LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062219\
Data File : BF115127.D
Acq On : 22 Jun 2019 18:10
Operator : HP/JU
Sample : K3421-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-1

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-BF062119.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	4.460	424	429	435	rVB	131126	149551	2.44%	0.241%
2	5.213	551	557	560	rBV	4976390	5175015	84.41%	8.345%
3	6.248	727	733	736	rBV	4774683	5386856	87.87%	8.687%
4	6.284	736	739	742	rVB	97573	87160	1.42%	0.141%
5	6.378	750	755	759	rBV	5341681	5581424	91.04%	9.001%
6	6.613	791	795	798	rVB	1899702	1704940	27.81%	2.749%
7	6.766	817	821	825	rVB	4802926	4392665	71.65%	7.084%
8	7.172	884	890	893	rBV	3557689	3415261	55.71%	5.507%
9	7.413	928	931	935	rVB	70721	61781	1.01%	0.100%
10	7.889	1008	1012	1015	rBV	2700008	2213290	36.10%	3.569%
11	8.966	1191	1195	1199	rBV	6086291	6130709	100.00%	9.886%
12	9.360	1258	1262	1265	rBV	880020	677606	11.05%	1.093%
13	9.636	1304	1309	1312	rBV	2929563	2524823	41.18%	4.071%
14	9.666	1312	1314	1317	rVB	315768	227749	3.71%	0.367%
15	9.836	1338	1343	1348	rBV	109646	105795	1.73%	0.171%
16	10.177	1398	1401	1404	rVB	222765	190795	3.11%	0.308%
17	10.313	1418	1424	1426	rBV2	95822	110417	1.80%	0.178%
18	10.413	1437	1441	1446	rBV	3428073	3150996	51.40%	5.081%
19	10.577	1467	1469	1475	rVB	152793	129219	2.11%	0.208%
20	10.724	1487	1494	1496	rBV4	59063	88206	1.44%	0.142%
21	10.971	1532	1536	1539	rBV4	65125	95846	1.56%	0.155%
22	11.007	1539	1542	1544	rVV2	125436	127182	2.07%	0.205%
23	11.042	1544	1548	1552	rVB	115974	125718	2.05%	0.203%
24	11.107	1555	1559	1561	rVV	3124498	2646150	43.16%	4.267%
25	11.130	1561	1563	1566	rVV	959764	745446	12.16%	1.202%
26	11.177	1568	1571	1575	rVB	275018	225405	3.68%	0.363%
27	11.430	1612	1614	1618	rVB	107649	91734	1.50%	0.148%
28	11.607	1637	1644	1646	rBV	163658	183783	3.00%	0.296%
29	11.630	1646	1648	1650	rVV	191033	139698	2.28%	0.225%
30	11.677	1654	1656	1659	rVB2	86826	74587	1.22%	0.120%
31	11.713	1659	1662	1665	rBV	303540	288657	4.71%	0.465%
32	11.836	1680	1683	1688	rVV	89123	78017	1.27%	0.126%
33	11.901	1691	1694	1704	rVB2	125435	173998	2.84%	0.281%
34	12.154	1733	1737	1739	rBV	57289	65277	1.06%	0.105%

