LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

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-BF091319.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	5.440	566	570	590	rVB	1284256	1202865	77.97%	7.053%
2	6.451	738	742	750	rBV	1275166	1348369	87.40%	7.906%
3	6.592	762	766	769	rBV	1607321	1370884	88.86%	8.038%
4	6.651	773	776	781	rVB3	15558	20082	1.30%	0.118%
5	6.822	801	805	813	rBV	442947	388036	25.15%	2.275%
6	6.975	828	831	847	rVB	1113561	1040529	67.44%	6.101%
7	7.381	896	900	915	rBV	843394	800489	51.89%	4.694%
8	8.104	1019	1023	1032	rBV	451977	515961	33.44%	3.025%
9	9.175	1201	1205	1216	rBV	1741832	1542792	100.00%	9.046%
10	9.257	1216	1219	1227	rVB5	26029	41333	2.68%	0.242%
11	9.563	1268	1271	1279	rVB	129082	127133	8.24%	0.745%
12	9.716	1294	1297	1300	rBV	25051	27859	1.81%	0.163%
13	9.786	1307	1309	1314	rVB	18288	17245	1.12%	0.101%
14	9.851	1316	1320	1324	rVV	677715	600886	38.95%	3.523%
15	9.880	1324	1325	1332	rVB4	26418	27762	1.80%	0.163%
16	10.057	1350	1355	1359	rBV3	15144	21572	1.40%	0.126%
17	10.257	1386	1389	1391	rBV3	18021	20073	1.30%	0.118%
18	10.398	1409	1413	1419	rBV	32447	41178	2.67%	0.241%
19	10.504	1426	1431	1433	rBV5	19221	21647	1.40%	0.127%
20	10.633	1449	1453	1464	rBV	921783	973512	63.10%	5.708%
21	10.763	1471	1475	1478	rBV2	43608	63630	4.12%	0.373%
22	11.227	1552	1554	1560	rVB	40163	47135	3.06%	0.276%
23	11.333	1568	1572	1574	rBV	603317	566276	36.70%	3.320%
24	11.357	1574	1576	1582	rVV	254888	237104	15.37%	1.390%
25	11.410	1582	1585	1588	rVV	61427	62733	4.07%	0.368%
26	11.622	1619	1621	1625	rVB5	29126	25024	1.62%	0.147%
27	11.833	1655	1657	1658	rBV	37947	27128	1.76%	0.159%
28	11.857	1658	1661	1668	rVB4	178624	198399	12.86%	1.163%
29	11.945	1673	1676	1679	rBV	79843	74661	4.84%	0.438%
30	12.127	1704	1707	1709	rBV	37635	44152	2.86%	0.259%
31	12.310	1736	1738	1741	rBV3	32068	35723	2.32%	0.209%
32	12.545	1774	1778	1782	rBV	559241	502722	32.59%	2.948%
33	12.580	1782	1784	1788	rVV4	47707	44919	2.91%	0.263%
34	12.639	1792	1794	1797	rBV3	58399	59328	3.85%	0.348%

LSC Area Percent Report

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Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

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-BF091319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.769	1811	1816	1823	rBV	456564	541820	35.12%	3.177%
36	12.910	1836	1840	1847	rVB	1248711	1275984	82.71%	7.482%
37	13.098	1870	1872	1875	rVB	101506	89659	5.81%	0.526%
38	13.163	1881	1883	1886	rBV	58534	46275	3.00%	0.271%
39	13.963	2015	2019	2022	rBV2	435401	594094	38.51%	3.483%
40	13.992	2022	2024	2033	rVB	234971	238688	15.47%	1.400%
41	14.998	2191	2195	2202	rBV	267672	483132	31.32%	2.833%
42	15.292	2243	2245	2251	rVB	153345	190841	12.37%	1.119%
43	15.357	2252	2256	2261	rVV	209634	326258	21.15%	1.913%
44	15.415	2262	2266	2278	rVB2	350699	603511	39.12%	3.539%
45	16.521	2450	2454	2461	rVB3	97828	173359	11.24%	1.016%
46	16.845	2504	2509	2517	rVB4	109041	208330	13.50%	1.222%
47	17.280	2579	2583	2590	rVB2	69567	143830	9.32%	0.843%

