LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122817\
Data File : BF101805.D
Acq On : 28 Dec 2017 16:31
Operator : SJ/JU
Sample : I6970-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-0-5

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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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	5.004	492	496	516	rBV	300901	560550	16.93%	1.831%
2	5.410	561	565	590	rBV	2379755	3285647	99.24%	10.732%
3	6.433	735	739	756	rBV	2587311	3310972	100.00%	10.815%
4	6.557	756	760	777	rVB	3050278	3114323	94.06%	10.173%
5	6.781	795	798	807	rBV	850174	855073	25.83%	2.793%
6	6.939	821	825	846	rBV	2189974	2407734	72.72%	7.865%
7	7.357	892	896	914	rBV	1757710	2024752	61.15%	6.614%
8	7.510	919	922	931	rVB	27460	34907	1.05%	0.114%
9	8.063	1013	1016	1032	rBV	1025596	1122956	33.92%	3.668%
10	9.139	1195	1199	1207	rBV	3049547	2877433	86.91%	9.399%
11	9.204	1207	1210	1214	rVB	35123	34305	1.04%	0.112%
12	9.539	1264	1267	1272	rVB	113294	111300	3.36%	0.364%
13	9.733	1297	1300	1303	rVB	76455	56012	1.69%	0.183%
14	9.821	1311	1315	1318	rBV	1095215	1021432	30.85%	3.336%
15	9.851	1318	1320	1327	rVB	64123	72323	2.18%	0.236%
16	10.233	1382	1385	1388	rVB	87830	67716	2.05%	0.221%
17	10.374	1406	1409	1415	rVB	51215	49618	1.50%	0.162%
18	10.451	1415	1422	1425	rBV3	41558	73975	2.23%	0.242%
19	10.616	1447	1450	1462	rBV	1419568	1517821	45.84%	4.958%
20	10.704	1462	1465	1474	rVB	96213	122331	3.69%	0.400%
21	10.921	1495	1502	1505	rBV5	24919	50093	1.51%	0.164%
22	11.151	1538	1541	1543	rBV2	50682	51567	1.56%	0.168%
23	11.310	1565	1568	1571	rBV	932535	928191	28.03%	3.032%
24	11.339	1571	1573	1577	rVV	432663	400223	12.09%	1.307%
25	11.392	1579	1582	1589	rVB	100963	120130	3.63%	0.392%
26	11.574	1608	1613	1616	rBV7	27817	41424	1.25%	0.135%
27	11.815	1651	1654	1657	rBV	104778	124446	3.76%	0.406%
28	11.845	1657	1659	1663	rVB	102778	93580	2.83%	0.306%
29	11.927	1670	1673	1676	rBV	112928	133033	4.02%	0.435%
30	11.951	1676	1677	1681	rVB	67165	49888	1.51%	0.163%
31	12.110	1701	1704	1713	rBV	58779	71199	2.15%	0.233%
32	12.368	1744	1748	1751	rBV2	55127	68881	2.08%	0.225%
33	12.533	1772	1776	1780	rBV	416695	386269	11.67%	1.262%
34	12.686	1800	1802	1809	rVB4	22895	33757	1.02%	0.110%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6970-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-0-5

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:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.762	1809	1815	1821	rBV	473386	513218	15.50%	1.676%
36	12.892	1833	1837	1840	rBV	2326360	2035159	61.47%	6.648%
37	12.986	1849	1853	1857	rVB2	32296	46029	1.39%	0.150%
38	13.092	1869	1871	1875	rVB2	68578	69240	2.09%	0.226%
39	13.157	1880	1882	1886	rVB	45908	39781	1.20%	0.130%
40	13.198	1886	1889	1892	rBV2	41626	44986	1.36%	0.147%
41	13.292	1902	1905	1907	rBV	37043	34610	1.05%	0.113%
42	13.768	1983	1986	1993	rBV3	112530	158203	4.78%	0.517%
43	13.962	2014	2019	2022	rBV2	869515	1018723	30.77%	3.328%
44	13.992	2022	2024	2032	rVB	185194	190258	5.75%	0.621%
45	15.015	2194	2198	2201	rBV	134873	189552	5.72%	0.619%
46	15.315	2246	2249	2253	rVB	73300	88564	2.67%	0.289%
47	15.380	2256	2260	2265	rBV	136596	172974	5.22%	0.565%
48	15.433	2265	2269	2279	rBV2	534706	739032	22.32%	2.414%

