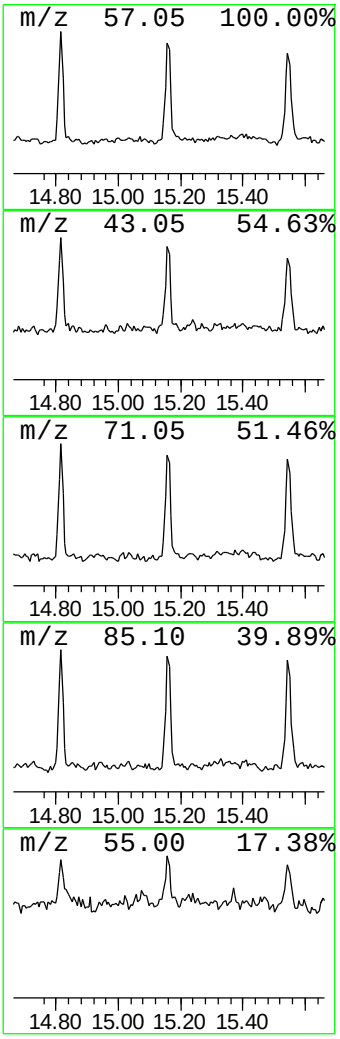
Peak Number 8 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	9.40 ng	532220	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Tricosane	324	C23H48	000638-67-5	87
3	1-Iodoundecane	282	C11H23I	004282-44-4	87
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	80
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119463.D
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Operator : CG/JU
Sample : L1913-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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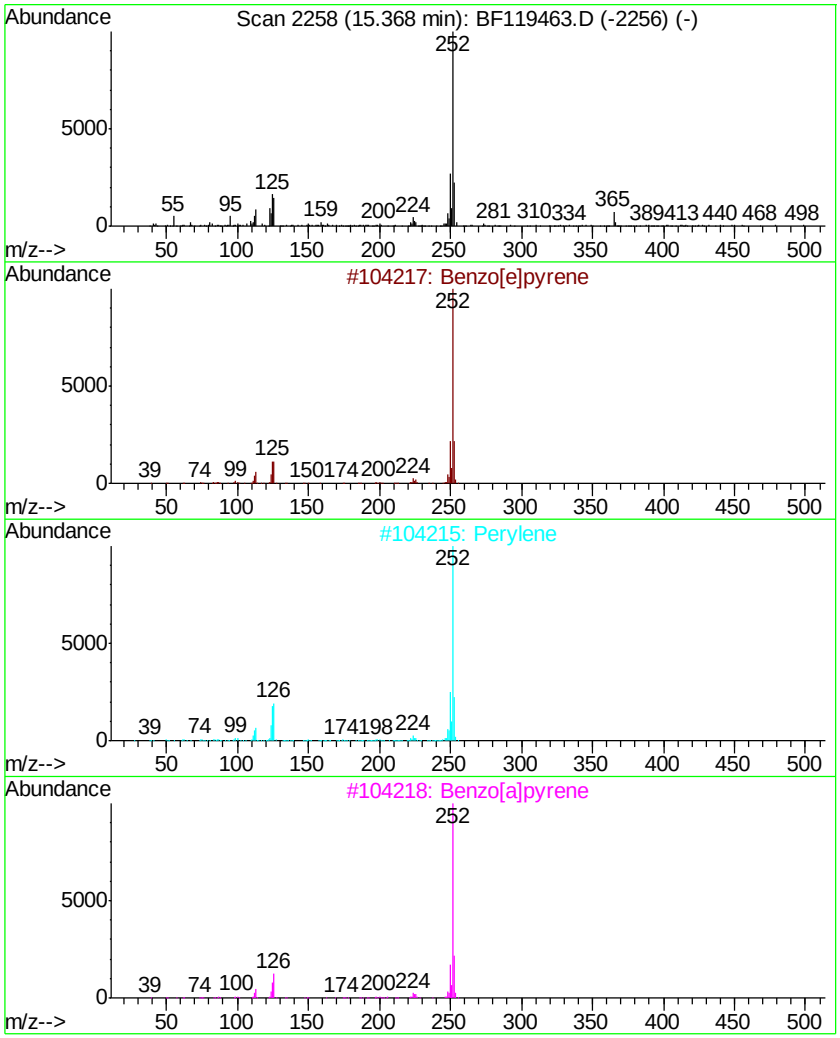
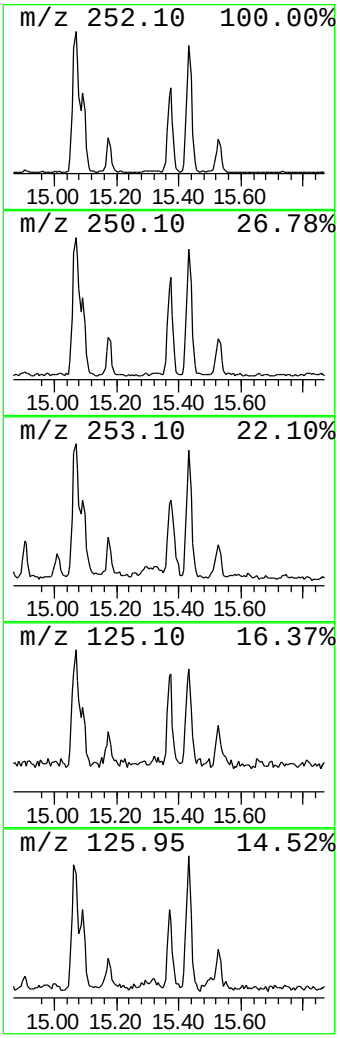
Peak Number 9 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	7.71 ng	436181	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	94
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031920\
Data File : BF119463.D
Acq On : 20 Mar 2020 3:13
Operator : CG/JU
Sample : L1913-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-2-5-COMP-B4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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
n-Hexadecanoic acid	11.91	9.0	ng	882488	4	11.38	1956090	20.0
Anthracene, 1-met...	11.99	2.4	ng	230282	4	11.38	1956090	20.0
Octadecanoic acid	12.70	3.3	ng	320294	4	11.38	1956090	20.0
1-Docosene	13.87	9.7	ng	1263680	5	14.03	2611230	20.0
Heptadecane	14.50	2.5	ng	330803	5	14.03	2611230	20.0
Heneicosane	14.82	4.8	ng	274658	6	15.50	1132180	20.0
Heptacosane	15.16	9.4	ng	532220	6	15.50	1132180	20.0
Benzo[e]pyrene	15.37	7.7	ng	436181	6	15.50	1132180	20.0