Sum of corrected areas: 17054922

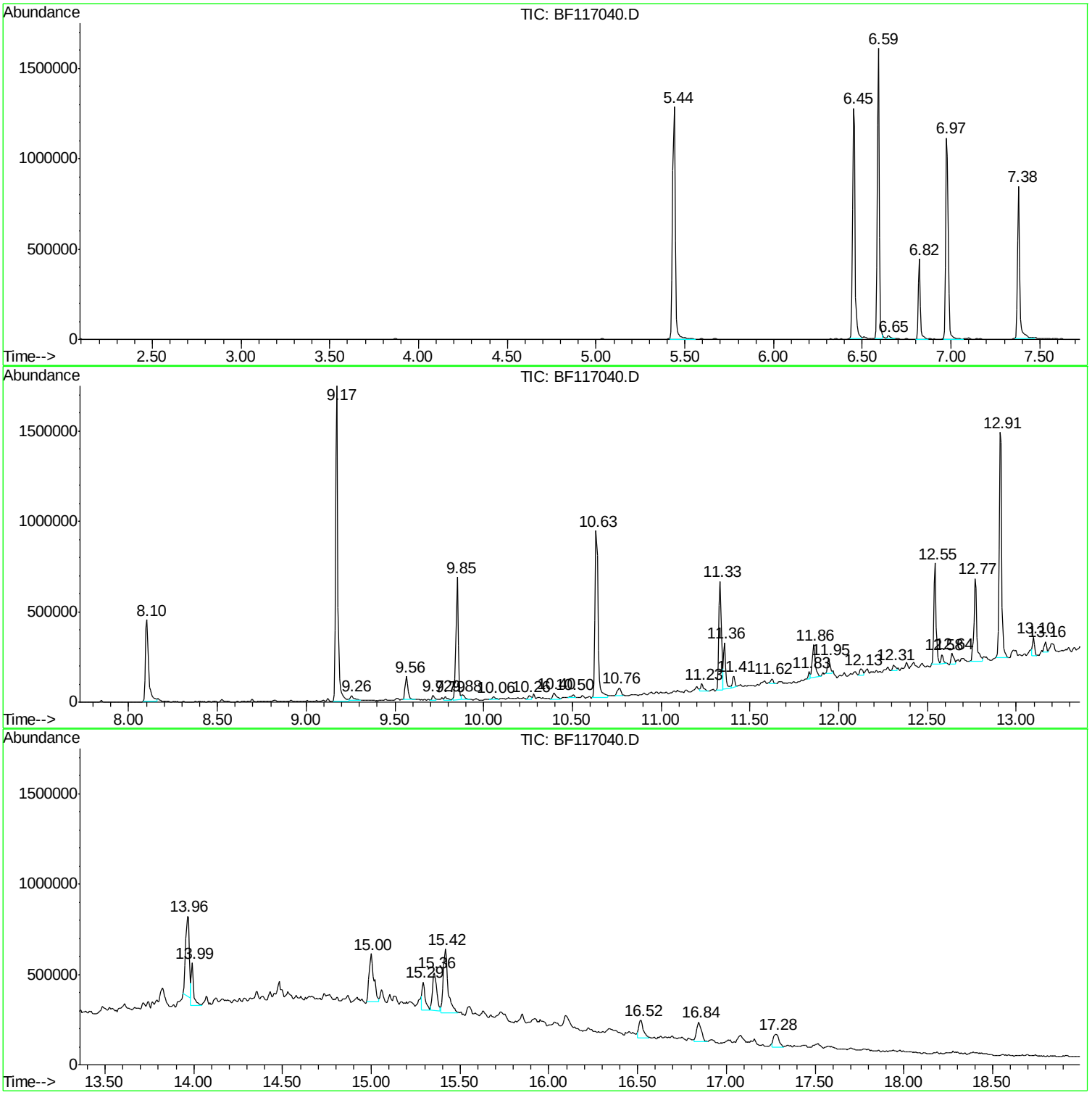
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

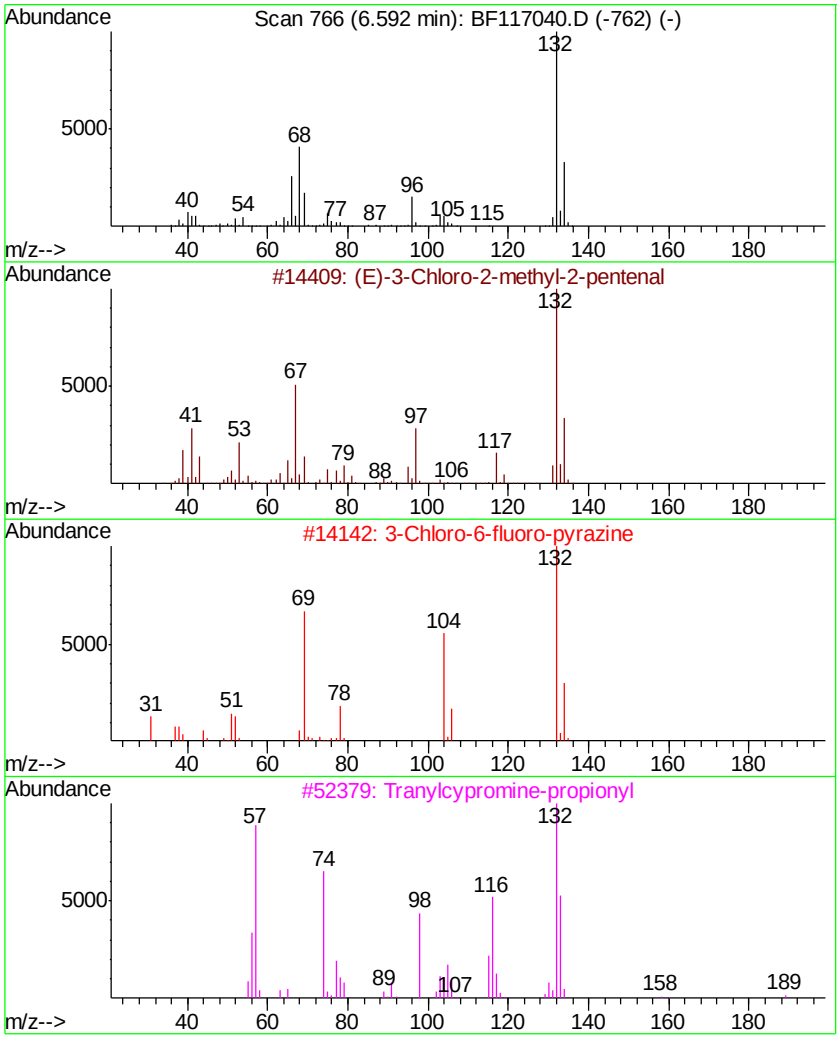
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

