LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097907.D
Acq On : 21 Aug 2017 15:38
Operator : SJ/JU
Sample : I4852-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-207

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	4.940	481	485	495	rVB	412515	572845	18.11%	1.916%
2	5.322	546	550	551	rBV	50198	46087	1.46%	0.154%
3	5.357	551	556	559	rVB	2905830	3053208	96.54%	10.213%
4	5.587	592	595	598	rVB	43480	40662	1.29%	0.136%
5	6.351	720	725	726	rBV	53382	55189	1.75%	0.185%
6	6.386	726	731	734	rVB	2881432	3162553	100.00%	10.579%
7	6.522	749	754	757	rBV	3034635	2993869	94.67%	10.015%
8	6.575	760	763	769	rVB2	52686	57053	1.80%	0.191%
9	6.751	789	793	796	rBV	1006111	864034	27.32%	2.890%
10	6.904	815	819	822	rBV	2392061	2217224	70.11%	7.417%
11	7.316	883	889	892	rBV	1930434	1918111	60.65%	6.416%
12	7.404	898	904	907	rBV	36121	40353	1.28%	0.135%
13	8.033	1006	1011	1013	rBV	1211601	1066308	33.72%	3.567%
14	8.051	1013	1014	1016	rVB	67848	37424	1.18%	0.125%
15	9.110	1188	1194	1197	rBV	3058356	2661122	84.14%	8.902%
16	9.498	1257	1260	1265	rBV	355070	307199	9.71%	1.028%
17	9.780	1302	1308	1312	rBV	1001516	944209	29.86%	3.158%
18	9.816	1312	1314	1318	rVB	69223	54895	1.74%	0.184%
19	9.986	1339	1343	1346	rVB	52371	43962	1.39%	0.147%
20	10.222	1380	1383	1385	rVB	41610	32721	1.03%	0.109%
21	10.327	1398	1401	1406	rVB2	79952	69750	2.21%	0.233%
22	10.569	1437	1442	1445	rBV	1535527	1370871	43.35%	4.586%
23	10.692	1459	1463	1471	rVB	64861	76902	2.43%	0.257%
24	11.263	1556	1560	1562	rBV	948006	790707	25.00%	2.645%
25	11.286	1562	1564	1567	rVV	365403	271541	8.59%	0.908%
26	11.339	1567	1573	1576	rVB	79879	82786	2.62%	0.277%
27	11.763	1642	1645	1647	rBV	48423	39020	1.23%	0.131%
28	11.792	1647	1650	1654	rVB	69764	59307	1.88%	0.198%
29	11.874	1660	1664	1666	rBV	86201	84975	2.69%	0.284%
30	12.080	1697	1699	1704	rVB4	33360	32939	1.04%	0.110%
31	12.310	1735	1738	1741	rBV	43137	44399	1.40%	0.149%
32	12.392	1750	1752	1758	rVB3	34613	36025	1.14%	0.121%
33	12.474	1762	1766	1769	rBV	621423	567614	17.95%	1.899%
34	12.515	1770	1773	1779	rVV4	61189	65841	2.08%	0.220%

LSC Area Percent Report

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Operator : SJ/JU
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-207