LSC Area Percent Report

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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
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.177	1739	1741	1745	rVV2	87972	130385	2.13%	0.210%
36	12.224	1747	1749	1755	rVB3	121186	148891	2.43%	0.240%
37	12.307	1759	1763	1770	rBV	1453763	1170246	19.09%	1.887%
38	12.360	1770	1772	1781	rVB5	45193	82865	1.35%	0.134%
39	12.436	1781	1785	1793	rBV2	185247	319621	5.21%	0.515%
40	12.530	1796	1801	1804	rVV2	1061653	1047406	17.08%	1.689%
41	12.595	1808	1812	1817	rVB3	83801	120822	1.97%	0.195%
42	12.695	1824	1829	1832	rBV	5485476	5595941	91.28%	9.024%
43	12.754	1834	1839	1845	rVB5	65911	116253	1.90%	0.187%
44	12.842	1848	1854	1855	rBV4	58364	85928	1.40%	0.139%
45	12.860	1855	1857	1862	rVB	210821	188917	3.08%	0.305%
46	12.930	1865	1869	1871	rBV	165131	165378	2.70%	0.267%
47	12.960	1871	1874	1877	rVB2	93956	110440	1.80%	0.178%
48	13.265	1919	1926	1927	rBV6	36553	72263	1.18%	0.117%
49	13.289	1927	1930	1932	rVB2	83305	77798	1.27%	0.125%
50	13.607	1981	1984	1992	rBV5	291521	435386	7.10%	0.702%
51	13.724	1998	2004	2006	rBV2	2083338	2178817	35.54%	3.514%
52	13.742	2006	2007	2010	rVB	250845	198558	3.24%	0.320%
53	13.930	2036	2039	2045	rBV2	118631	128241	2.09%	0.207%
54	14.236	2087	2091	2097	rBV3	147860	201884	3.29%	0.326%
55	14.530	2137	2141	2144	rBV	103367	105486	1.72%	0.170%
56	14.706	2168	2171	2174	rBV	187654	241126	3.93%	0.389%
57	14.830	2189	2192	2197	rVB	102614	103538	1.69%	0.167%
58	14.971	2213	2216	2221	rVB	101809	101521	1.66%	0.164%
59	15.024	2222	2225	2230	rVB	132465	139974	2.28%	0.226%
60	15.083	2230	2235	2243	rBV	1586063	1842536	30.05%	2.971%
61	15.165	2246	2249	2254	rVB	84411	114016	1.86%	0.184%
62	15.548	2310	2314	2318	rBV	69936	124377	2.03%	0.201%
63	16.336	2444	2448	2455	rVB2	50994	97786	1.60%	0.158%

