LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109144.D
Acq On : 19 Sep 2018 15:35
Operator : JU/SJ
Sample : J4967-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

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-BF091418.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	4.919	435	439	446	rVB	99878	121153	4.91%	0.412%
2	5.301	501	504	505	rBV	29442	27889	1.13%	0.095%
3	5.337	505	510	513	rVB	2312688	2190610	88.73%	7.455%
4	6.360	680	684	690	rVB2	2401689	2446355	99.09%	8.325%
5	6.489	702	706	710	rBV	2369439	2290841	92.79%	7.796%
6	6.554	714	717	719	rBV	43449	36965	1.50%	0.126%
7	6.719	742	745	749	rBV	901204	800964	32.44%	2.726%
8	6.878	768	772	775	rBV	2218686	1861285	75.39%	6.334%
9	7.278	835	840	843	rBV	1393033	1372714	55.60%	4.672%
10	8.001	959	963	969	rBV	1187195	992368	40.20%	3.377%
11	9.078	1142	1146	1149	rBV	2868779	2468824	100.00%	8.402%
12	9.472	1210	1213	1216	rBV	375966	288855	11.70%	0.983%
13	9.613	1234	1237	1240	rVB	55508	44054	1.78%	0.150%
14	9.754	1256	1261	1264	rBV	1171313	989560	40.08%	3.368%
15	9.954	1292	1295	1299	rVB2	35958	35830	1.45%	0.122%
16	10.295	1350	1353	1360	rVB	38594	39159	1.59%	0.133%
17	10.536	1390	1394	1399	rBV	1559803	1308930	53.02%	4.455%
18	10.666	1413	1416	1423	rVB5	33789	49564	2.01%	0.169%
19	11.036	1476	1479	1484	rVB	41650	43486	1.76%	0.148%
20	11.124	1490	1494	1497	rBV2	33695	38635	1.56%	0.131%
21	11.230	1508	1512	1514	rBV	1060875	898996	36.41%	3.059%
22	11.254	1514	1516	1519	rVV	640001	478235	19.37%	1.628%
23	11.301	1519	1524	1528	rVB	97991	101283	4.10%	0.345%
24	11.460	1546	1551	1553	rBV2	54397	53062	2.15%	0.181%
25	11.730	1594	1597	1599	rBV	107964	92874	3.76%	0.316%
26	11.760	1599	1602	1607	rVV2	159688	256527	10.39%	0.873%
27	11.801	1607	1609	1612	rVV2	39268	40906	1.66%	0.139%
28	11.842	1612	1616	1618	rVV	123431	138496	5.61%	0.471%
29	11.866	1618	1620	1622	rVB	66763	55166	2.23%	0.188%
30	12.024	1644	1647	1648	rBV	80565	61665	2.50%	0.210%
31	12.042	1648	1650	1657	rVB	106384	99150	4.02%	0.337%
32	12.277	1687	1690	1693	rBV	82971	89155	3.61%	0.303%
33	12.313	1694	1696	1698	rVV2	39651	39202	1.59%	0.133%
34	12.360	1701	1704	1708	rVB2	63919	73572	2.98%	0.250%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109144.D
Acq On : 19 Sep 2018 15:35
Operator : JU/SJ
Sample : J4967-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

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-BF091418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.436	1713	1717	1721	rVV	1005065	848705	34.38%	2.888%
36	12.666	1750	1756	1759	rBV	806248	870396	35.26%	2.962%
37	12.783	1774	1776	1777	rBV	54352	37766	1.53%	0.129%
38	12.813	1777	1781	1784	rVV	2214616	1917028	77.65%	6.524%
39	12.883	1791	1793	1796	rVB	62969	61679	2.50%	0.210%
40	13.060	1820	1823	1825	rVB	67193	57477	2.33%	0.196%
41	13.095	1826	1829	1832	rBV2	110416	111855	4.53%	0.381%
42	13.218	1848	1850	1853	rBV	53462	42102	1.71%	0.143%
43	13.495	1895	1897	1903	rVB	120273	121457	4.92%	0.413%
44	13.607	1913	1916	1919	rBV2	80026	89060	3.61%	0.303%
45	13.636	1919	1921	1923	rBV	68064	54116	2.19%	0.184%
46	13.701	1930	1932	1933	rBV	78063	61622	2.50%	0.210%
47	13.718	1933	1935	1939	rVB	146517	149101	6.04%	0.507%
48	13.860	1954	1959	1961	rBV2	1117715	1368289	55.42%	4.657%
49	13.883	1961	1963	1965	rVB	496285	360679	14.61%	1.227%
50	14.865	2127	2130	2133	rBV	446064	607291	24.60%	2.067%
51	14.959	2143	2146	2150	rBV2	274742	306026	12.40%	1.041%
52	15.148	2175	2178	2184	rVB	296854	350302	14.19%	1.192%
53	15.207	2184	2188	2191	rVV	386351	447078	18.11%	1.521%
54	15.265	2194	2198	2201	rVV	691875	887878	35.96%	3.022%
55	15.312	2204	2206	2214	rVB	333568	395515	16.02%	1.346%
56	15.718	2272	2275	2281	rVB	223942	312284	12.65%	1.063%