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.698	1798	1804	1807	rBV	578981	590618	18.68%	1.976%
36	12.815	1822	1824	1826	rBV	34440	33161	1.05%	0.111%
37	12.851	1826	1830	1833	rVV	2118475	1891678	59.81%	6.328%
38	12.915	1837	1841	1845	rBV2	44939	74316	2.35%	0.249%
39	13.027	1857	1860	1863	rVB2	82365	79571	2.52%	0.266%
40	13.092	1868	1871	1874	rBV	57403	55938	1.77%	0.187%
41	13.133	1874	1878	1880	rBV2	66504	67158	2.12%	0.225%
42	13.221	1890	1893	1896	rVB	39826	37393	1.18%	0.125%
43	13.251	1896	1898	1902	rBV2	37467	44929	1.42%	0.150%
44	13.533	1943	1946	1950	rVB	52239	56077	1.77%	0.188%
45	13.645	1961	1965	1968	rBV2	63511	93624	2.96%	0.313%
46	13.674	1968	1970	1972	rVV	48328	37294	1.18%	0.125%
47	13.745	1979	1982	1989	rVB2	154162	174636	5.52%	0.584%
48	13.892	2002	2007	2010	rBV2	967569	1208935	38.23%	4.044%
49	13.921	2010	2012	2019	rVB	333920	286765	9.07%	0.959%
50	13.998	2023	2025	2029	rVB	46162	36255	1.15%	0.121%
51	14.909	2177	2180	2187	rVB	257244	458085	14.48%	1.532%
52	15.198	2226	2229	2234	rVB	168532	199651	6.31%	0.668%
53	15.251	2235	2238	2242	rBV	174612	210023	6.64%	0.703%
54	15.315	2245	2249	2252	rBV	446817	497161	15.72%	1.663%

Sum of corrected areas: 29894973

LSC Report - Integrated Chromatogram

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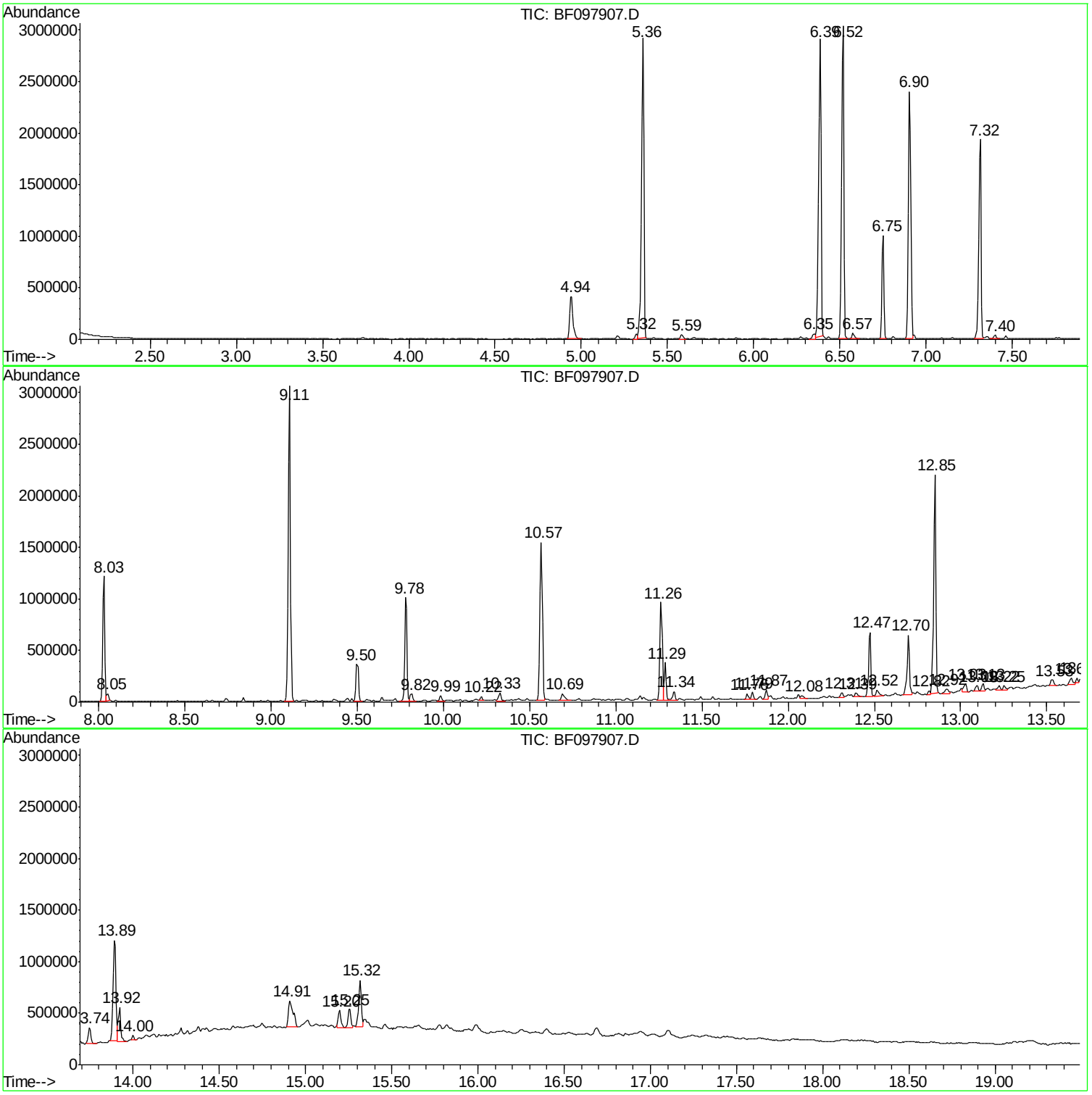
Operator : SJ/JU
Sample : I4852-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-207