Sum of corrected areas: 62012156

LSC Report - Integrated Chromatogram

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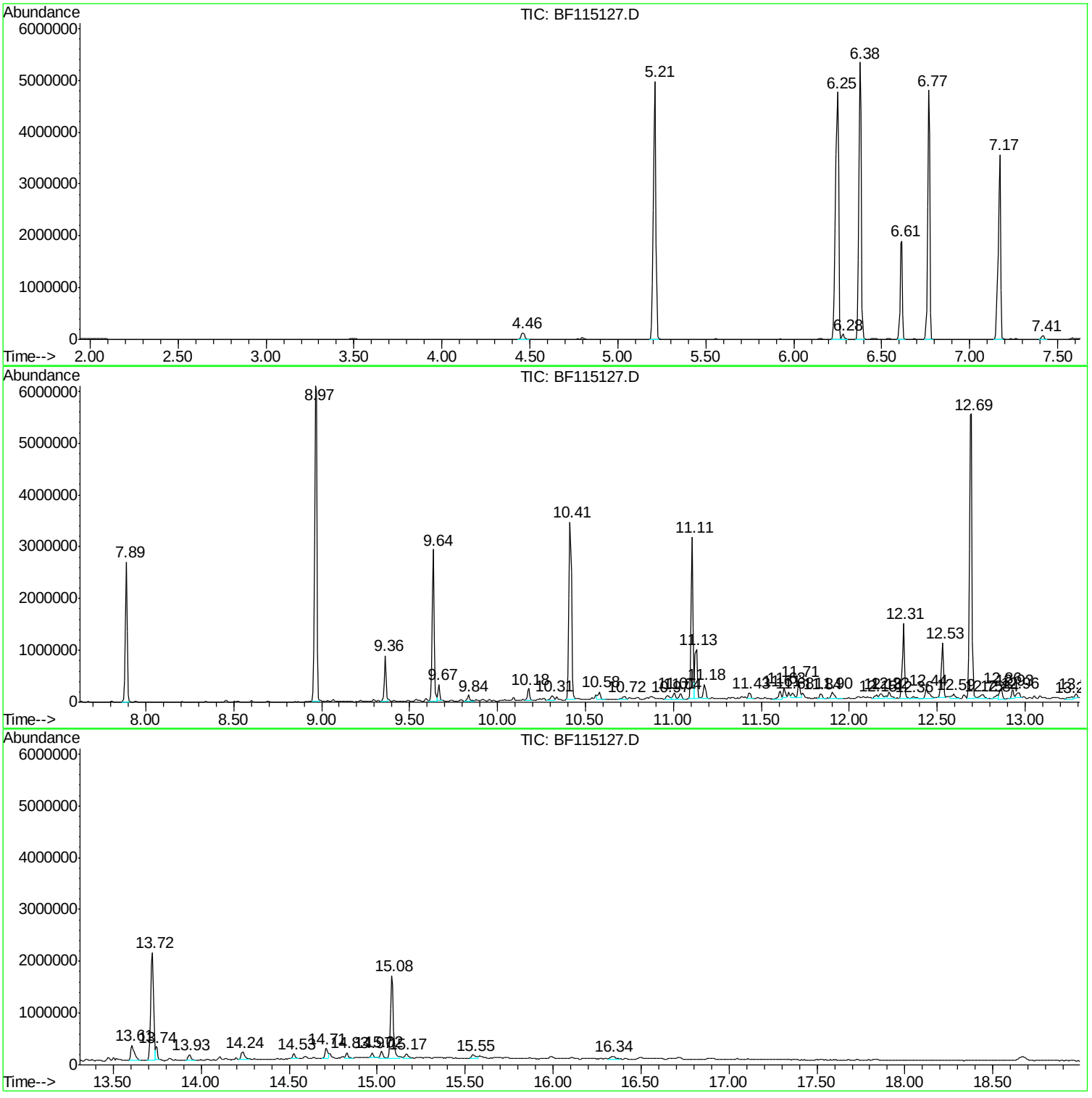
Sample : K3421-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.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\BF062219\
Data File : BF115127.D
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Instrument : BNA_F
ClientSampleId : SAMPLE-1

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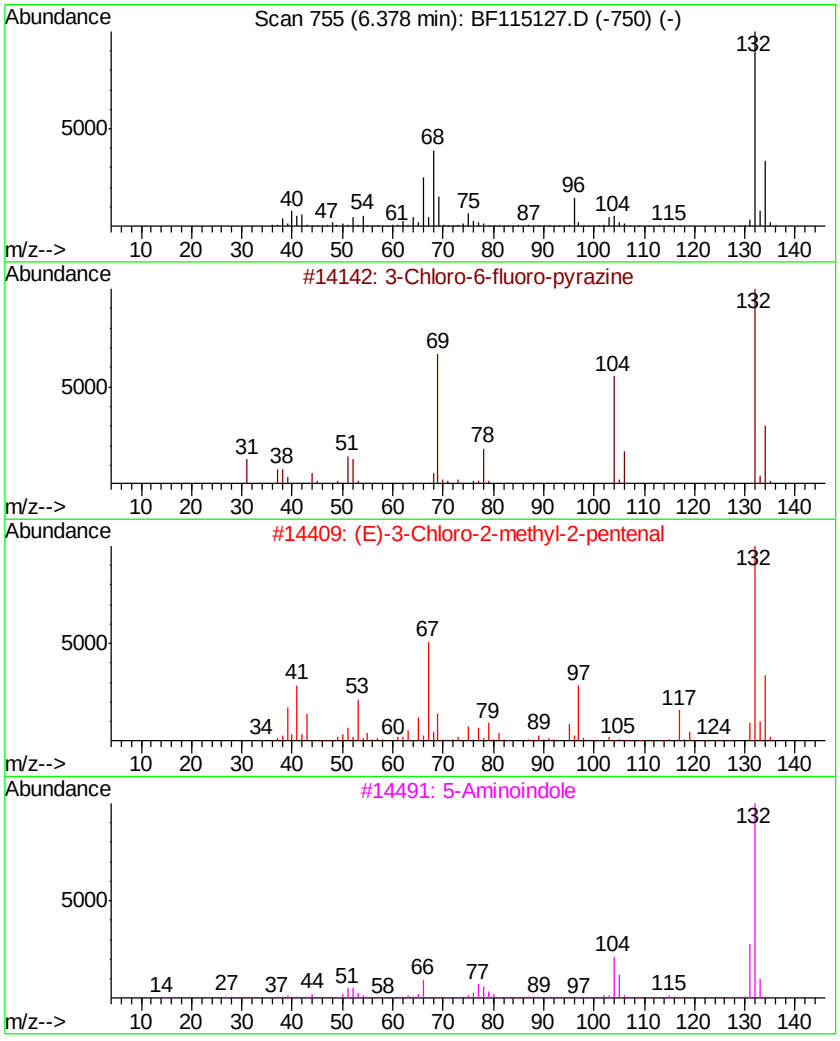
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