Sum of corrected areas: 30614190

LSC Report - Integrated Chromatogram

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Data File : BF101805.D
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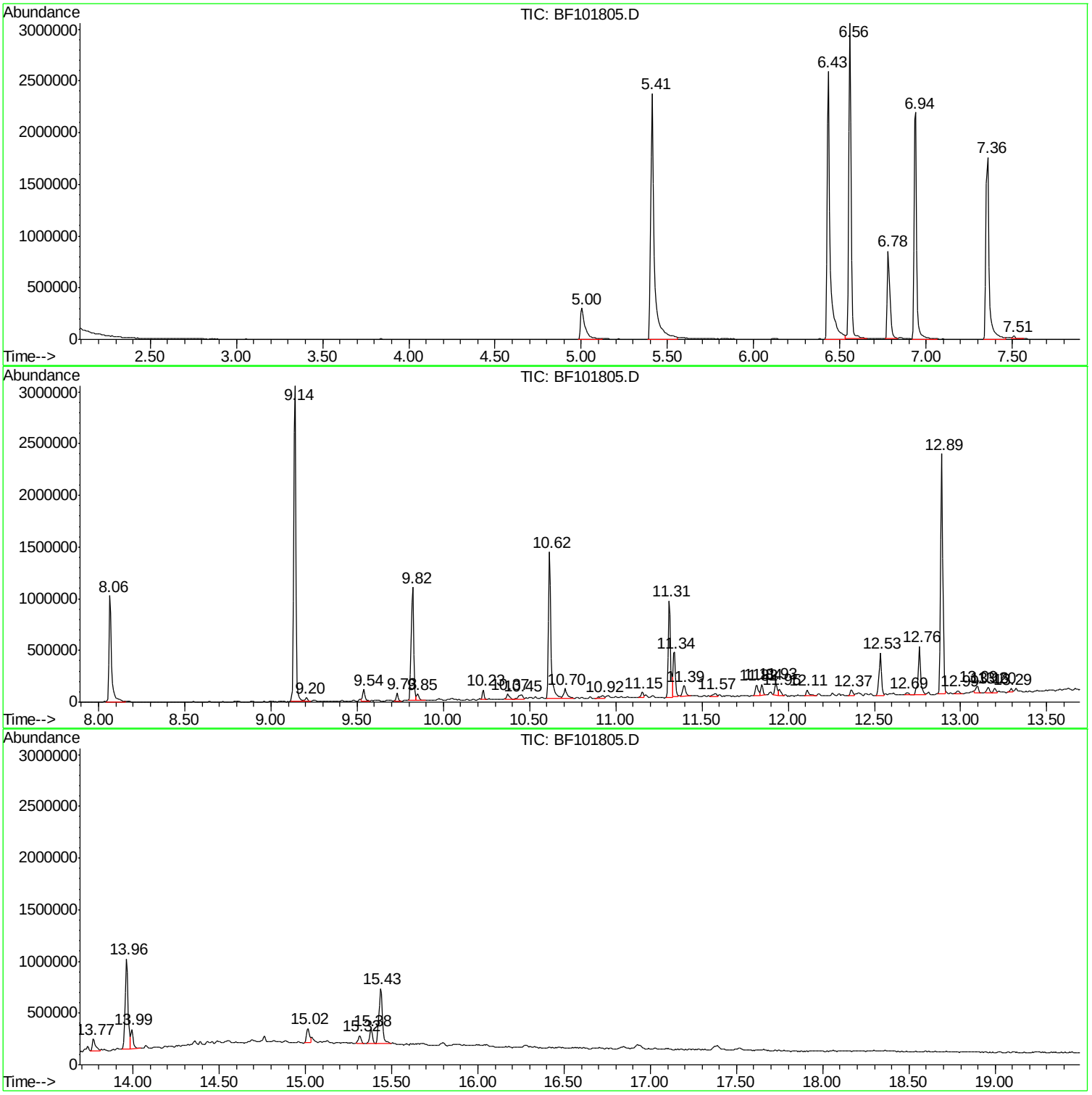
Operator : SJ/JU
Sample : I6970-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF122817\
Data File : BF101805.D
Acq On : 28 Dec 2017 16:31
Operator : SJ/JU
Sample : I6970-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