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
Data File : BF097907.D
Acq On : 21 Aug 2017 15:38
Operator : SJ/JU
Sample : I4852-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

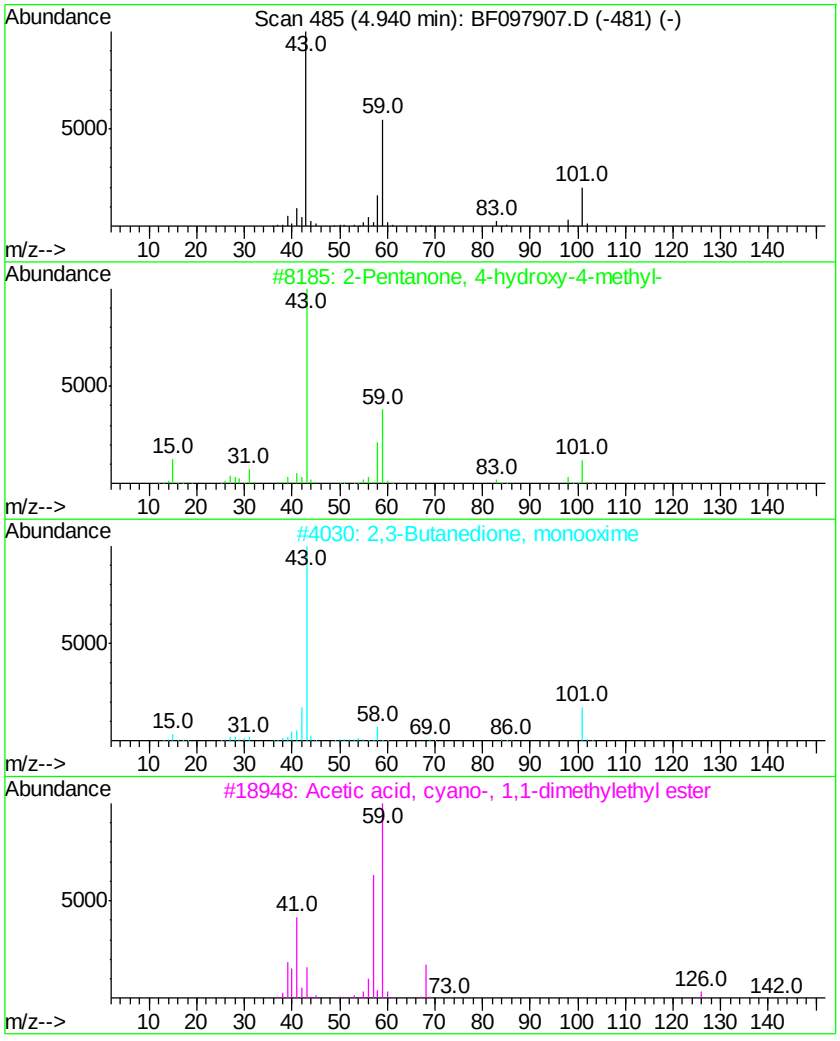
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