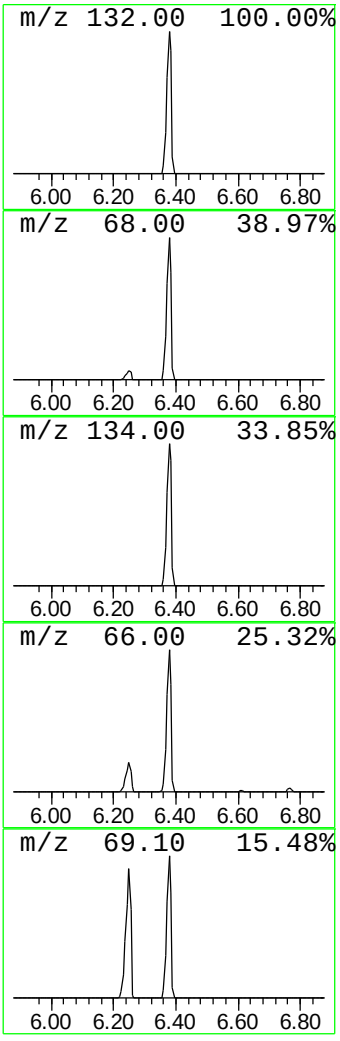
****

Peak Number 1 unknown6.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	65.47 ng	5581420	1,4-Dichlorobenzene-d4	6.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062219\
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Instrument : BNA_F
ClientSampleId : SAMPLE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