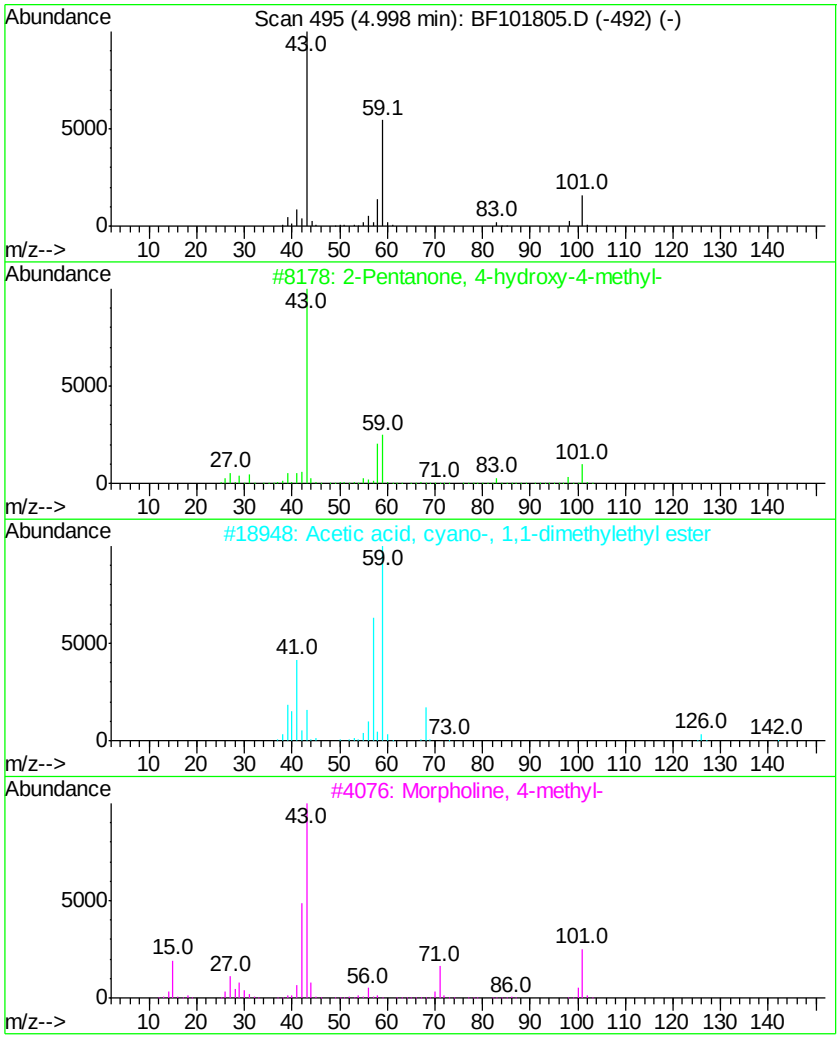
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

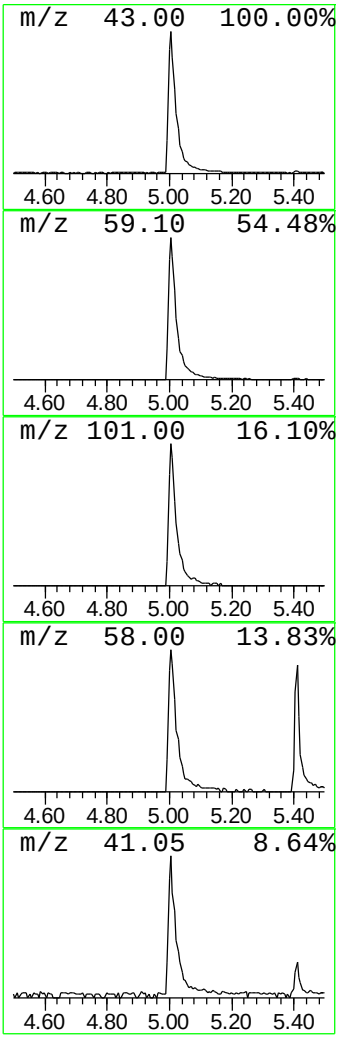
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	13.11 ng	560550	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122817\
Data File : BF101805.D
Acq On : 28 Dec 2017 16:31
Operator : SJ/JU
Sample : I6970-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