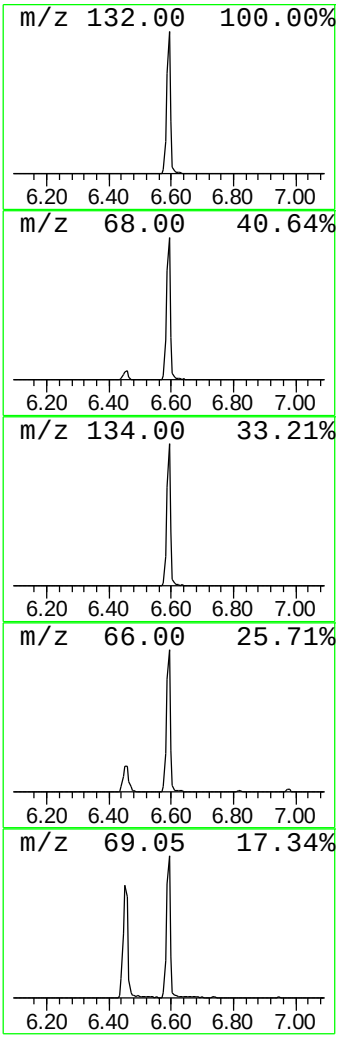
****

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	70.66 ng	1370880	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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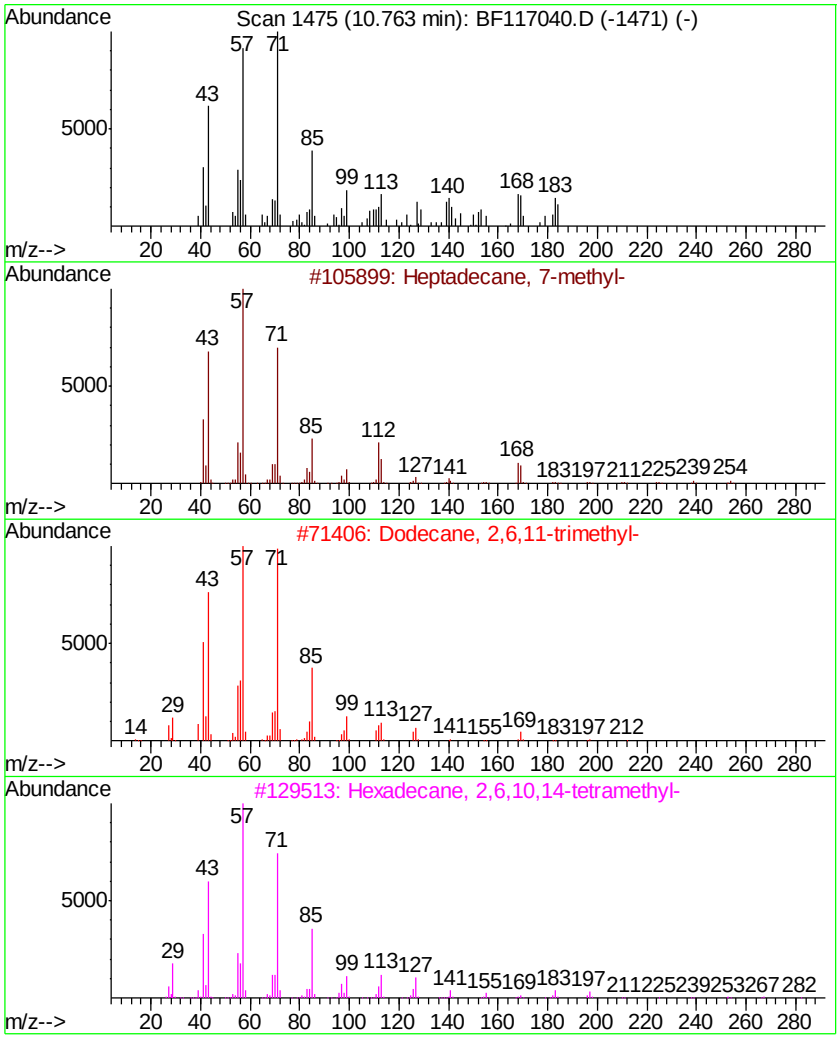
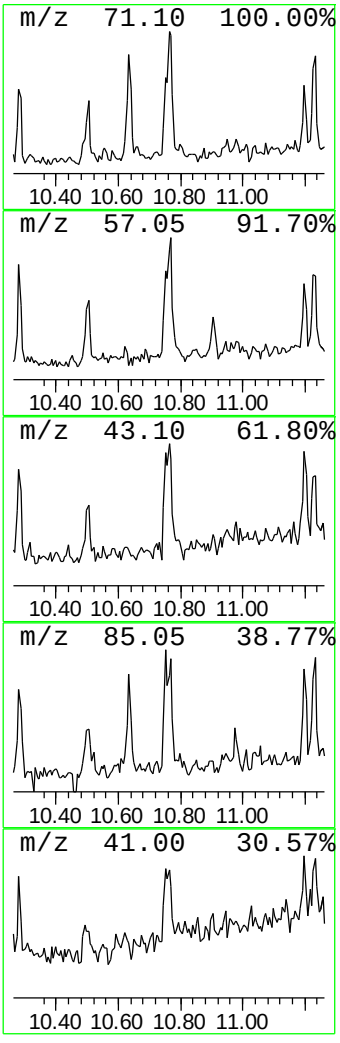
Peak Number 3 Heptadecane, 7-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.25 ng	63630	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	58
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	52
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	52
4	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	49
5	Tridecane, 4-methyl-	198	C14H30	026730-12-1	49