Sum of corrected areas: 29384036

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Misc :
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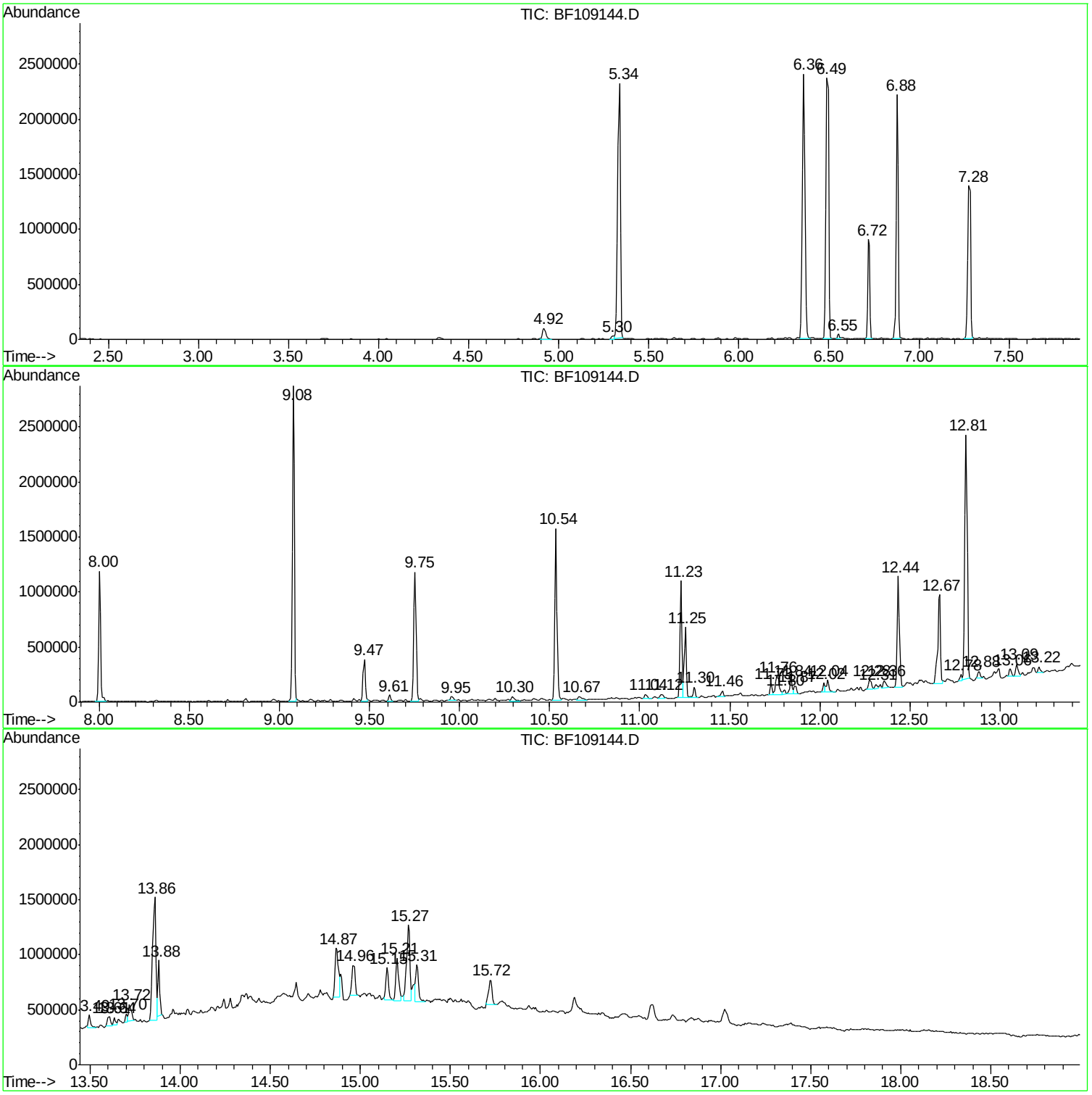
Instrument :
BNA_F
ClientSampleId :
SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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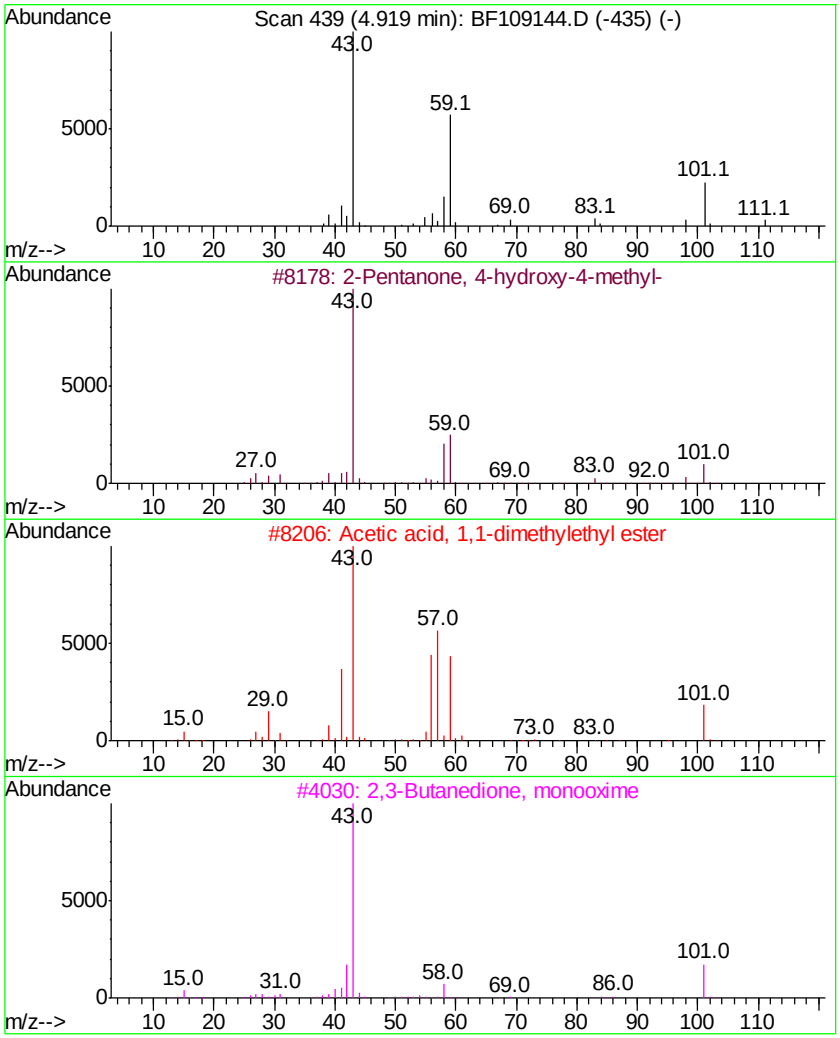
TIC Integration Parameters: LSCINT.P

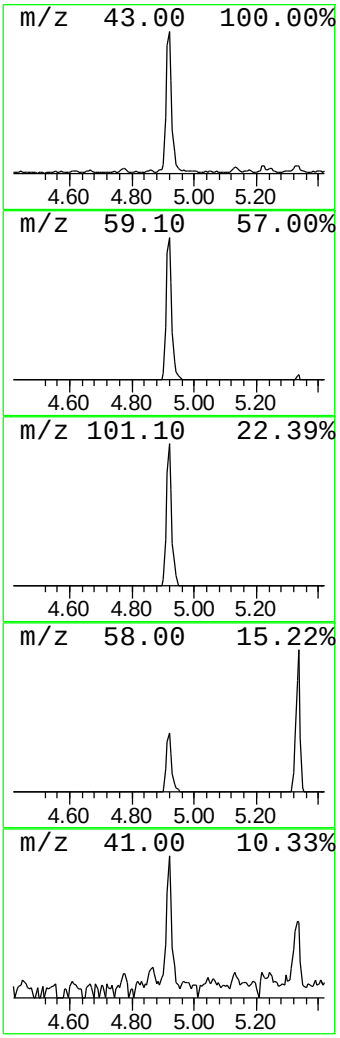
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.03 ng	121153	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	22