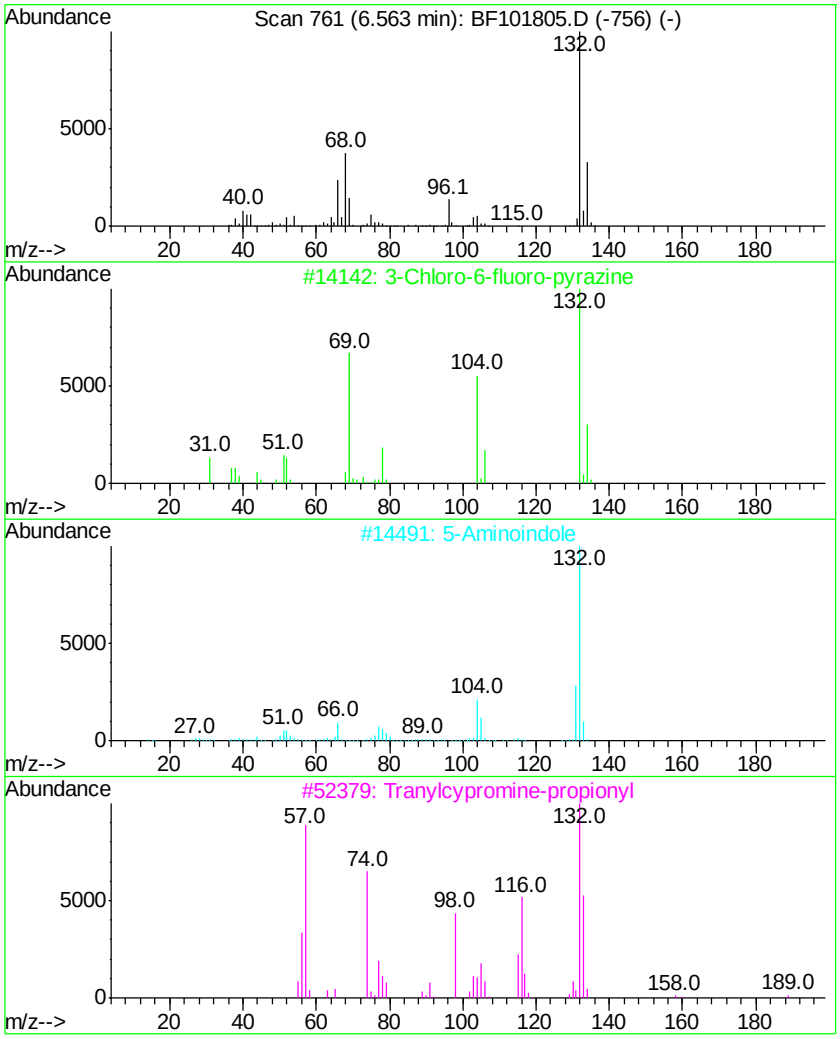
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

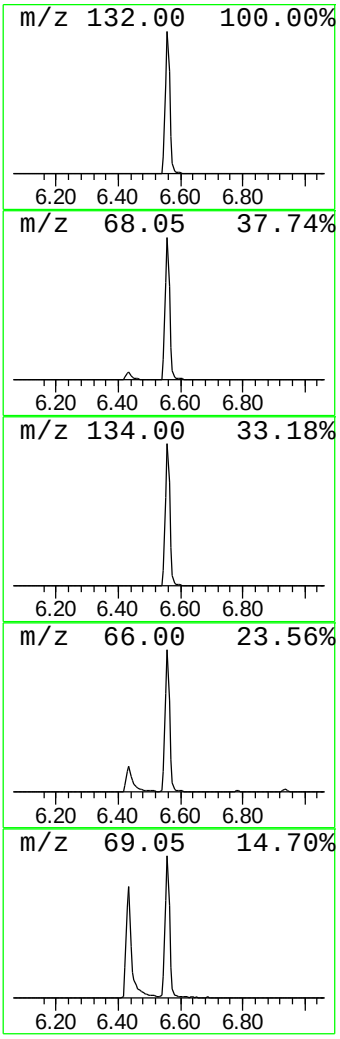
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	72.84 ng	3114320	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122817\
Data File : BF101805.D
Acq On : 28 Dec 2017 16:31
Operator : SJ/JU
Sample : I6970-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