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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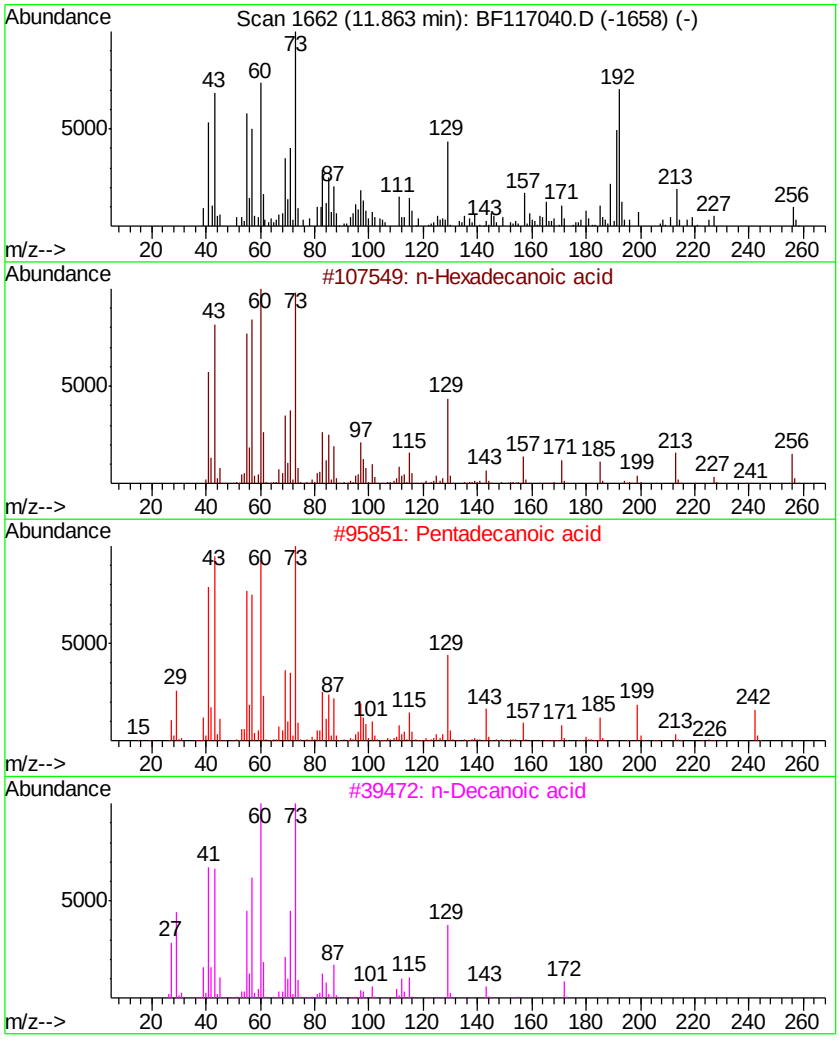
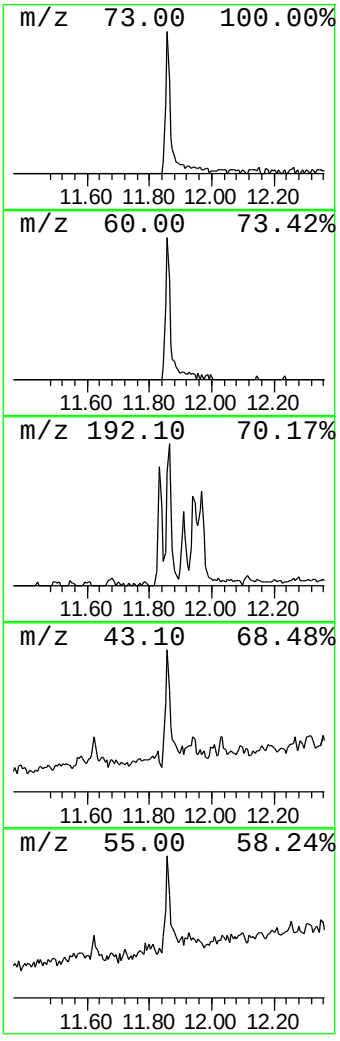
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	7.01 ng	198399	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

