LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101351.D
Acq On : 13 Dec 2017 00:55
Operator : SJ/JU
Sample : I6822-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(13-15)

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-BF113017.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	5.051	500	504	515	rBV	52651	79754	6.86%	0.713%
2	5.445	567	571	588	rVB	1068442	1082433	93.09%	9.671%
3	6.463	739	744	761	rBV	1125955	1160549	99.81%	10.368%
4	6.598	762	767	770	rBV	1243299	1146636	98.61%	10.244%
5	6.822	802	805	813	rBB	339410	271102	23.32%	2.422%
6	6.981	828	832	835	rBV	945158	848989	73.02%	7.585%
7	7.392	897	902	913	rBV	680647	643774	55.37%	5.752%
8	8.104	1019	1023	1026	rBV	405147	336373	28.93%	3.005%
9	9.180	1202	1206	1209	rBV	1421757	1162754	100.00%	10.388%
10	9.575	1269	1273	1281	rVB	192474	151624	13.04%	1.355%
11	9.863	1318	1322	1325	rBV	413054	336827	28.97%	3.009%
12	9.892	1325	1327	1330	rVB	21444	17813	1.53%	0.159%
13	10.280	1389	1393	1396	rVB	20326	15135	1.30%	0.135%
14	10.410	1411	1415	1419	rBV	15118	13592	1.17%	0.121%
15	10.657	1453	1457	1464	rBV	702323	613915	52.80%	5.485%
16	10.751	1471	1473	1479	rBV3	15478	21225	1.83%	0.190%
17	11.357	1572	1576	1578	rBV	327822	314768	27.07%	2.812%
18	11.380	1578	1580	1583	rVV	104627	85110	7.32%	0.760%
19	11.427	1583	1588	1592	rVV	29585	28270	2.43%	0.253%
20	11.857	1658	1661	1663	rBV	14065	13539	1.16%	0.121%
21	11.886	1663	1666	1669	rVB	20300	18077	1.55%	0.162%
22	11.968	1677	1680	1683	rBV2	24903	29614	2.55%	0.265%
23	12.404	1752	1754	1757	rBV	12064	13736	1.18%	0.123%