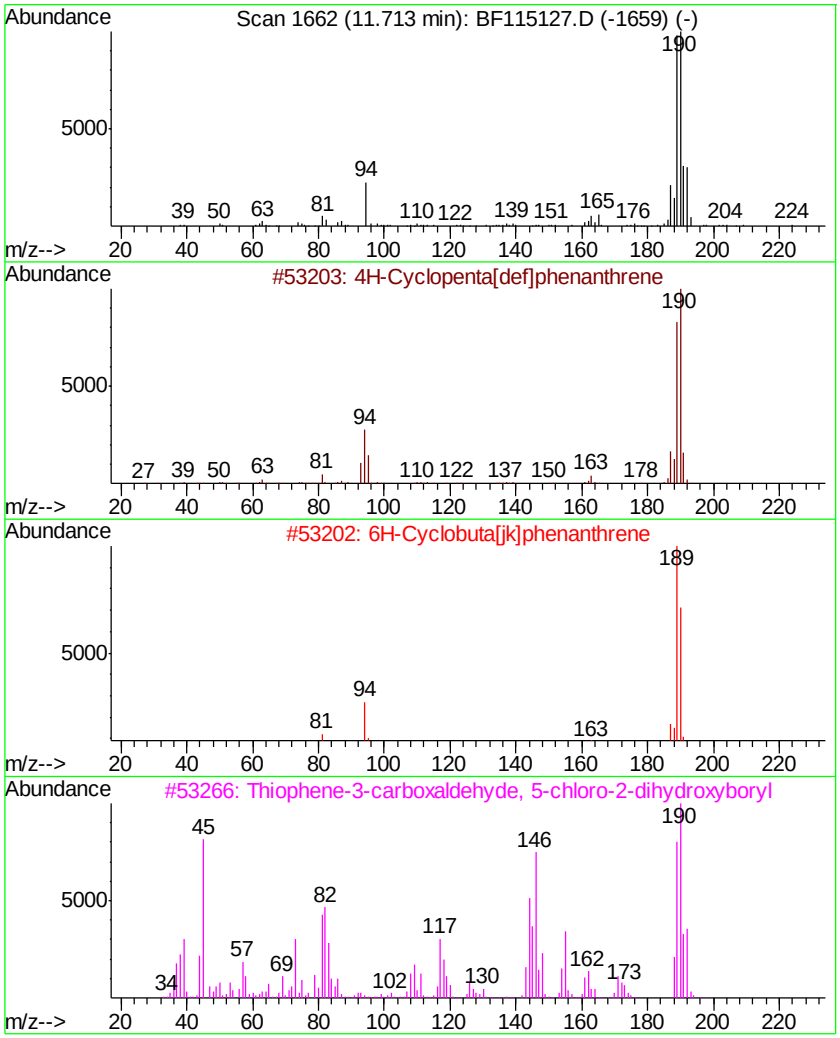
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

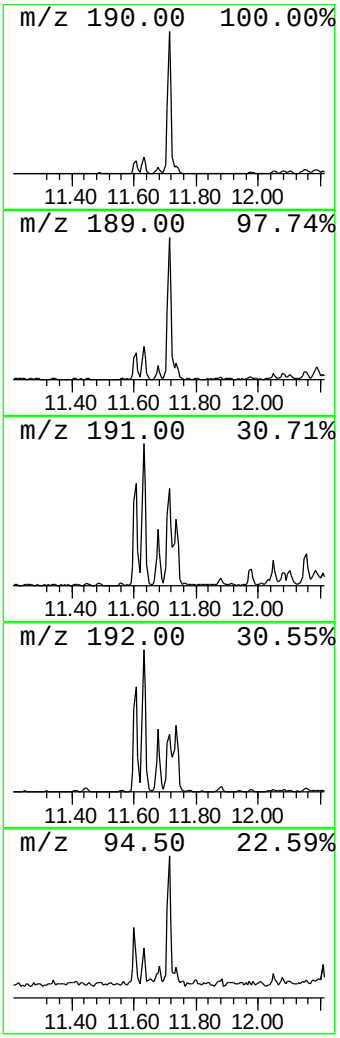
****

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	2.18 ng	288657	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	Megastigmatrienone	190	C13H18O	038818-55-2	25