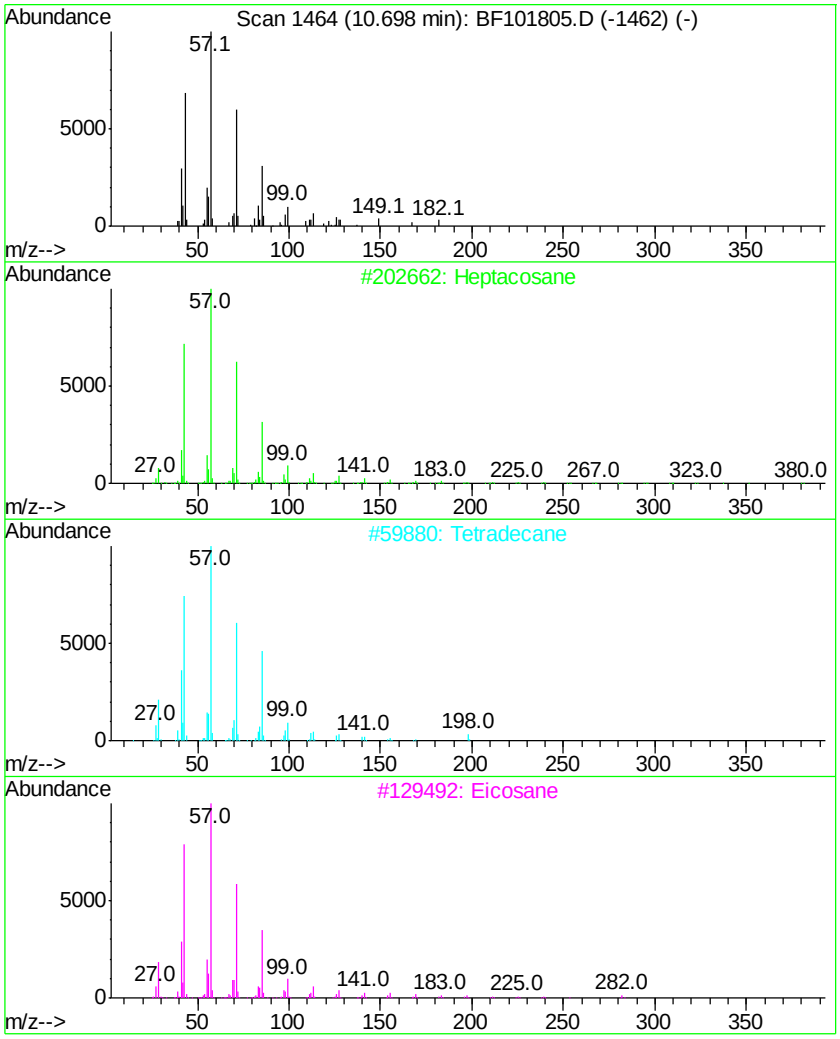
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