Library Search Compound Report

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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

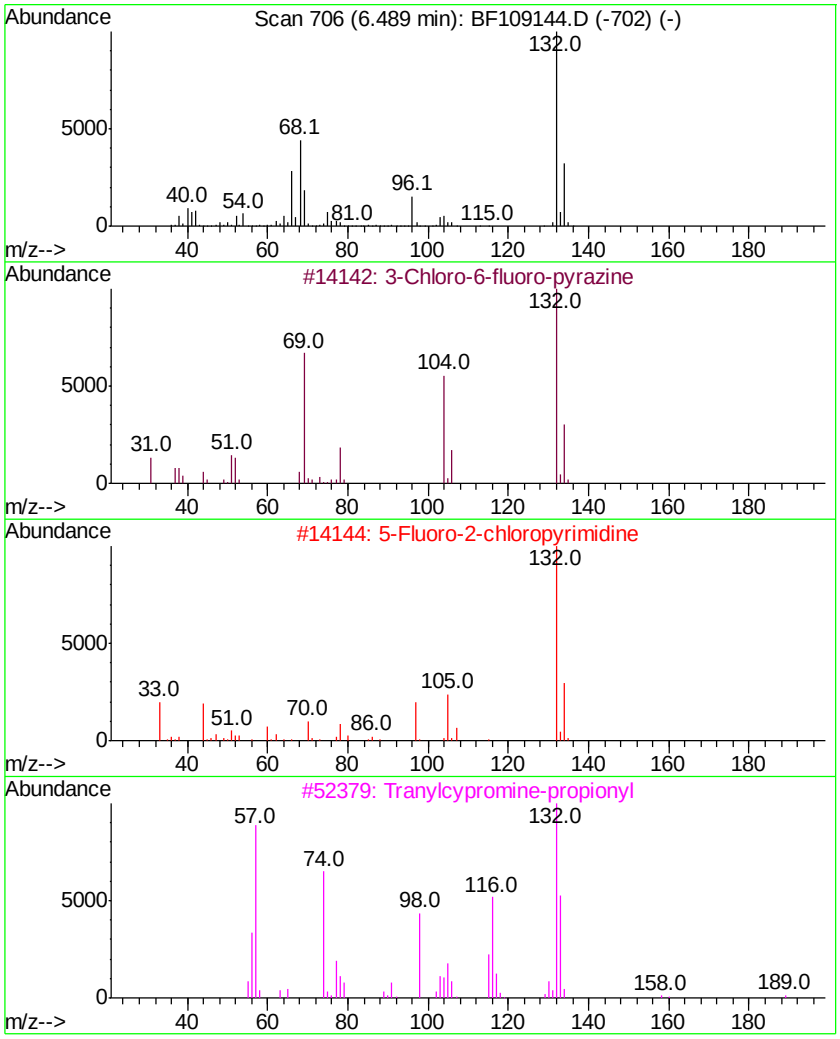
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

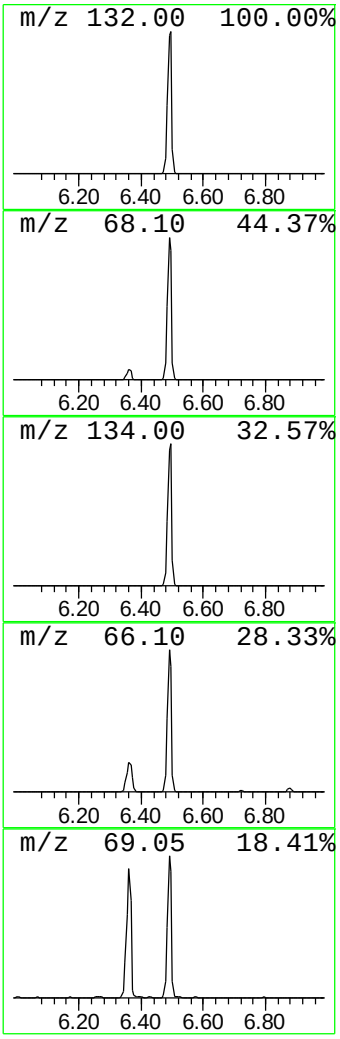
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	57.20 ng	2290840	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Sample : J4967-03
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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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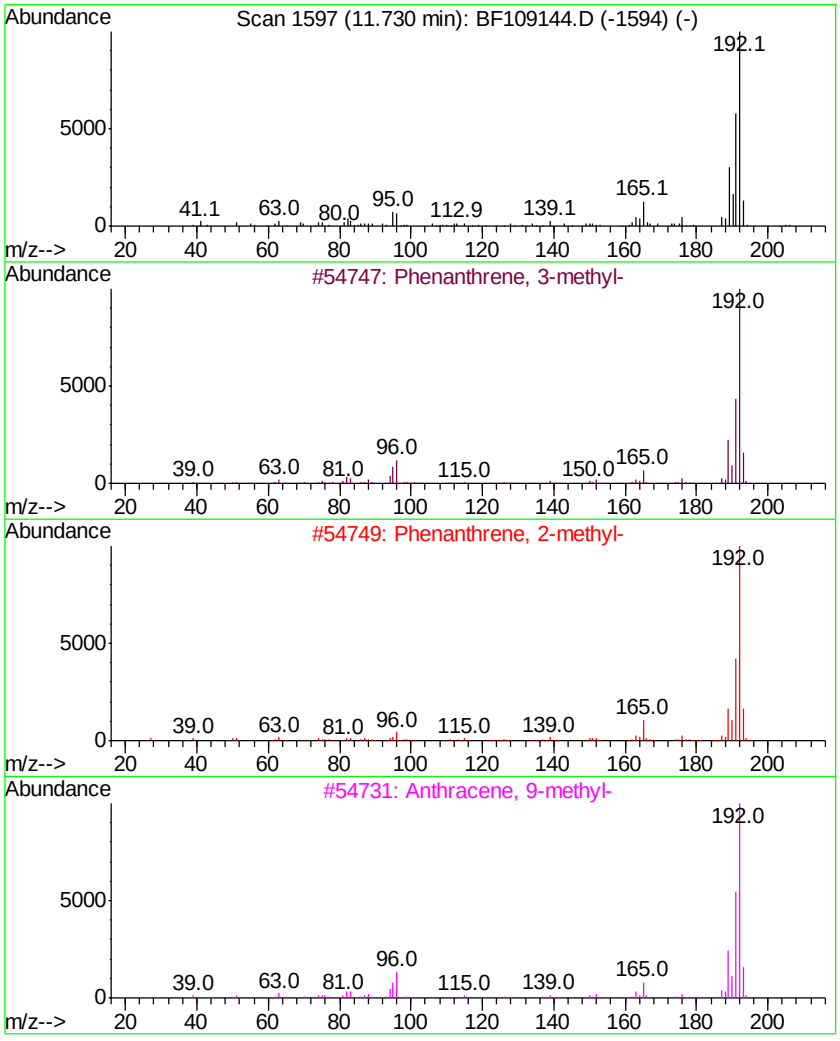
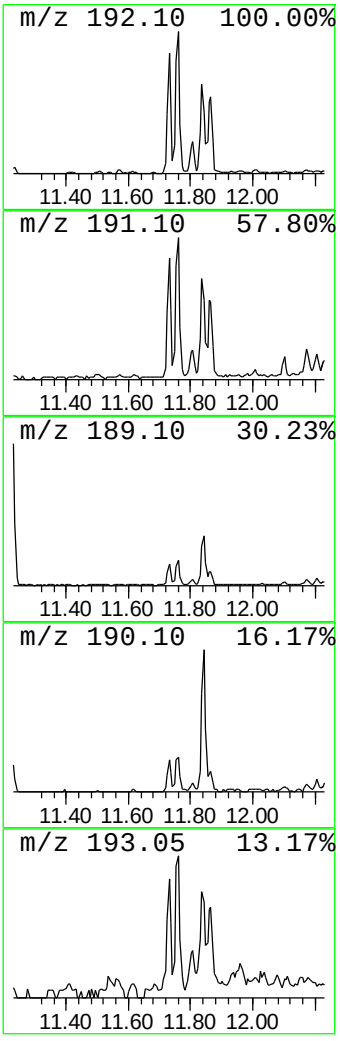
****