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-1

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

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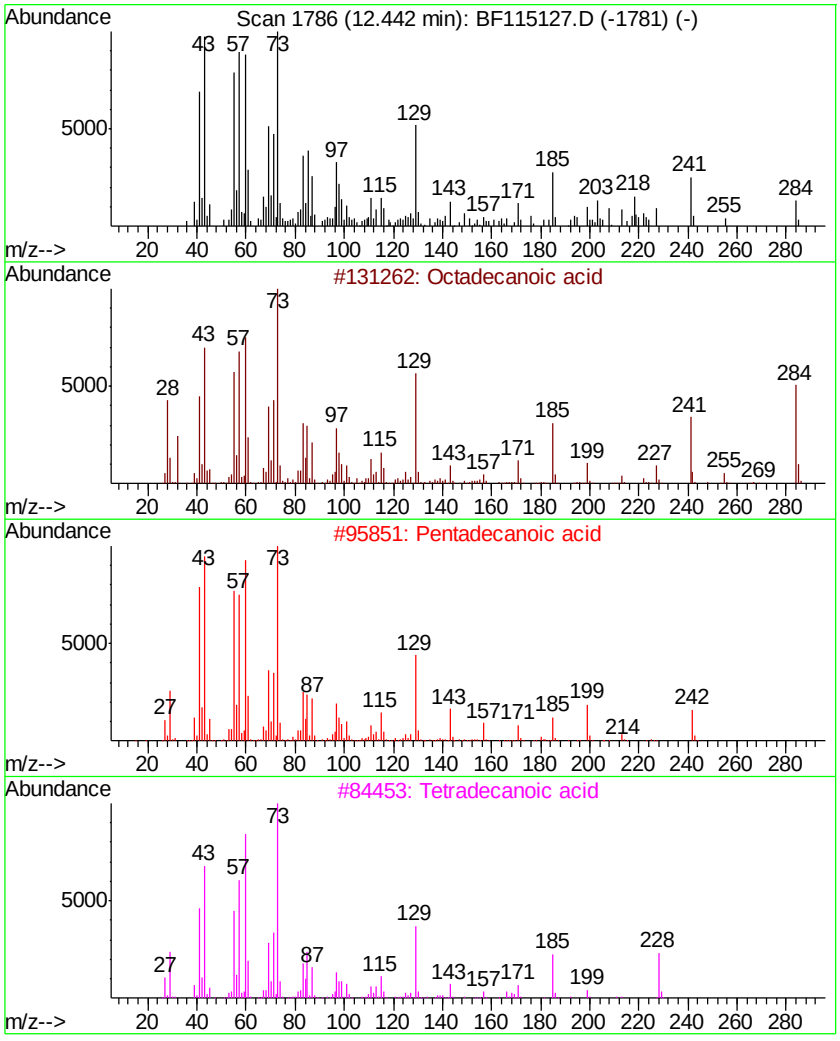
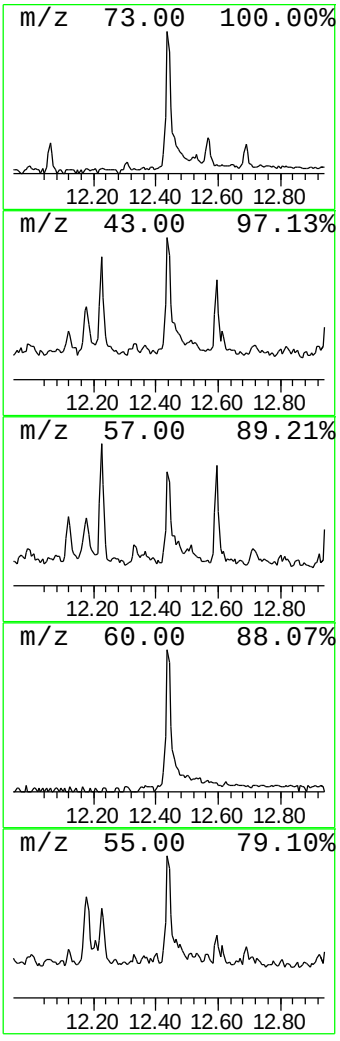
Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	2.93 ng	319621	Chrysene-d12	13.72

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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





Library Search Compound Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAMPLE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF062119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