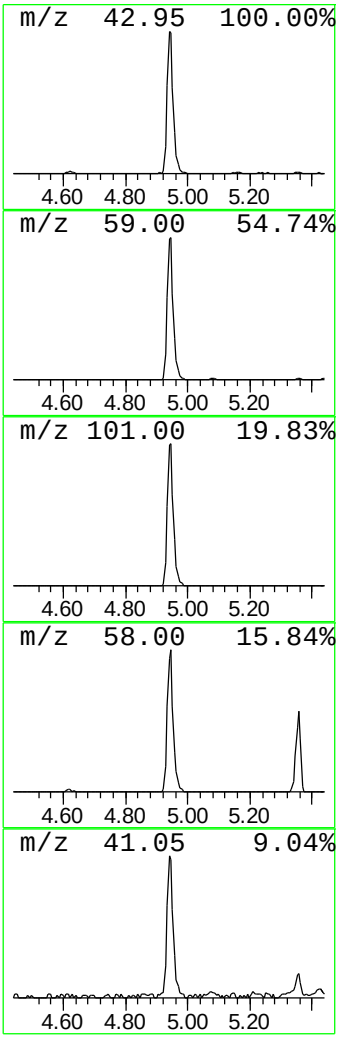
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	13.26 ng	572845	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
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Acq On : 21 Aug 2017 15:38
Operator : SJ/JU
Sample : I4852-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-207

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

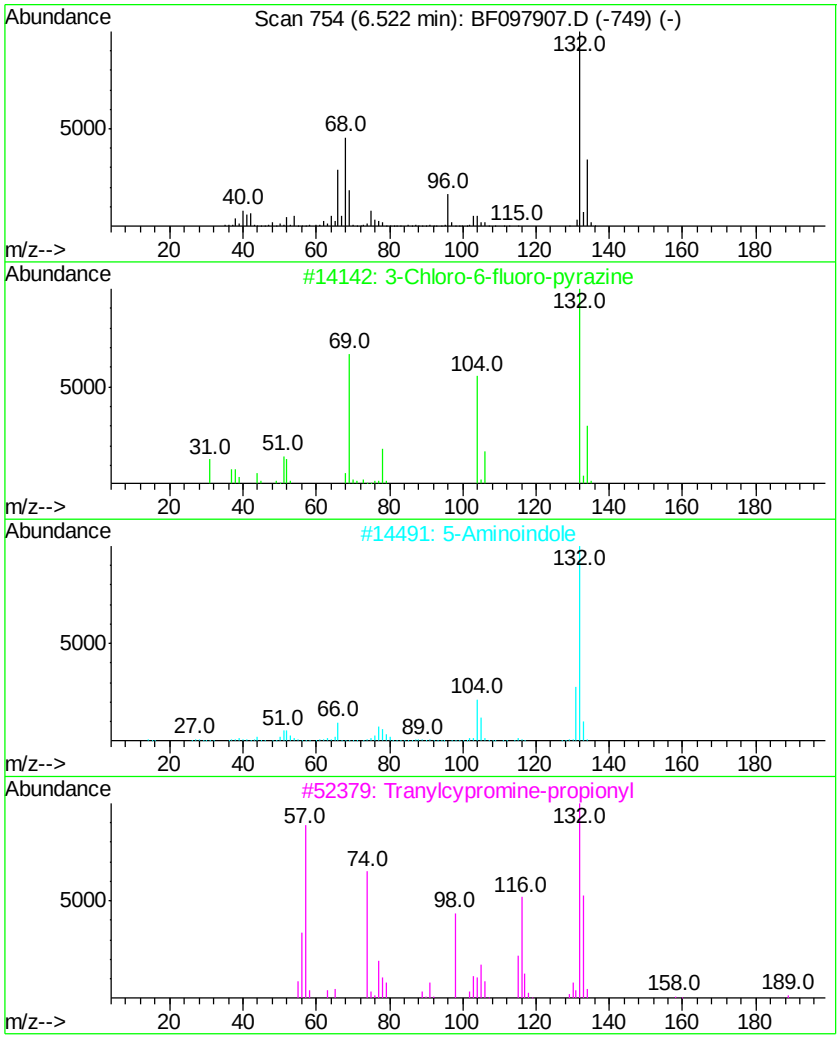
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