Peak Number 4 Phenanthrene, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	2.07 ng	92874	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	93
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91





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Sample : J4967-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

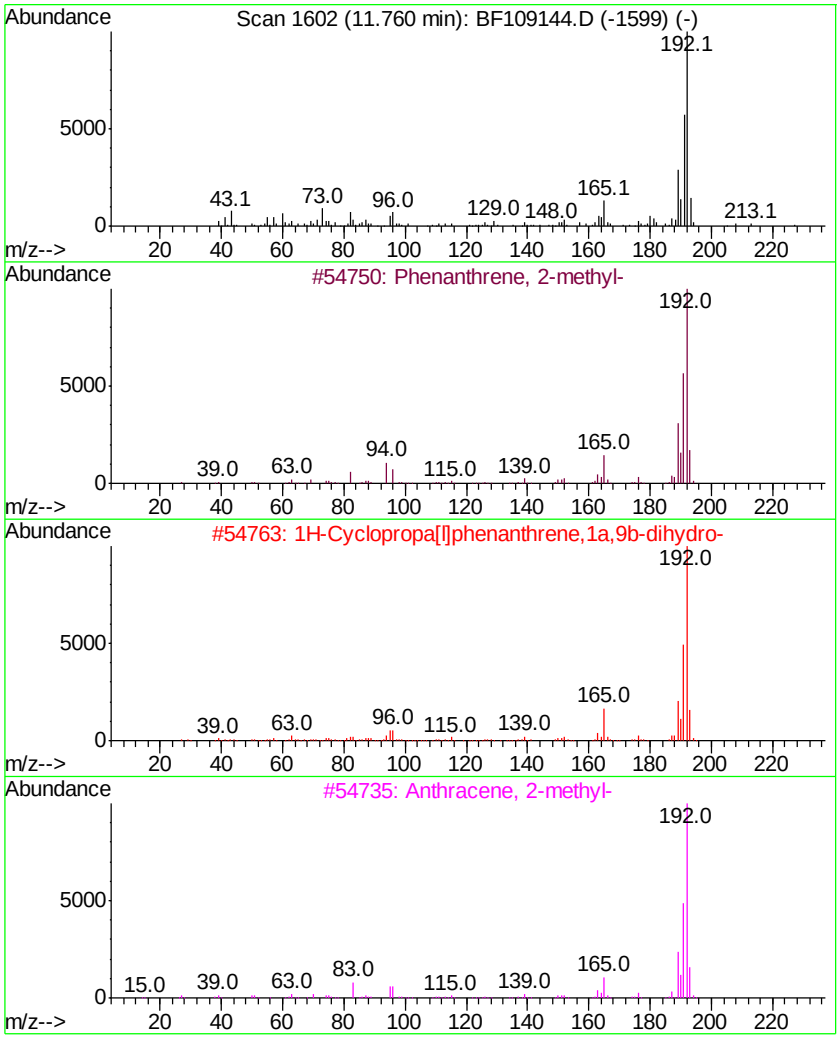
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

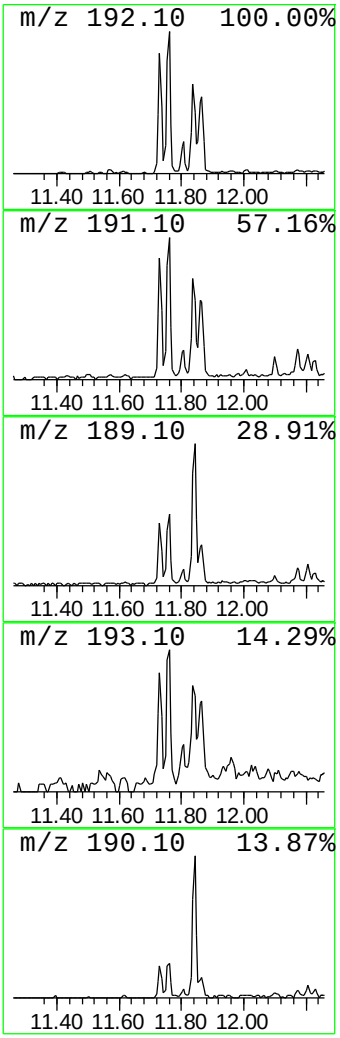
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	5.71 ng	256527	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	95
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