24	12.574	1779	1783	1786	rBV	139756	118219	10.17%	1.056%
25	12.786	1815	1819	1820	rBV2	35149	36881	3.17%	0.329%
26	12.804	1820	1822	1825	rVB	123527	95475	8.21%	0.853%
27	12.939	1841	1845	1848	rVB	1037189	899352	77.35%	8.035%
28	13.021	1854	1859	1862	rBV3	11483	17139	1.47%	0.153%
29	13.133	1875	1878	1880	rVB	24422	22259	1.91%	0.199%
30	13.198	1886	1889	1891	rBV	23610	20885	1.80%	0.187%
31	13.233	1891	1895	1898	rVV2	15610	19536	1.68%	0.175%
32	13.327	1907	1911	1914	rBV2	12790	13698	1.18%	0.122%
33	13.757	1979	1984	1986	rBV2	12203	14654	1.26%	0.131%
34	13.827	1990	1996	2004	rVB4	60251	89256	7.68%	0.797%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-8(13-15)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.004	2021	2026	2029	rBV2	351379	393467	33.84%	3.515%
36	14.033	2029	2031	2033	rVB	82230	63488	5.46%	0.567%
37	14.110	2042	2044	2048	rBV	26137	23003	1.98%	0.206%
38	14.357	2083	2086	2088	rBV2	14205	15488	1.33%	0.138%
39	14.392	2088	2092	2095	rVB	27511	29731	2.56%	0.266%
40	15.051	2200	2204	2207	rBV	96539	138571	11.92%	1.238%
41	15.162	2219	2223	2226	rVB	23713	27522	2.37%	0.246%
42	15.257	2233	2239	2243	rBV6	10674	24685	2.12%	0.221%
43	15.356	2253	2256	2263	rVB	57746	71224	6.13%	0.636%
44	15.421	2263	2267	2271	rVB	94355	113489	9.76%	1.014%
45	15.480	2271	2277	2281	rBV	190047	239476	20.60%	2.139%
46	15.515	2281	2283	2289	rVB2	26563	34539	2.97%	0.309%
47	15.968	2356	2360	2364	rVB6	10218	16628	1.43%	0.149%
48	16.968	2522	2530	2538	rVB	52790	103345	8.89%	0.923%
49	17.139	2554	2559	2564	rBV5	8902	22180	1.91%	0.198%
50	17.198	2565	2569	2575	rVV7	7659	15561	1.34%	0.139%