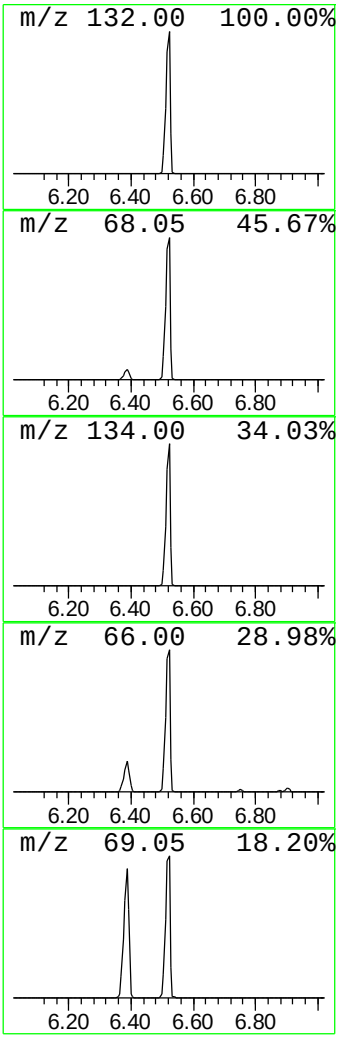
****

Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	69.30 ng	2993870	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	10
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Sample : I4852-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VNJ-207

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

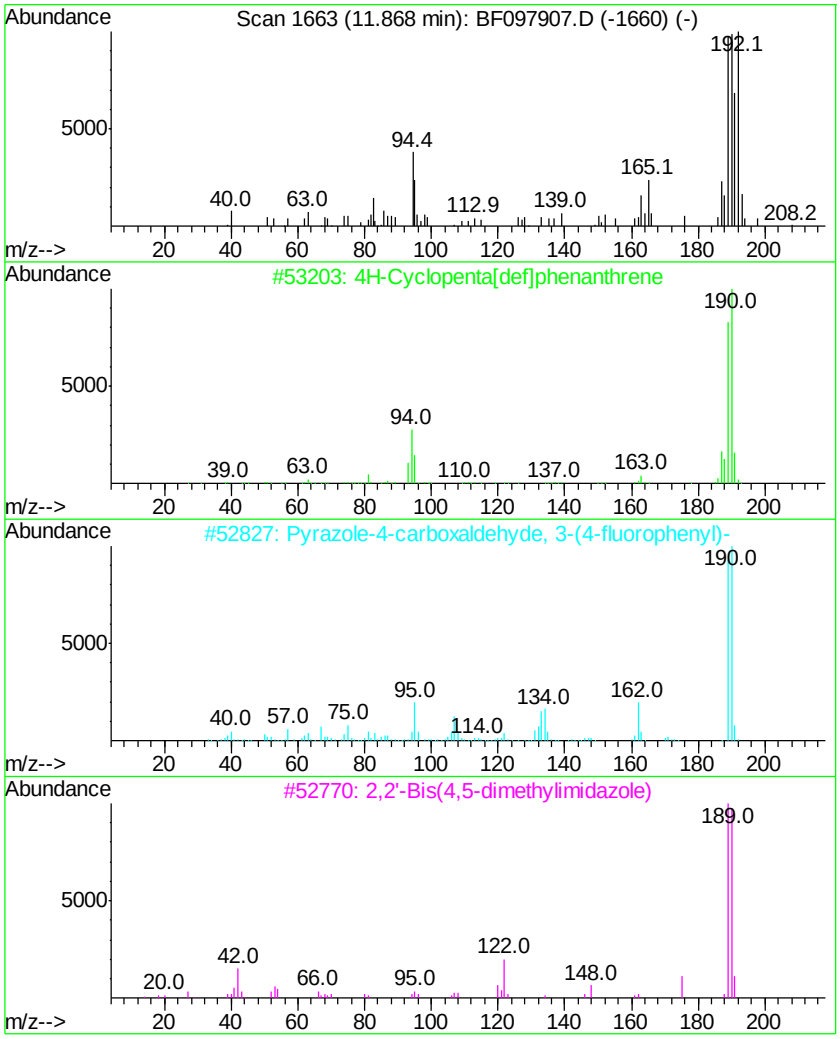
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