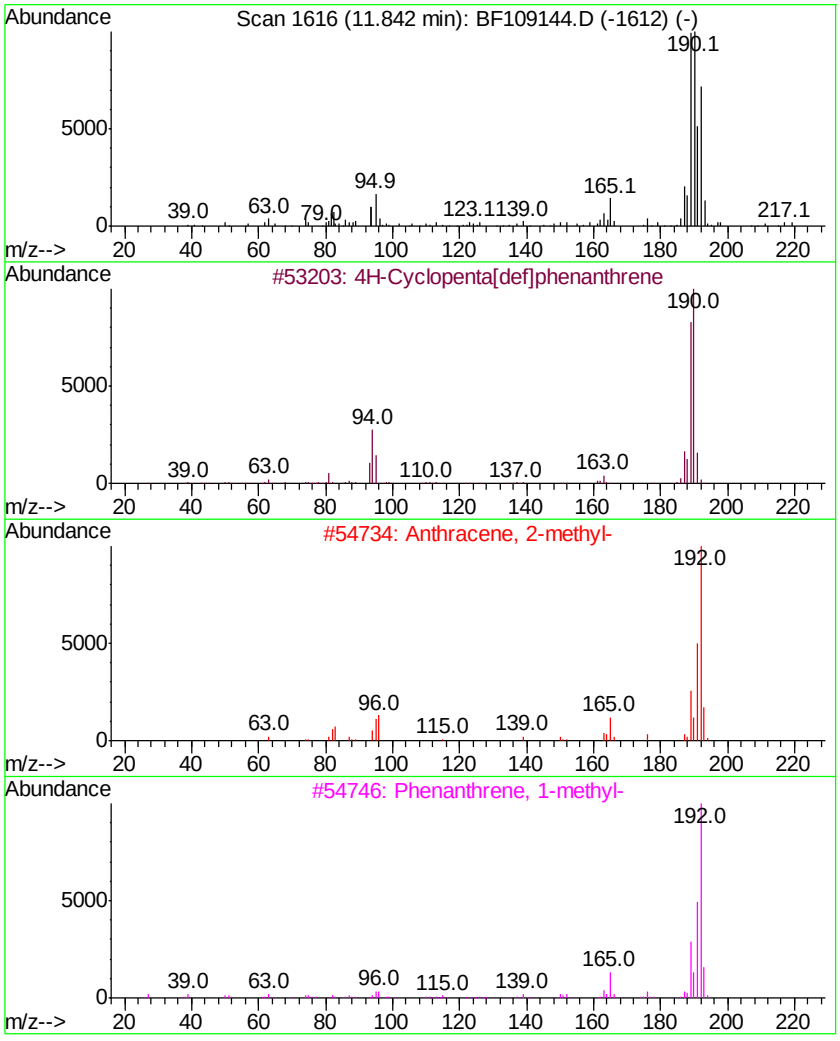
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

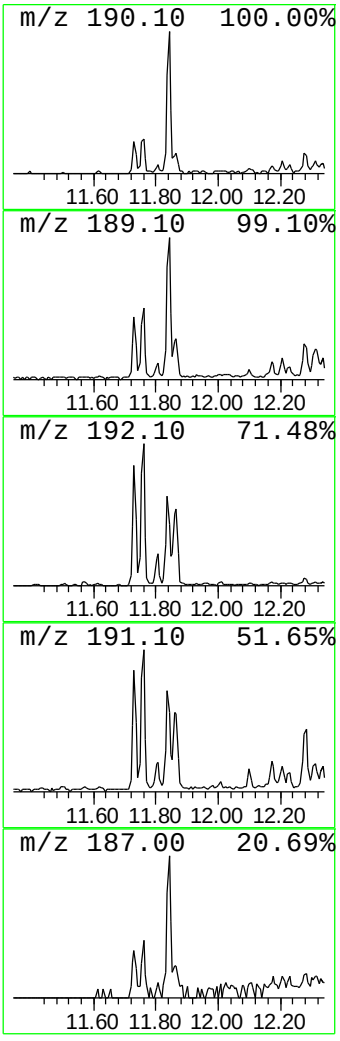
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.08 ng	138496	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	42
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	38
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

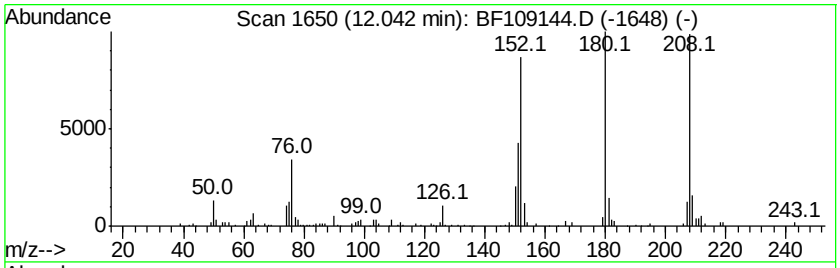
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

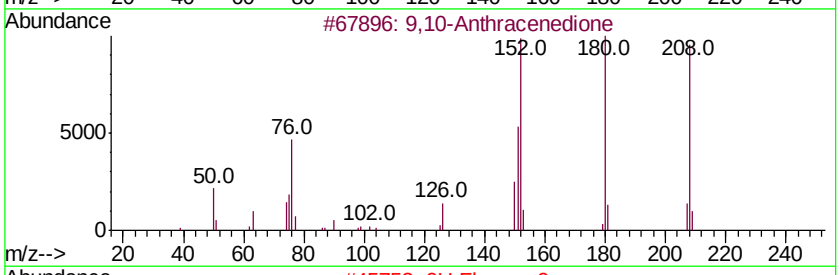
****

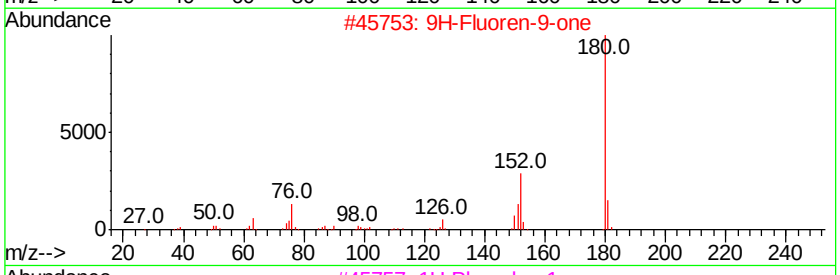
Peak Number 7 9,10-Anthracenedione Concentration Rank 9

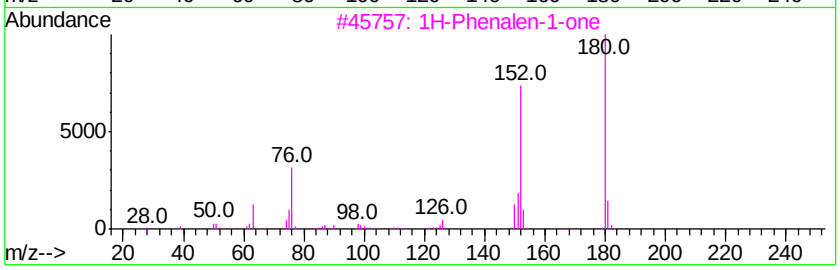
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	2.21 ng	99150	Phenanthrene-d10	11.23