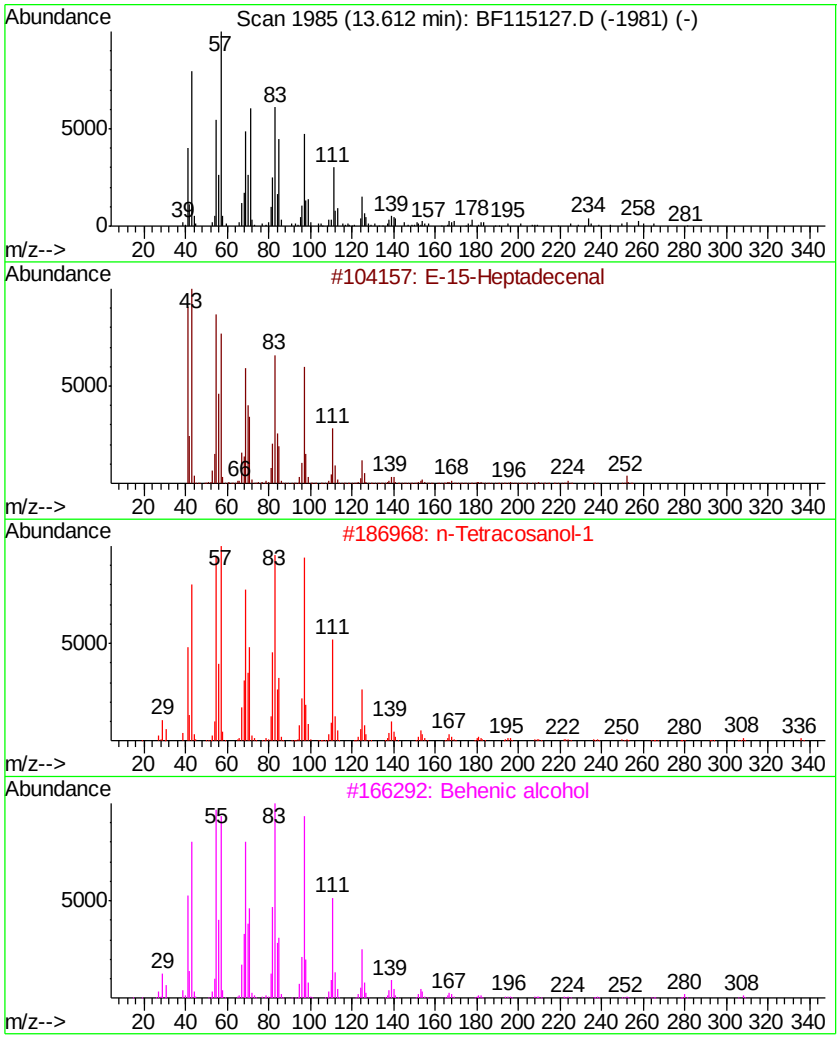
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

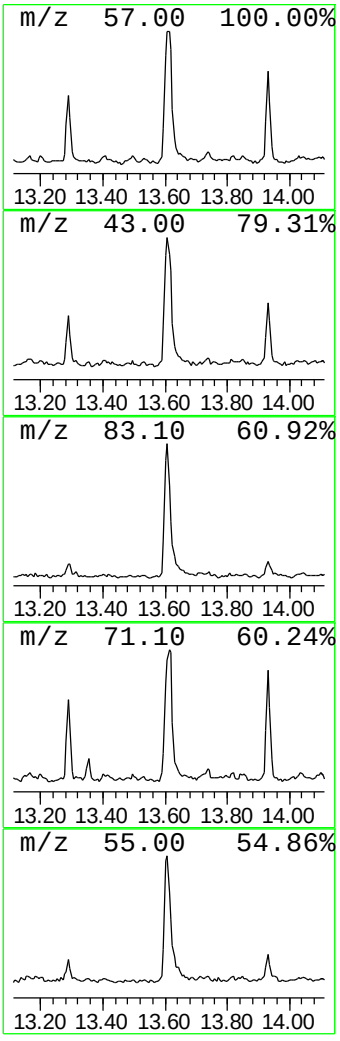
****

Peak Number 5 E-15-Heptadecenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	4.00 ng	435386	Chrysene-d12	13.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94





Tentatively Identified Compound (LSC) summary

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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
unknown6.38	6.38	65.5	ng	5581420	1	6.61	1704940	20.0
4H-Cyclopenta[def...	11.71	2.2	ng	288657	4	11.11	2646150	20.0
Octadecanoic acid	12.44	2.9	ng	319621	5	13.72	2178820	20.0
E-15-Heptadecenal	13.61	4.0	ng	435386	5	13.72	2178820	20.0