51	17.421	2601	2607	2614	rBV2	34692	66651	5.73%	0.595%
52	17.662	2642	2648	2656	rVB2	15274	41074	3.53%	0.367%

Sum of corrected areas: 11193085

LSC Report - Integrated Chromatogram

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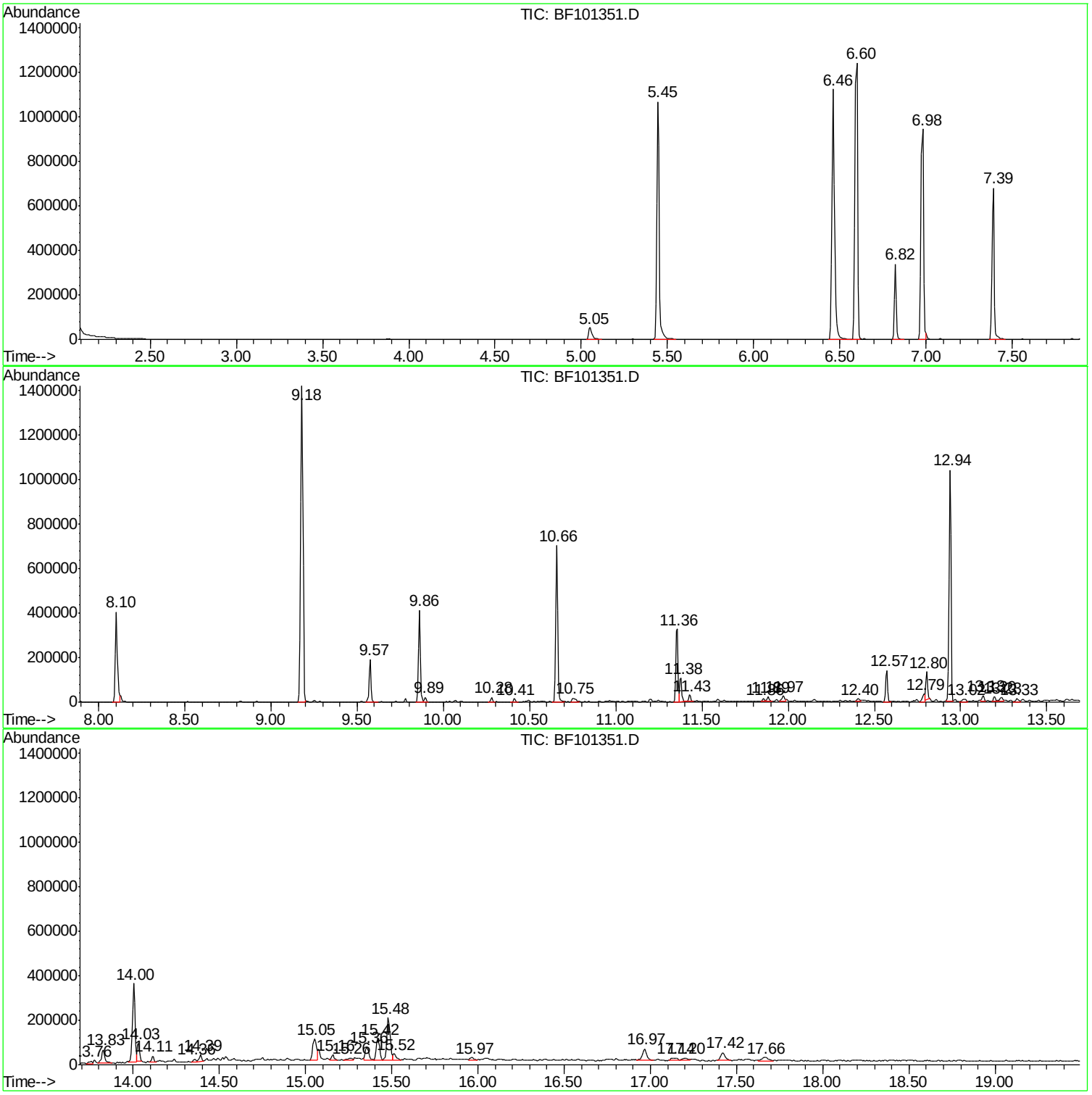
Operator : SJ/JU
Sample : I6822-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101351.D
Acq On : 13 Dec 2017 00:55
Operator : SJ/JU
Sample : I6822-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

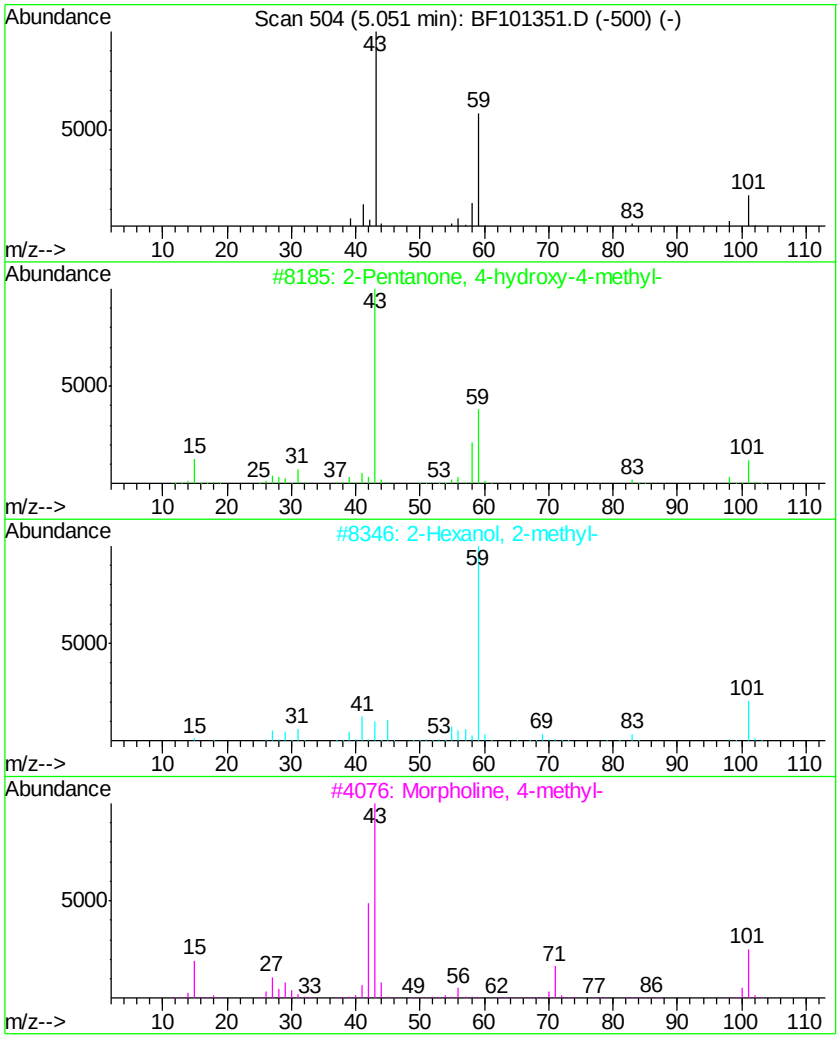
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

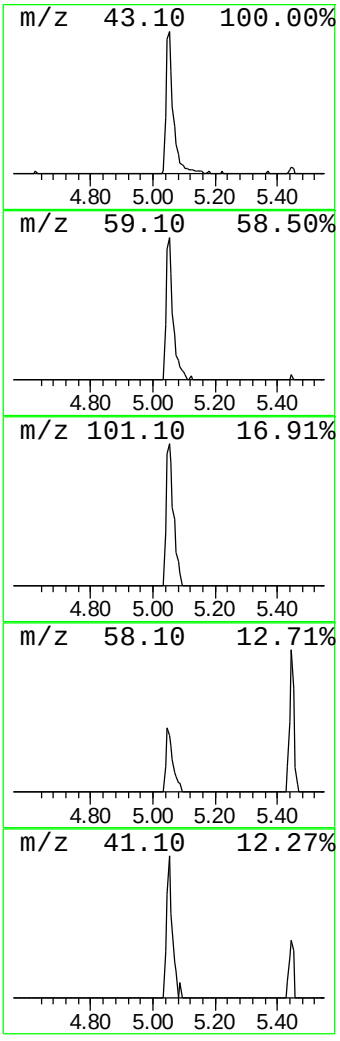
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	5.88 ng	79754	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121217\