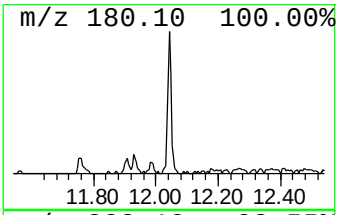
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	98
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	60
3	1H-Phenalen-1-one	180	C13H8O	000548-39-0	60
4	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	58
5	1,4-Anthracenedione	208	C14H8O2	000635-12-1	52

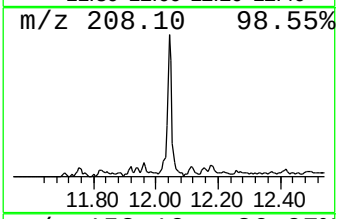


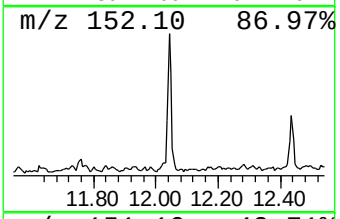


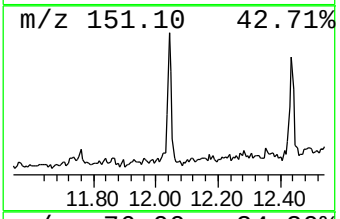


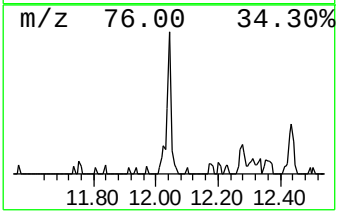












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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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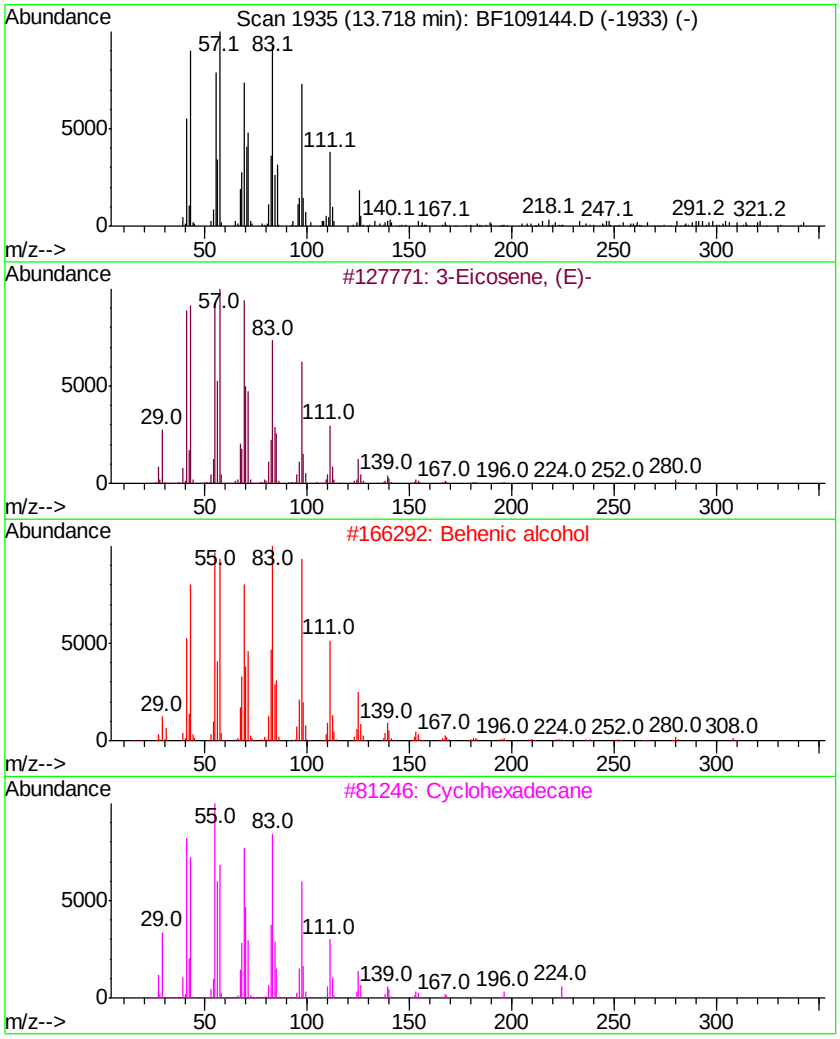
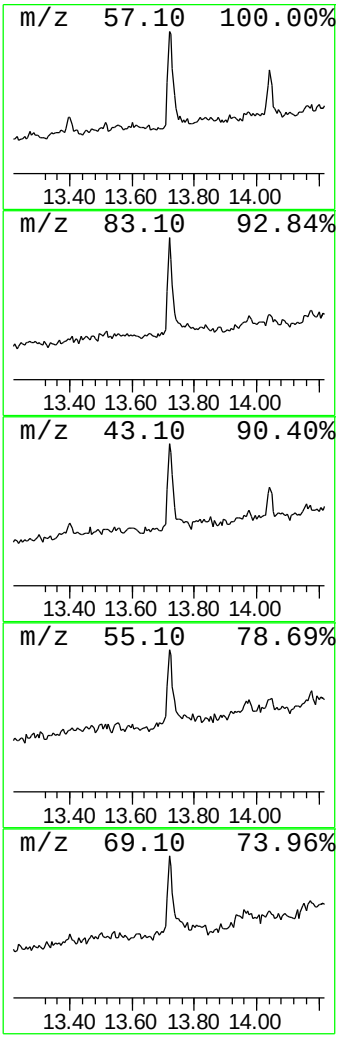
Peak Number 8 3-Eicosene, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.18 ng	149101	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Cyclohexadecane	224	C16H32	000295-65-8	93
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109144.D
Acq On : 19 Sep 2018 15:35
Operator : JU/SJ
Sample : J4967-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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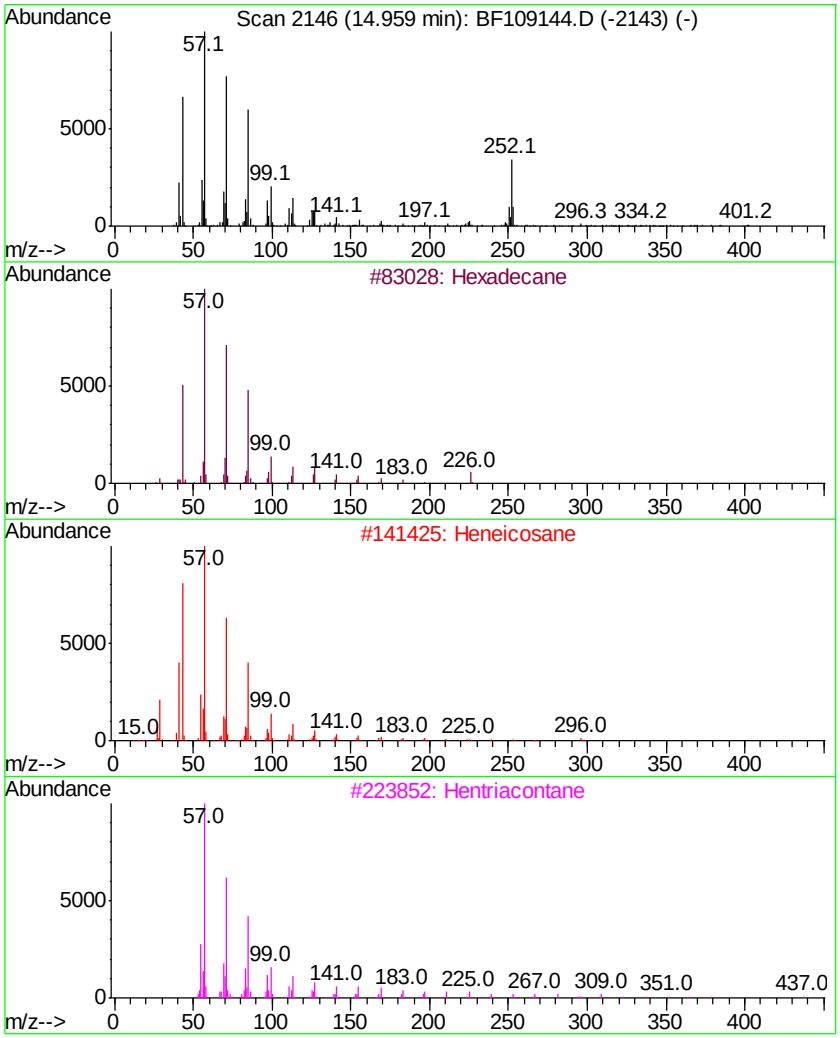