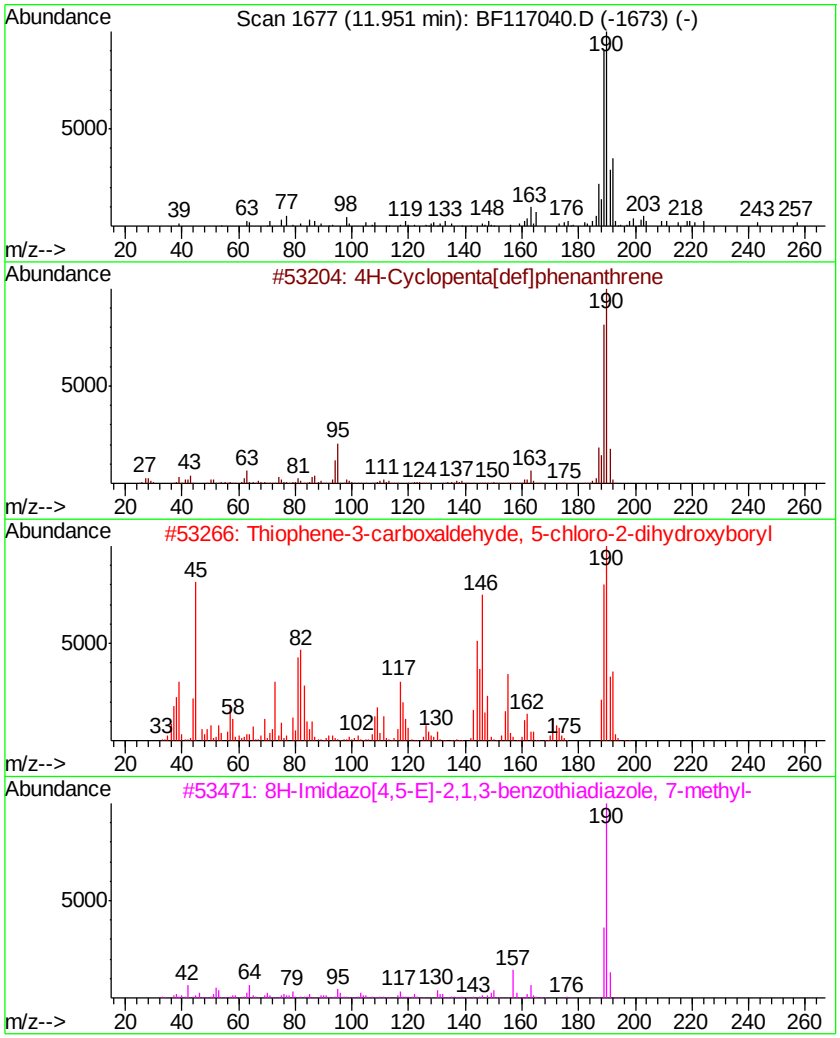
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

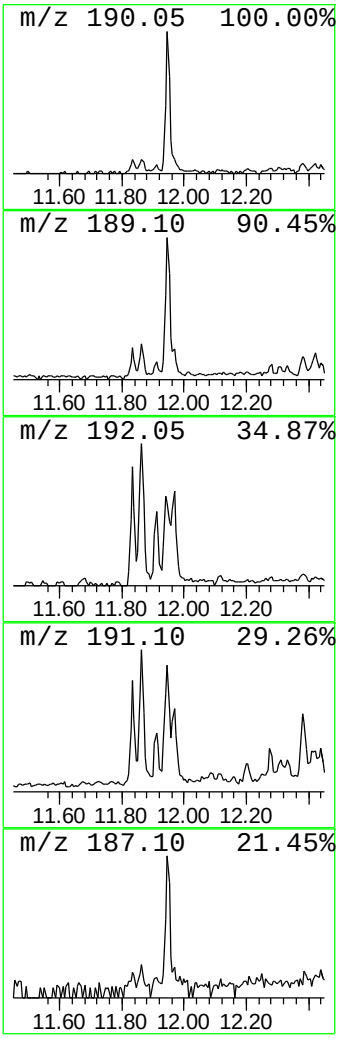
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.64 ng	74661	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	64
3	8H-Imidazo[4,5-E]-2,1,3-benzothi...	190	C8H6N4S	129485-68-3	38
4	5,8-Quinoxalinediol, 2,3-dimethyl-	190	C10H10N2O2	007698-00-2	30
5	Glaucyl alcohol	220	C15H24O	087745-32-2	30





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

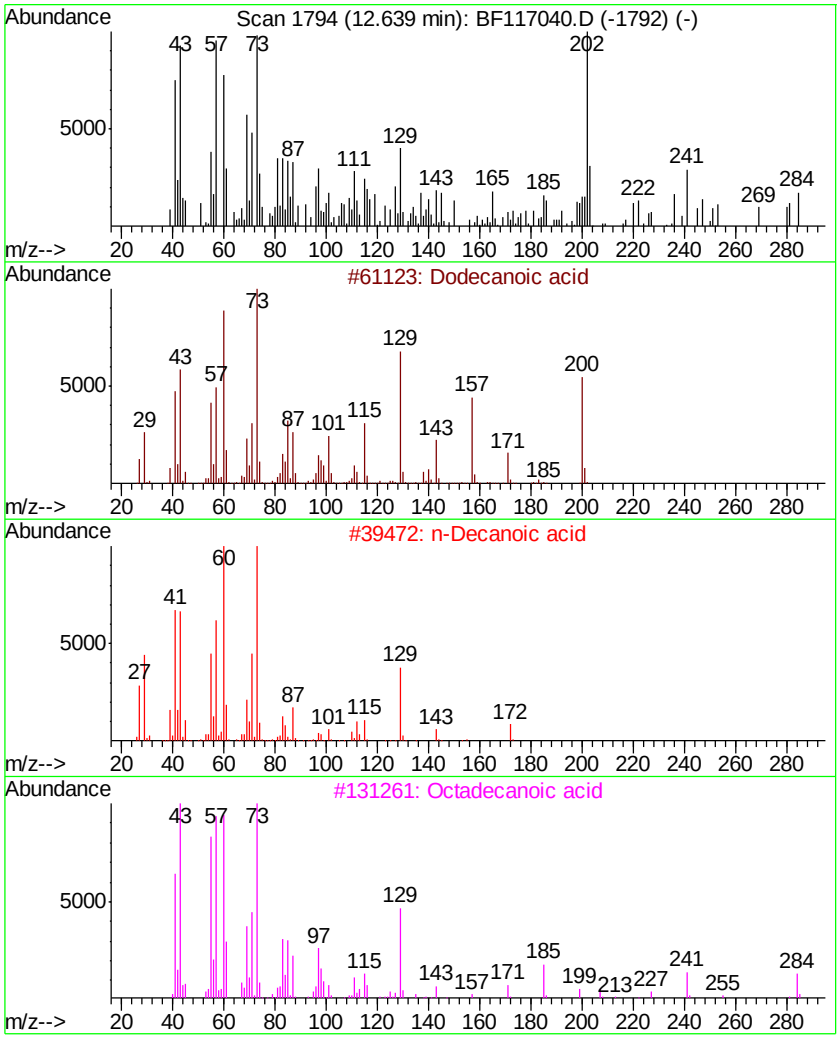
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