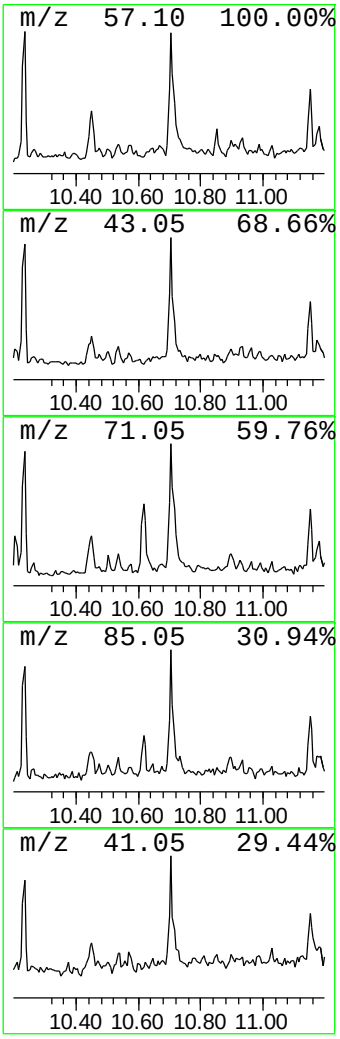
****

Peak Number 4 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.64 ng	122331	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Eicosane	282	C20H42	000112-95-8	86
4	Tridecane	184	C13H28	000629-50-5	78
5	Hexadecane	226	C16H34	000544-76-3	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122817\
Data File : BF101805.D
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Sample : I6970-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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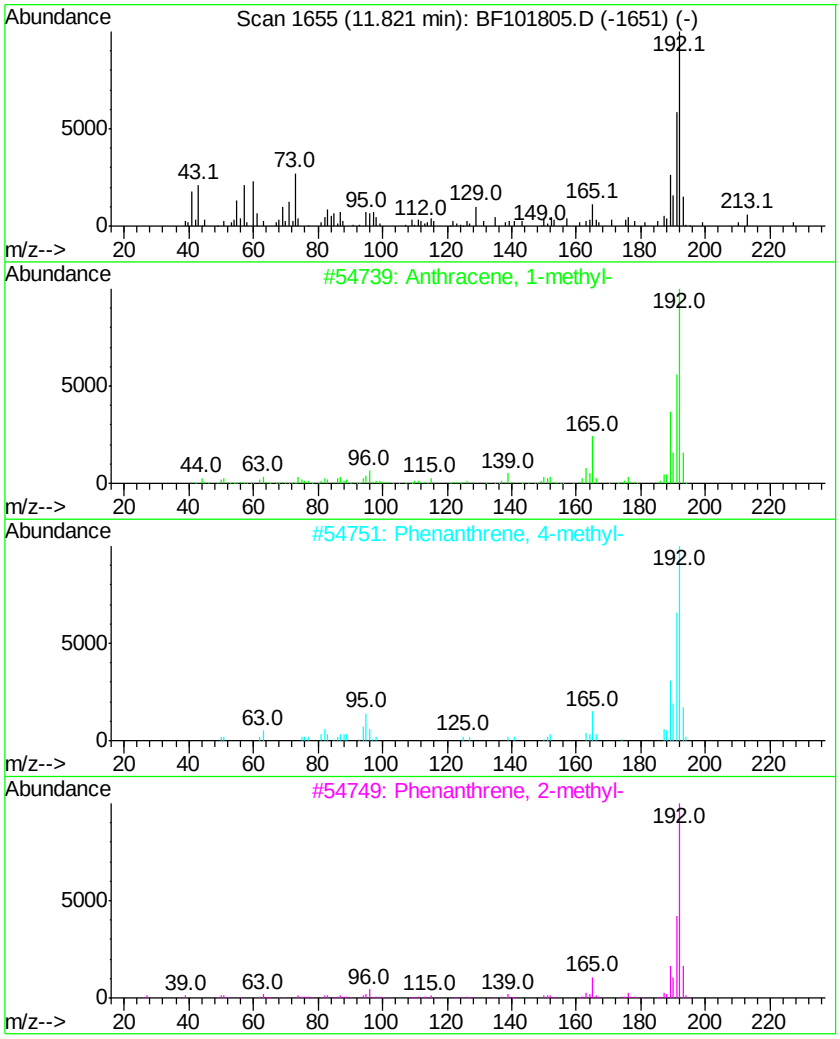
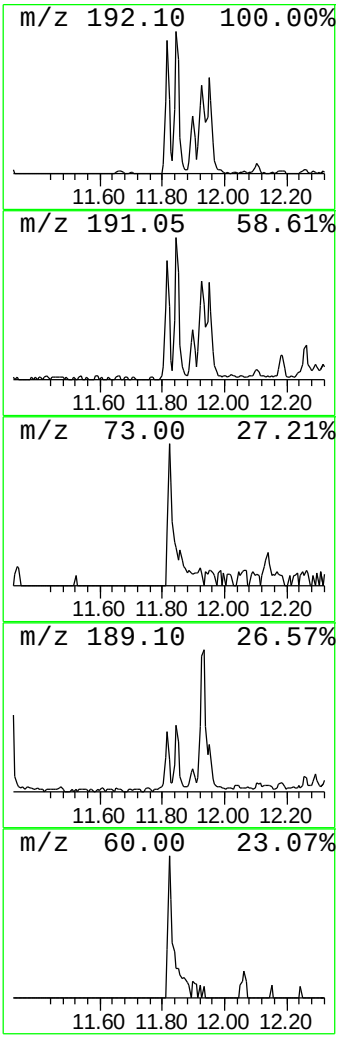
Peak Number 5 Anthracene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.68 ng	124446	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	89
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	87