Data File : BF101351.D
Acq On : 13 Dec 2017 00:55
Operator : SJ/JU
Sample : I6822-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-8(13-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

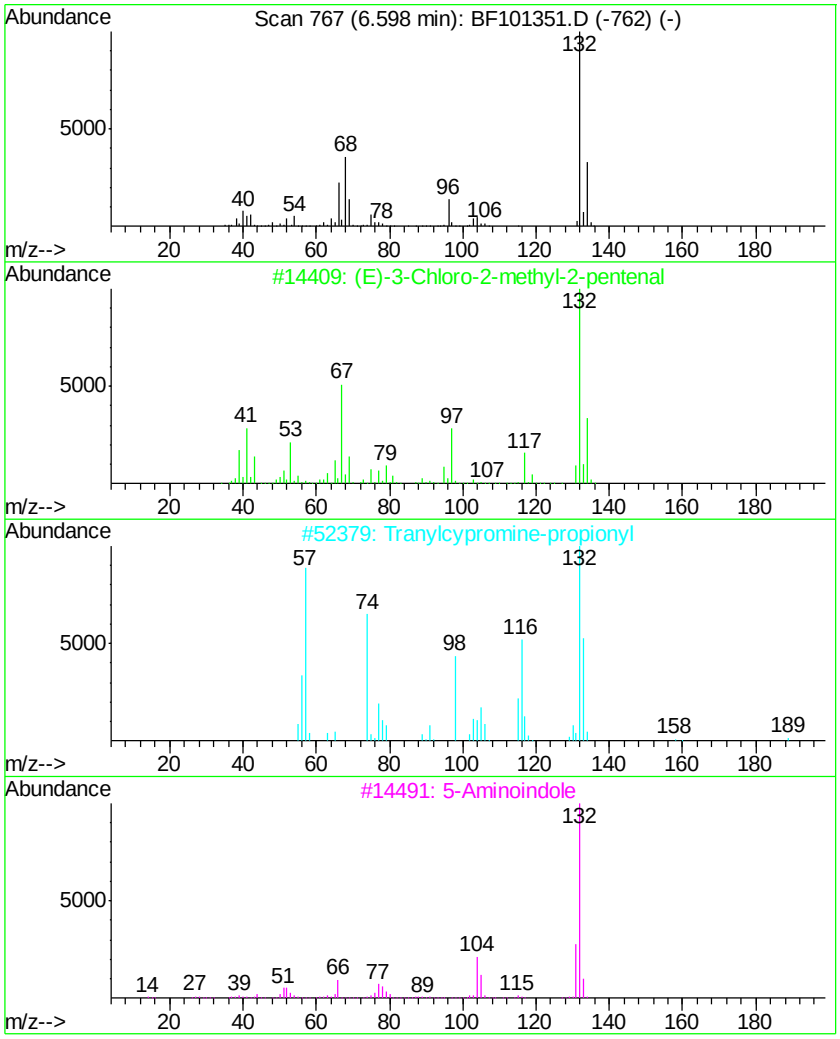
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

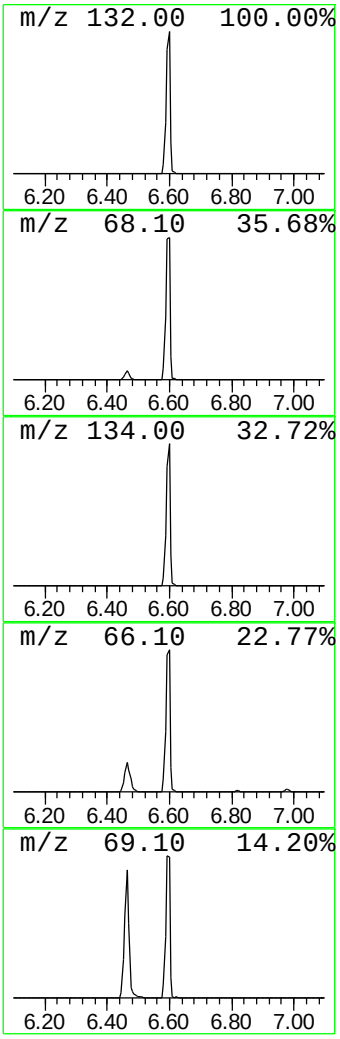
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	84.59 ng	1146640	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	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Xenon	132	Xe	007440-63-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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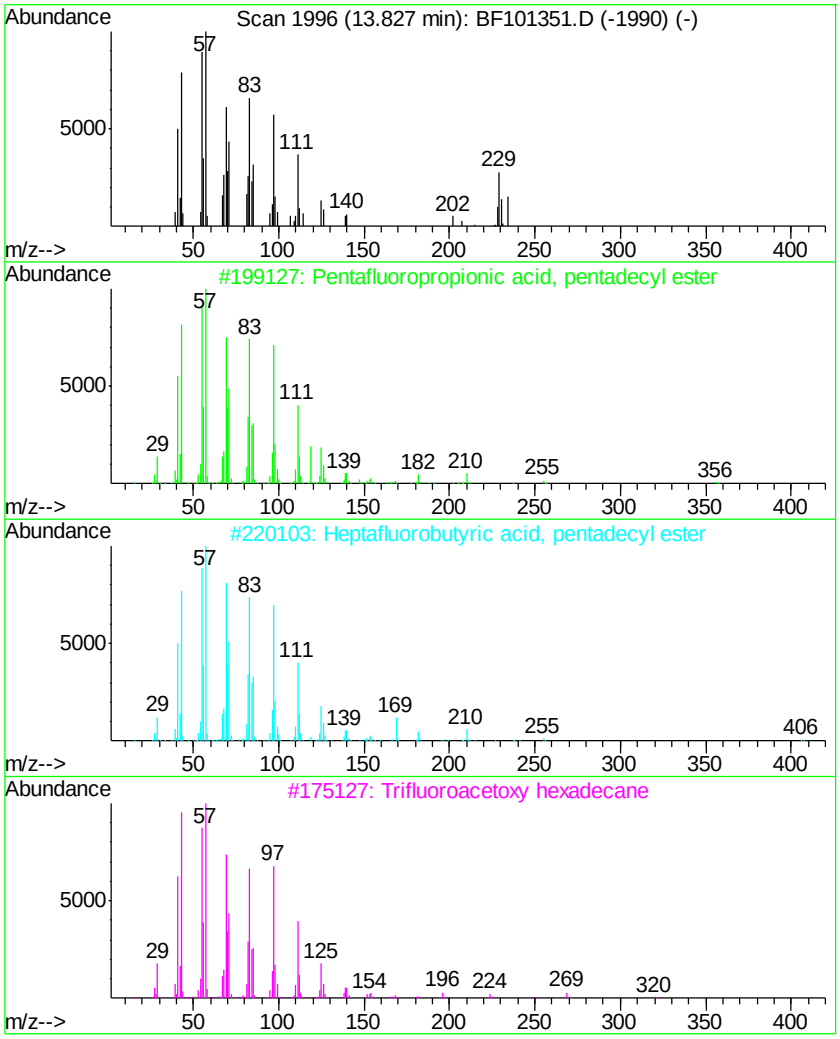
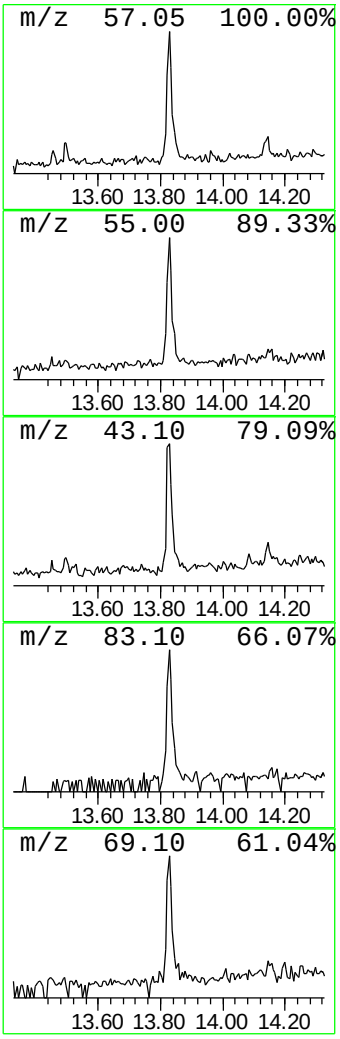
Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.54 ng	89256	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	92