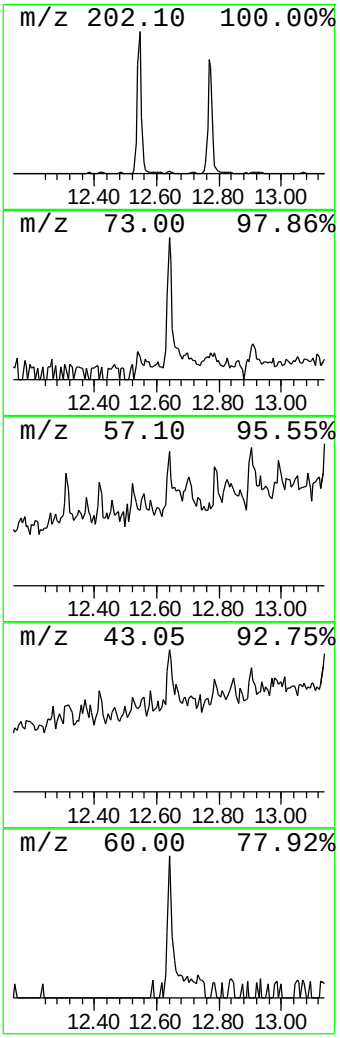
****

Peak Number 6 Dodecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.10 ng	59328	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	80
2	n-Decanoic acid	172	C10H20O2	000334-48-5	38
3	Octadecanoic acid	284	C18H36O2	000057-11-4	38
4	1-Methoxy-naphthoic acid	202	C12H10O3	000883-21-6	30
5	Anthracene, 9-(2-nitroethenyl)-	249	C16H11NO2	058349-77-2	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

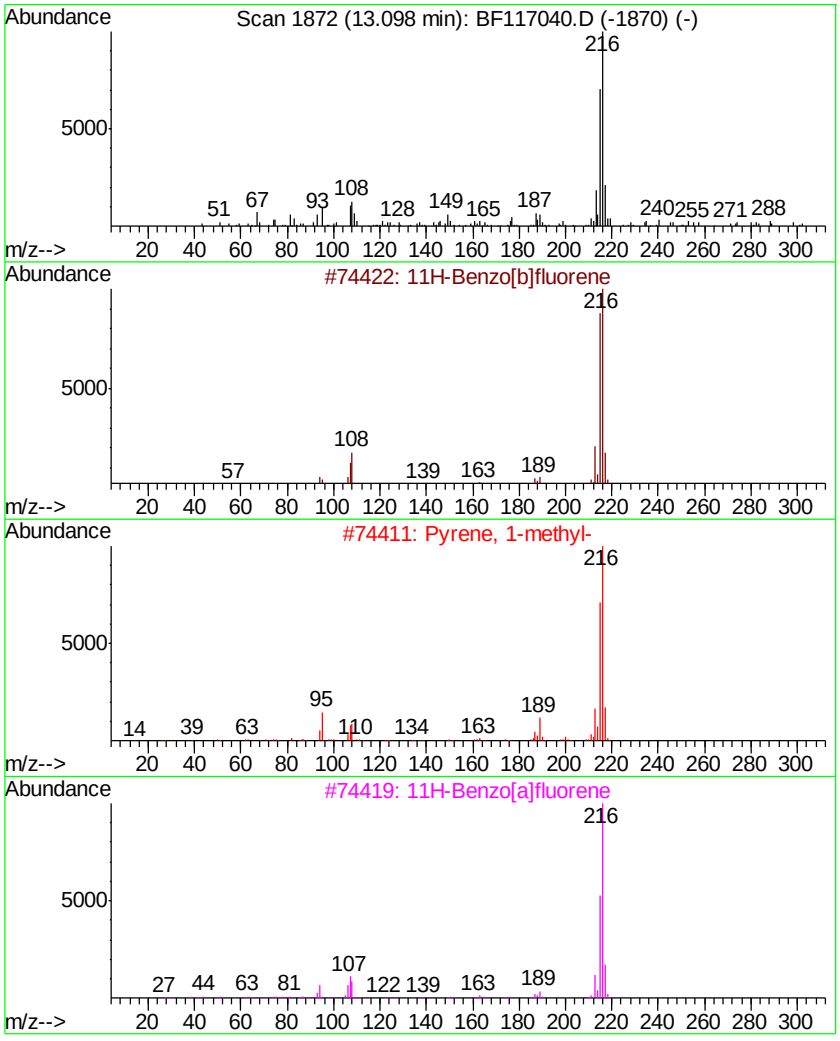
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