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Sample : I6970-06
Misc :
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Instrument : BNA_F
ClientSampleId : S6-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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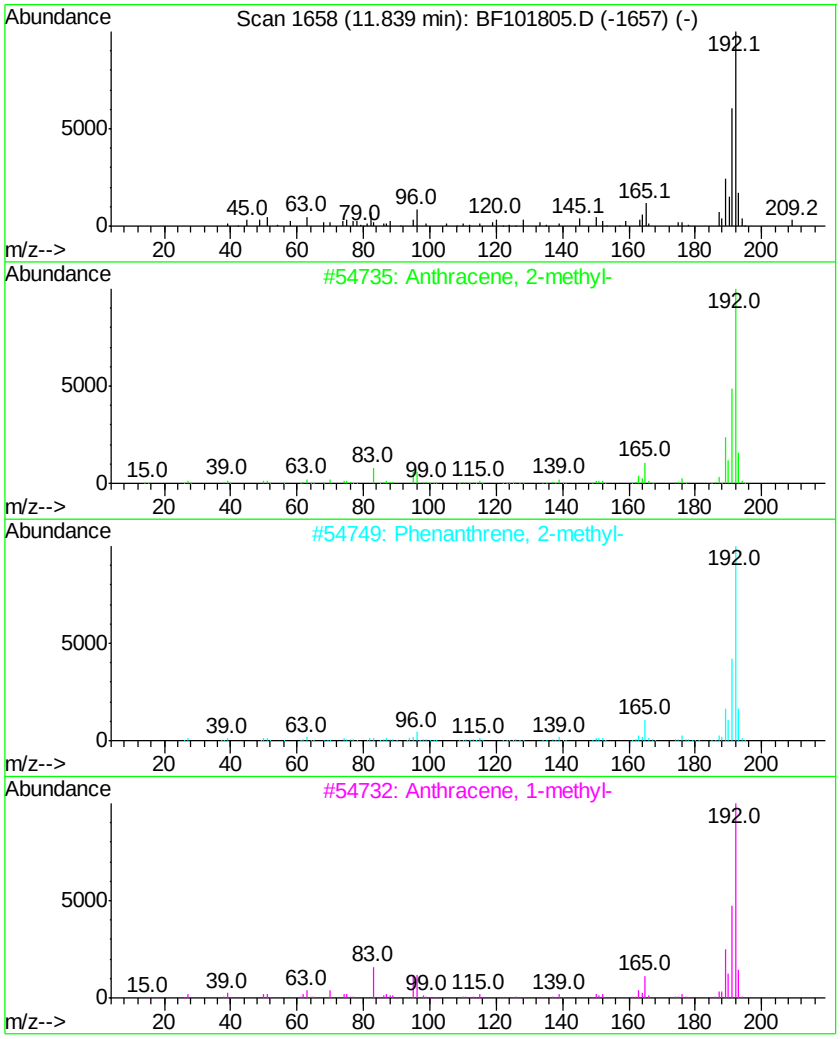
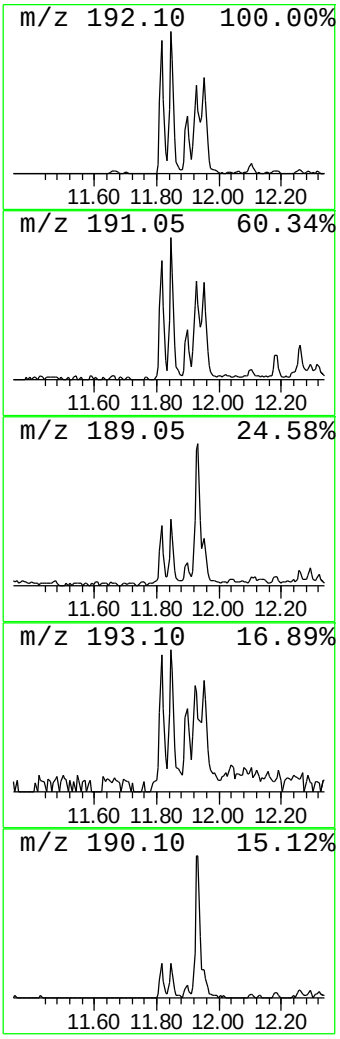
****

Peak Number 6 Anthracene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.02 ng	93580	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90