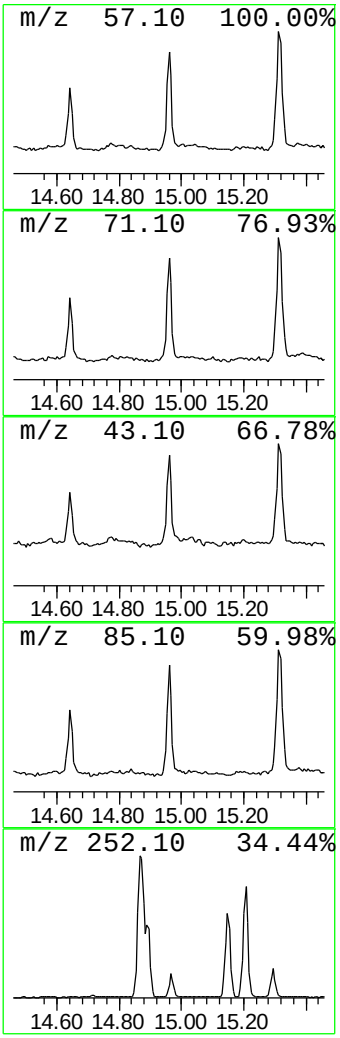
Peak Number 9 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	6.89 ng	306026	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Heneicosane	296	C21H44	000629-94-7	83
3	Hentriacontane	437	C31H64	000630-04-6	74
4	Hexacosane	366	C26H54	000630-01-3	74
5	2-methyloctacosane	408	C29H60	1000376-72-8	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109144.D
Acq On : 19 Sep 2018 15:35
Operator : JU/SJ
Sample : J4967-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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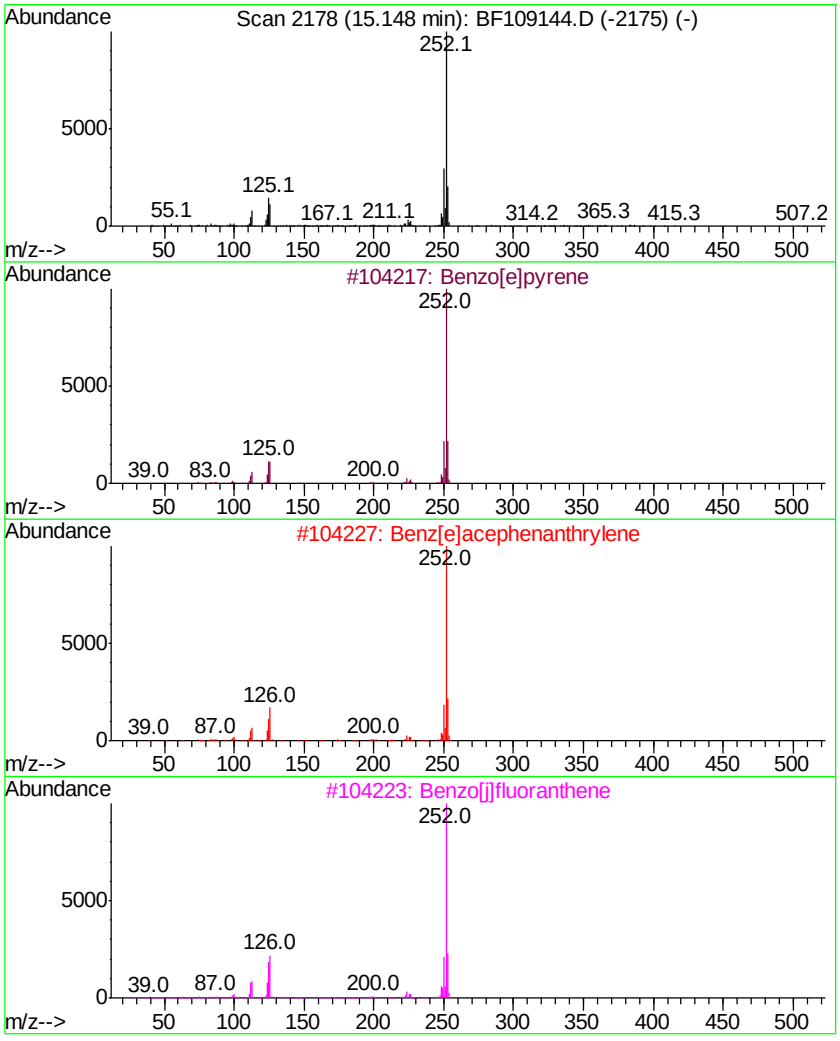
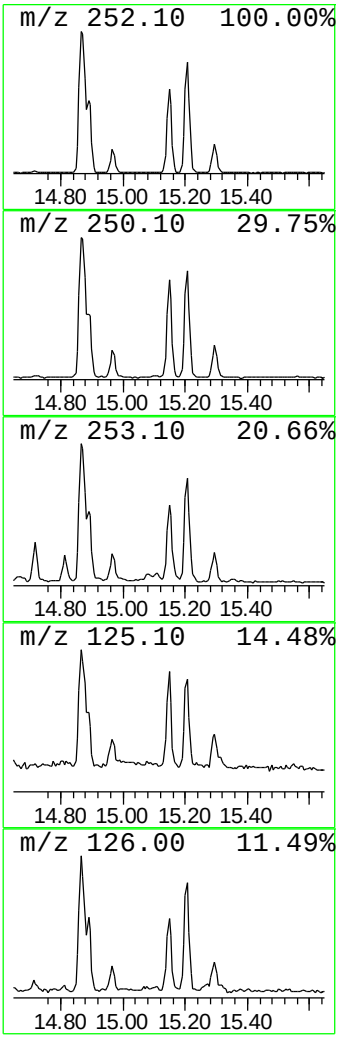
Peak Number 10 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	7.89 ng	350302	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	94
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091918\
Data File : BF109144.D
Acq On : 19 Sep 2018 15:35
Operator : JU/SJ
Sample : J4967-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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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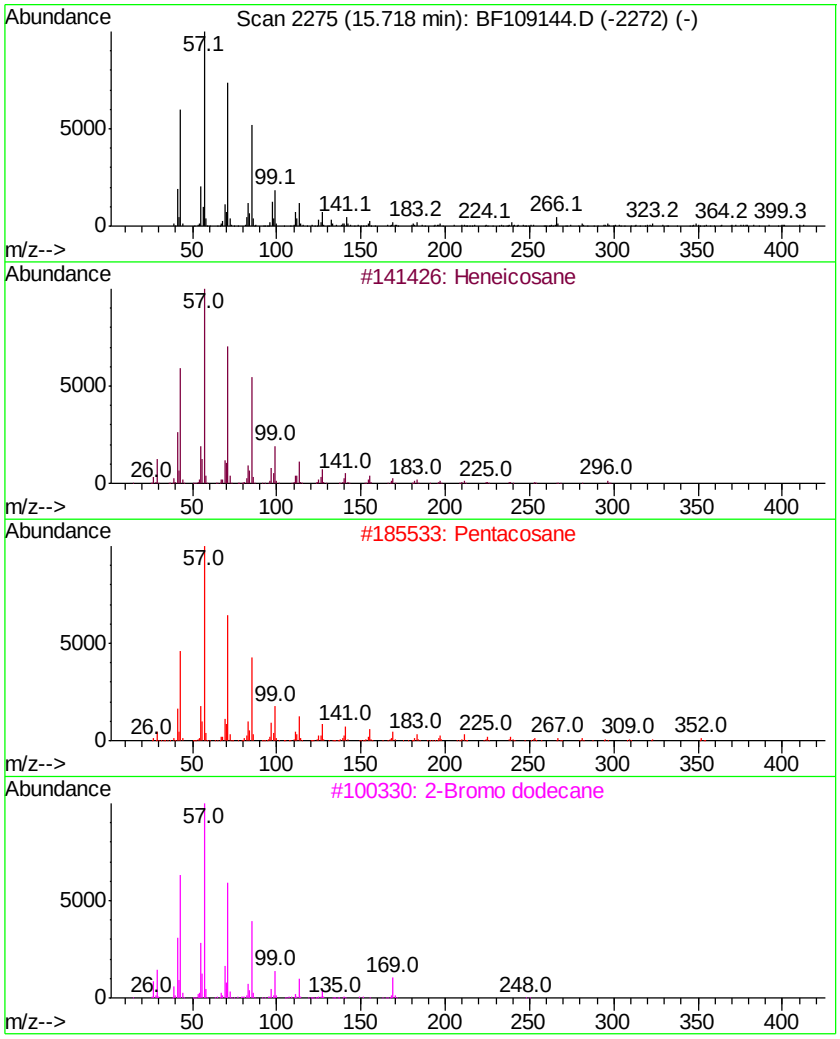