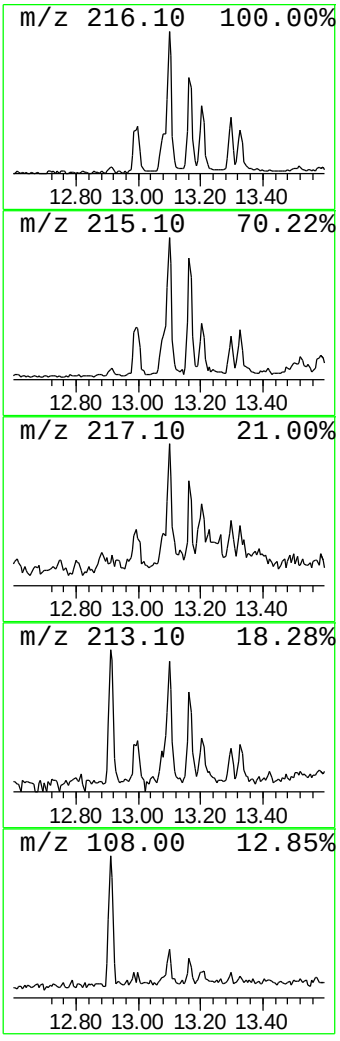
****

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	3.02 ng	89659	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	94
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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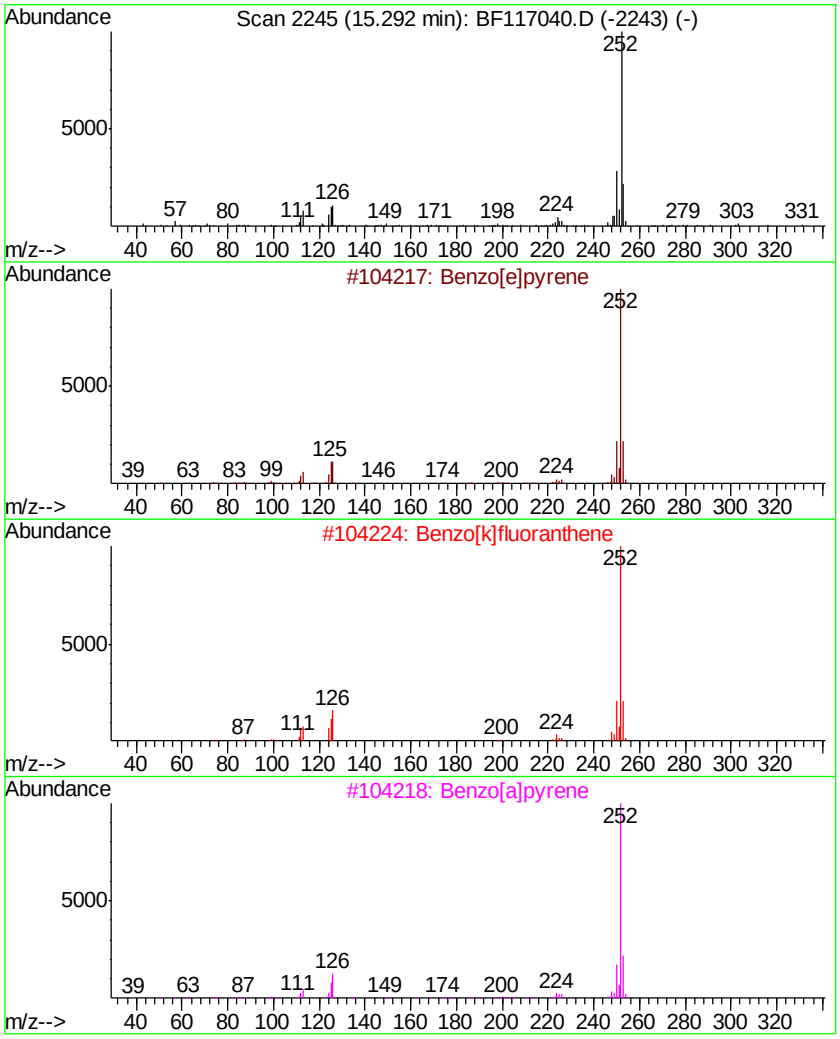
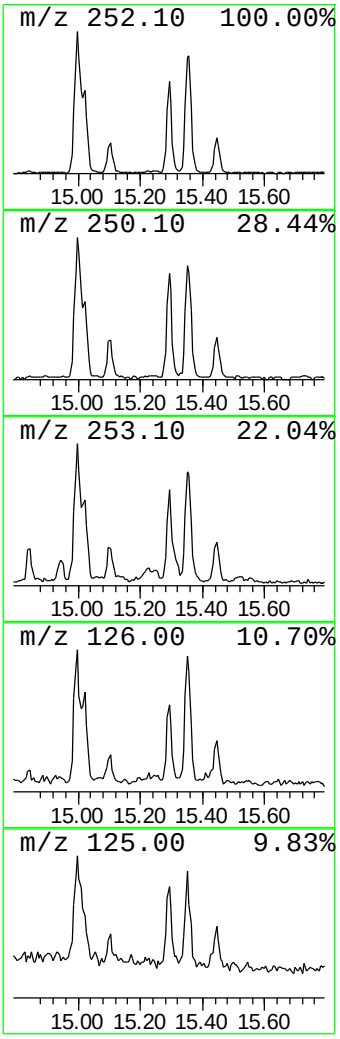
Peak Number 8 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	6.32 ng	190841	Perylene-d12	15.42