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Misc :
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Instrument : BNA_F
ClientSampleId : S6-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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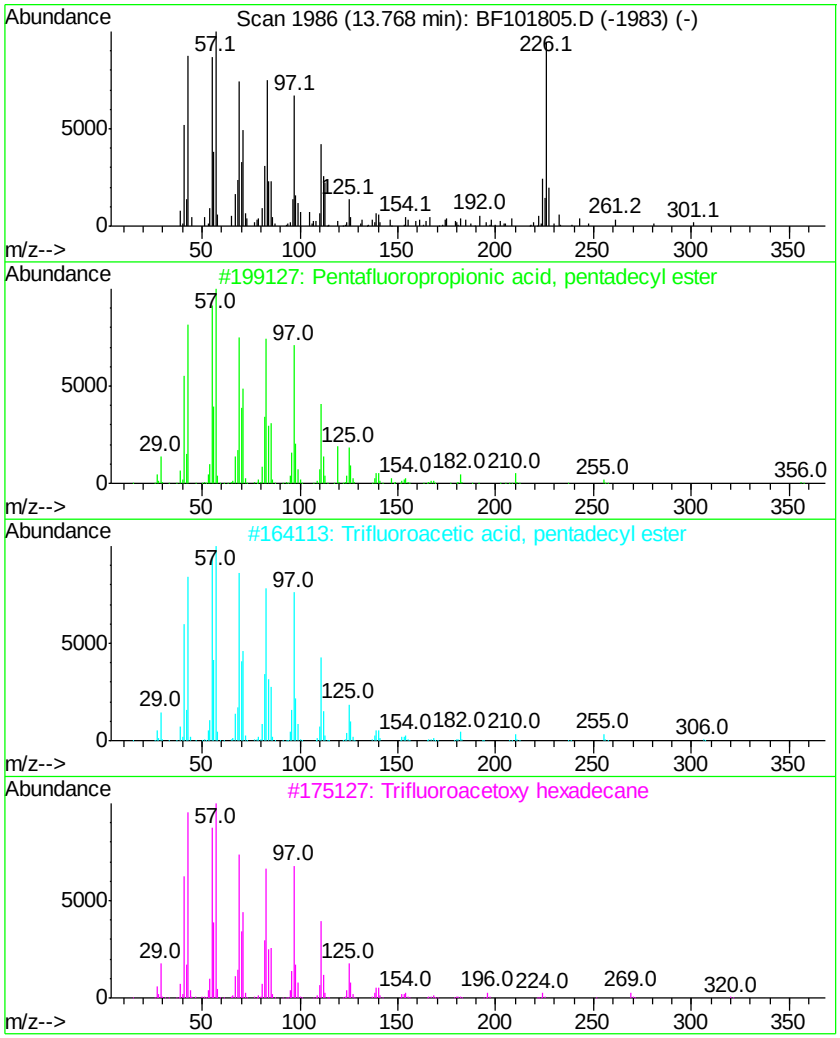
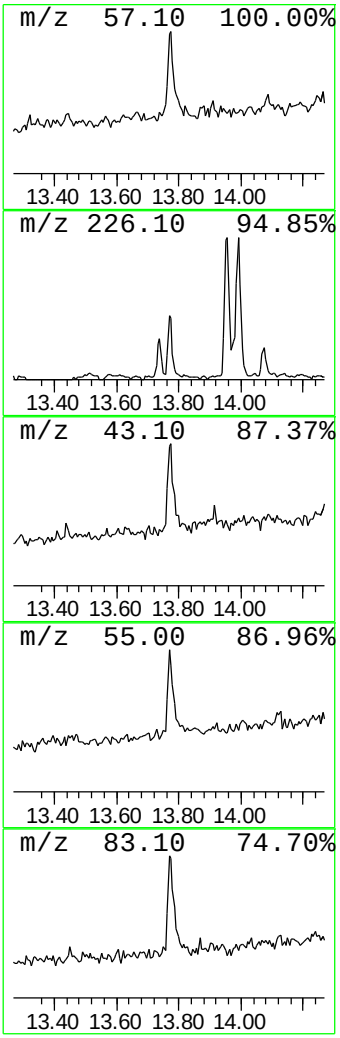
Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	3.11 ng	158203	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	83
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	83
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	64
4	Behenic alcohol	326	C22H46O	000661-19-8	60
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122817\
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Operator : SJ/JU
Sample : I6970-06
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.00	13.1	ng	560550	1	6.78	855073	20.0
unknown6.56	6.56	72.8	ng	3114320	1	6.78	855073	20.0
Heptacosane	10.70	2.6	ng	122331	4	11.31	928191	20.0
Anthracene, 1-met...	11.82	2.7	ng	124446	4	11.31	928191	20.0
Anthracene, 2-met...	11.84	2.0	ng	93580	4	11.31	928191	20.0
Pentafluoropropio...	13.77	3.1	ng	158203	5	13.96	1018720	20.0