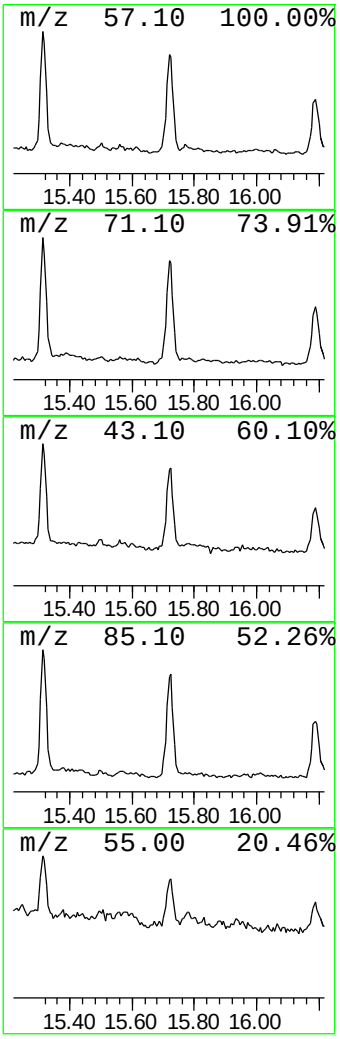
Peak Number 11 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	7.03 ng	312284	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Pentacosane	352	C25H52	000629-99-2	90
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091918\
Data File : BF109144.D
Acq On : 19 Sep 2018 15:35
Operator : JU/SJ
Sample : J4967-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-UST-091718-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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
2-Pentanone, 4-hy...	4.92	3.0	ng	121153	1	6.72	800964	20.0
unknown6.49	6.49	57.2	ng	2290840	1	6.72	800964	20.0
Phenanthrene, 3-m...	11.73	2.1	ng	92874	4	11.23	898996	20.0
Phenanthrene, 2-m...	11.76	5.7	ng	256527	4	11.23	898996	20.0
4H-Cyclopenta[def...	11.84	3.1	ng	138496	4	11.23	898996	20.0
9,10-Anthracenedione	12.04	2.2	ng	99150	4	11.23	898996	20.0
3-Eicosene, (E)-	13.72	2.2	ng	149101	5	13.86	1368290	20.0
Hexadecane	14.96	6.9	ng	306026	6	15.27	887878	20.0
Benzo[e]pyrene	15.15	7.9	ng	350302	6	15.27	887878	20.0
Heneicosane	15.72	7.0	ng	312284	6	15.27	887878	20.0