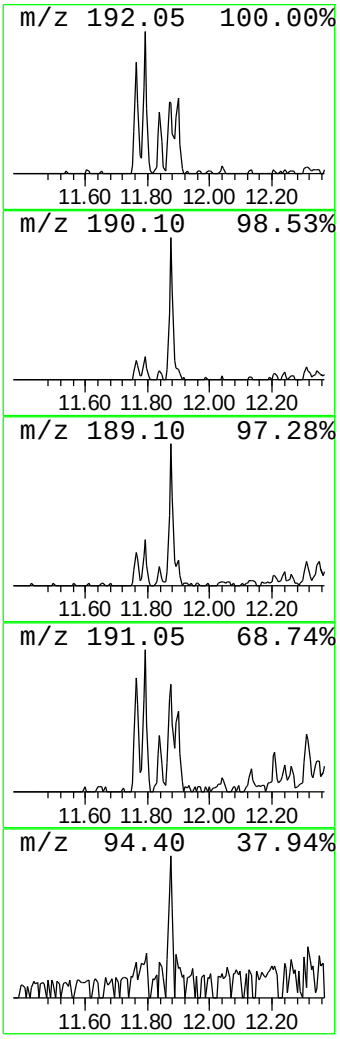
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.15 ng	84975	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	37
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	23
5	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	17





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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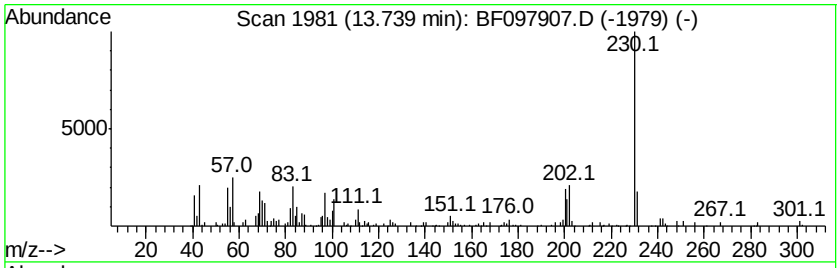
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