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	97
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
5	Perylene	252	C20H12	000198-55-0	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

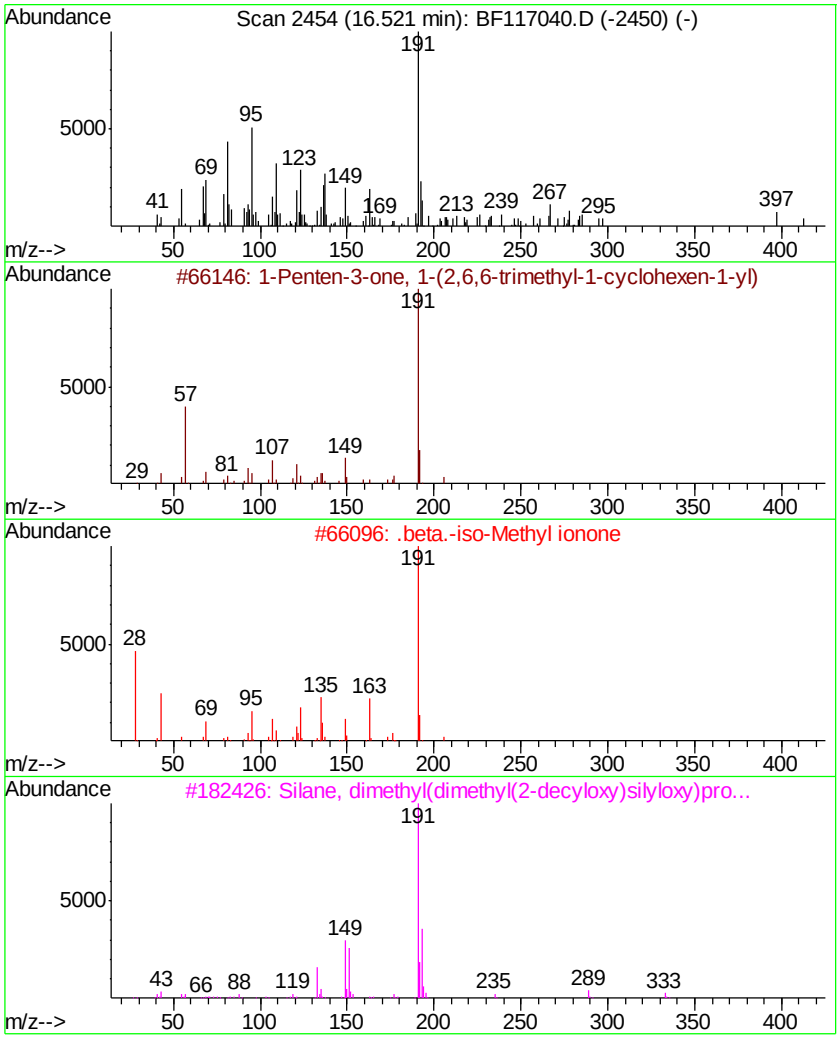
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

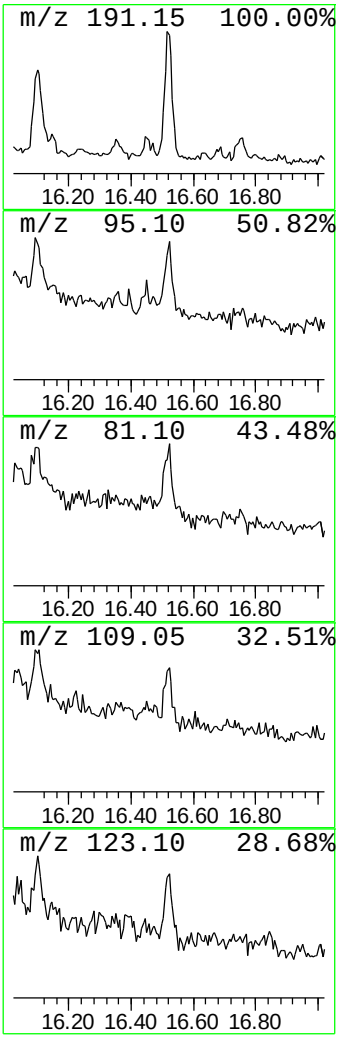
****

Peak Number 9 unknown16.52 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	5.75 ng	173359	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
3	Silane, dimethyl(dimethyl(2-decy...	348	C17H40O3Si2	1000347-63-3	35
4	N,N-Tetramethylene-3,4-dimethoxy...	261	C15H19NO3	327079-67-4	27
5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091319\
Data File : BF117040.D
Acq On : 13 Sep 2019 23:19
Operator : HP/JU
Sample : K4852-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BUS-3(0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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
unknown6.59	6.59	70.7	ng	1370880	1	6.82	388036	20.0
Heptadecane, 7-me...	10.76	2.3	ng	63630	4	11.33	566276	20.0
n-Hexadecanoic acid	11.86	7.0	ng	198399	4	11.33	566276	20.0
4H-Cyclopenta[def...	11.95	2.6	ng	74661	4	11.33	566276	20.0
Dodecanoic acid	12.64	2.1	ng	59328	4	11.33	566276	20.0
11H-Benzo[b]fluorene	13.10	3.0	ng	89659	5	13.97	594094	20.0
Benzo[e]pyrene	15.29	6.3	ng	190841	6	15.42	603511	20.0
unknown16.52	16.52	5.8	ng	173359	6	15.42	603511	20.0