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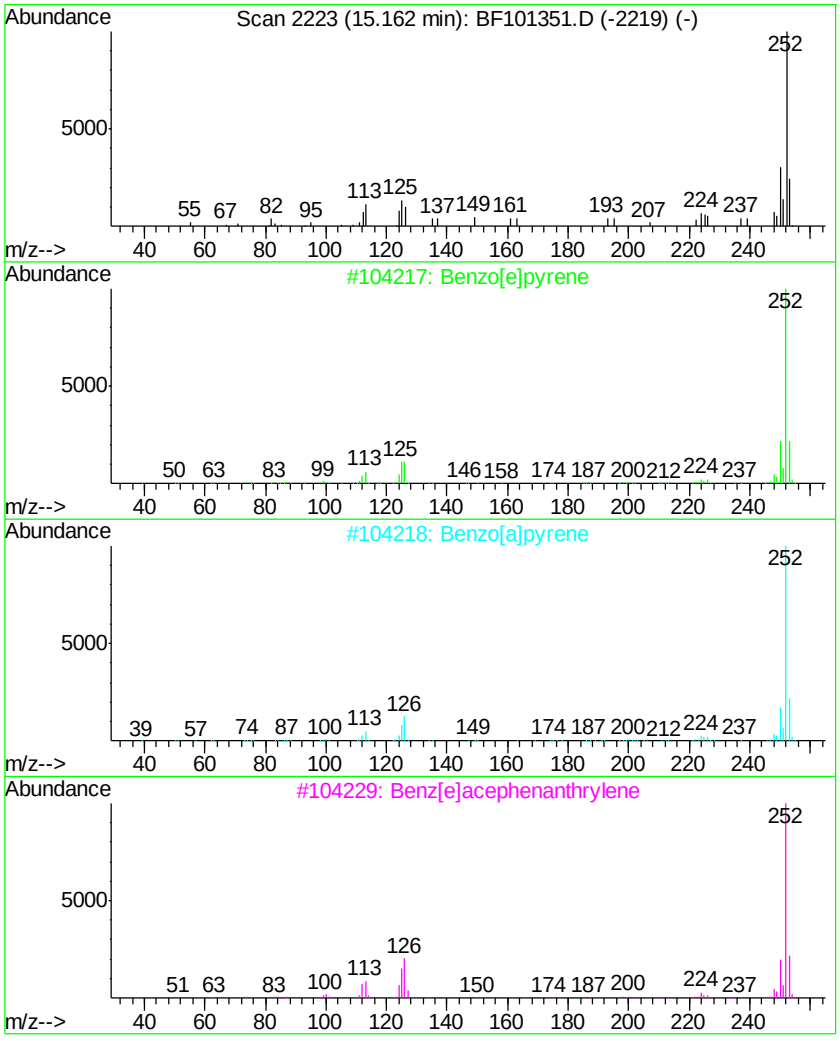
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

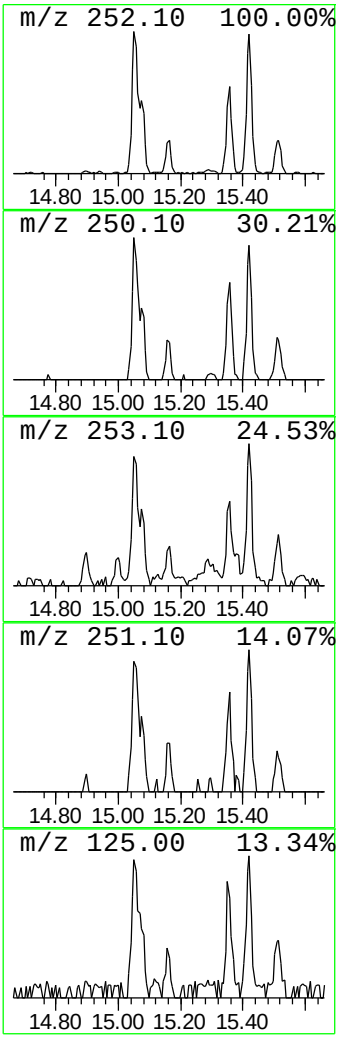
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.30 ng	27522	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	81
2	Benzo[a]pyrene	252	C20H12	000050-32-8	76
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	70
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	68
5	Perylene	252	C20H12	000198-55-0	59





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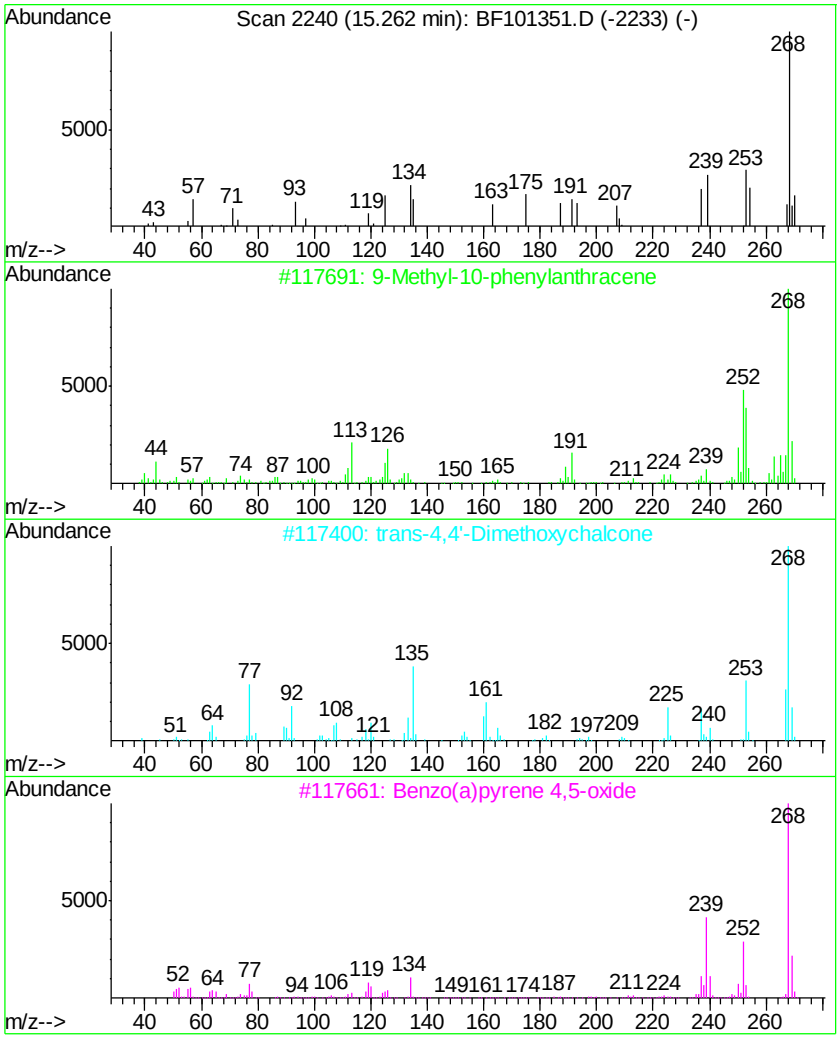
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

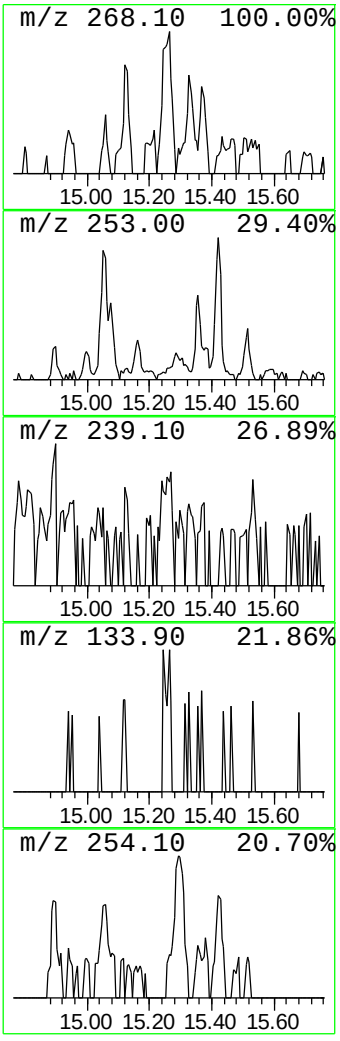
****

Peak Number 6 unknown15.26 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	2.06 ng	24685	Perylene-d12	15.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Methyl-10-phenylanthracene	268	C21H16	013425-08-6	46
2	trans-4,4'-Dimethoxychalcone	268	C17H16O3	041564-67-4	43
3	Benzo(a)pyrene 4,5-oxide	268	C20H12O	037574-47-3	43
4	Dinaphtho[1,2-b:1',2'-d]furan	268	C20H12O	000207-93-2	38
5	2-Hydroxy-4,5-methylenedioxy-2-(...	268	C16H12O4	1000284-51-7	38





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
2-Pentanone, 4-hy...	5.05	5.9	ng	79754	1	6.82	271102	20.0
unknown6.60	6.60	84.6	ng	1146640	1	6.82	271102	20.0
Pentafluoropropio...	13.83	4.5	ng	89256	5	14.00	393467	20.0
Benzo[e]pyrene	15.16	2.3	ng	27522	6	15.48	239476	20.0
unknown15.26	15.26	2.1	ng	24685	6	15.48	239476	20.0