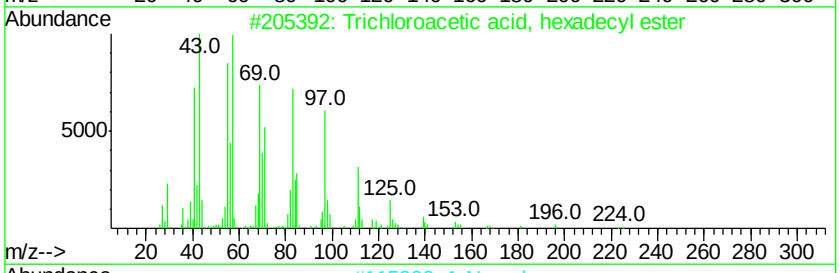
****

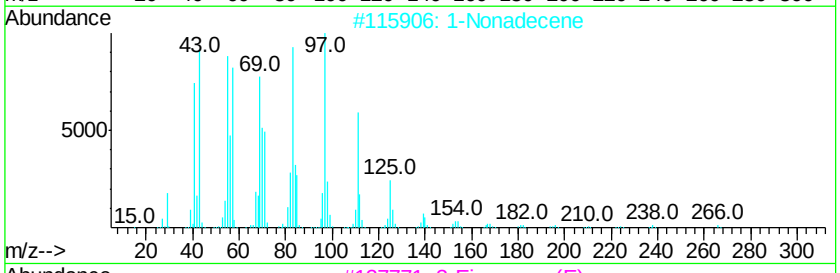
Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 5

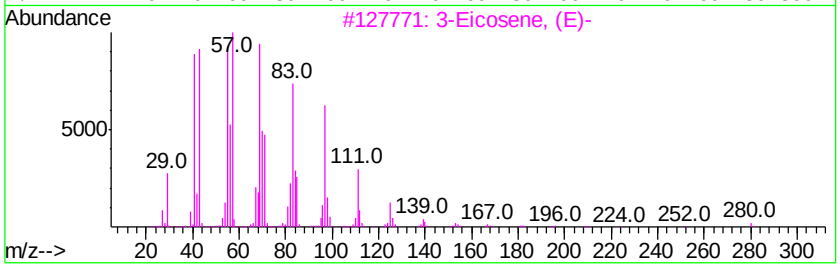
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.89 ng	174636	Chrysene-d12	13.90

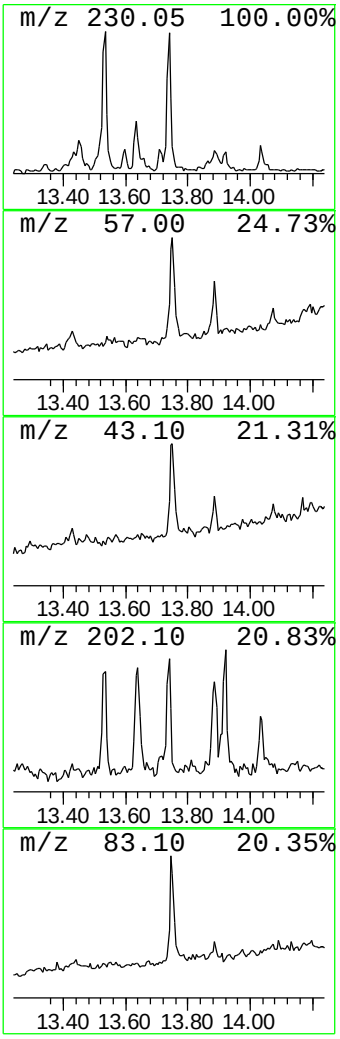
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
2	1-Nonadecene	266	C19H38	018435-45-5	87
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
5	Behenic alcohol	326	C22H46O	000661-19-8	87











Library Search Compound Report

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Data File : BF097907.D
Acq On : 21 Aug 2017 15:38
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Sample : I4852-01
Misc :
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Instrument : BNA_F
ClientSampleId : VNJ-207

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

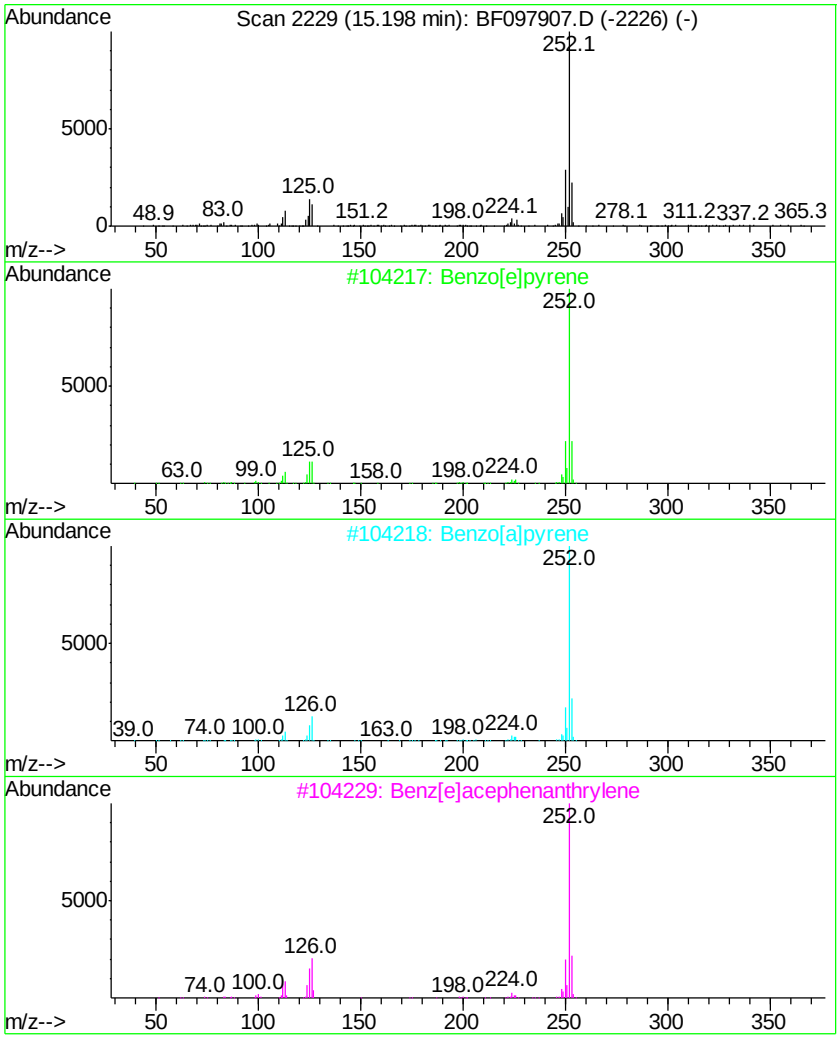
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

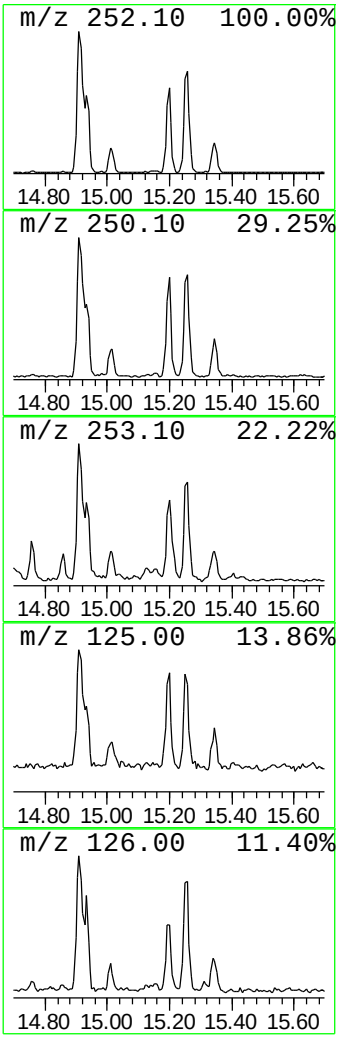
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	8.03 ng	199651	Perylene-d12	15.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
Data File : BF097907.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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	13.3	ng	572845	1	6.75	864034	20.0
unknown6.52	6.52	69.3	ng	2993870	1	6.75	864034	20.0
4H-Cyclopenta[def...	11.87	2.1	ng	84975	4	11.26	790707	20.0
Trichloroacetic a...	13.74	2.9	ng	174636	5	13.90	1208940	20.0
Benzo[e]pyrene	15.20	8.0	ng	199651	6	15.32	497161	20.0