LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112717\
Data File : BF100893.D
Acq On : 27 Nov 2017 15:46
Operator : SJ/JU
Sample : I6570-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P003-S003-0001-01

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-BF110817.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	2.475	61	66	72	rVB2	13421	22589	1.19%	0.148%
2	5.087	506	510	517	rBV	86221	112890	5.94%	0.738%
3	5.475	571	576	579	rBV	1488978	1453969	76.47%	9.505%
4	6.487	743	748	751	rBV	1440694	1541795	81.08%	10.080%
5	6.628	767	772	775	rBV	1738184	1558311	81.95%	10.187%
6	6.857	807	811	814	rBV	543101	434102	22.83%	2.838%
7	7.016	833	838	841	rBV	1329142	1224628	64.40%	8.006%
8	7.422	902	907	910	rBV	1026725	967171	50.86%	6.323%
9	8.140	1024	1029	1032	rBV	706230	582059	30.61%	3.805%
10	9.216	1206	1212	1215	rBV	2087307	1901472	100.00%	12.431%
11	9.286	1221	1224	1227	rVB	28601	20535	1.08%	0.134%
12	9.604	1274	1278	1281	rBV	223988	174717	9.19%	1.142%
13	9.816	1307	1314	1317	rBV	78861	67074	3.53%	0.438%
14	9.892	1323	1327	1331	rBV2	748148	646357	33.99%	4.226%
15	10.316	1396	1399	1402	rVB	85175	61147	3.22%	0.400%
16	10.533	1431	1436	1439	rBV	17992	23203	1.22%	0.152%
17	10.686	1458	1462	1465	rBV	1135677	1076894	56.63%	7.040%
18	10.786	1476	1479	1488	rVB	56425	55483	2.92%	0.363%
19	11.380	1576	1580	1583	rBV	804281	653486	34.37%	4.272%
20	11.898	1664	1668	1672	rBV	35007	34865	1.83%	0.228%
21	12.969	1845	1850	1853	rBV	1662809	1665180	87.57%	10.886%
22	13.845	1996	1999	2008	rBV	152282	150780	7.93%	0.986%
23	14.016	2025	2028	2032	rBV	433649	423831	22.29%	2.771%
24	15.486	2273	2278	2287	rBV	332618	417126	21.94%	2.727%
25	15.980	2358	2362	2371	rBV6	13125	26658	1.40%	0.174%

Sum of corrected areas: 15296322

LSC Report - Integrated Chromatogram

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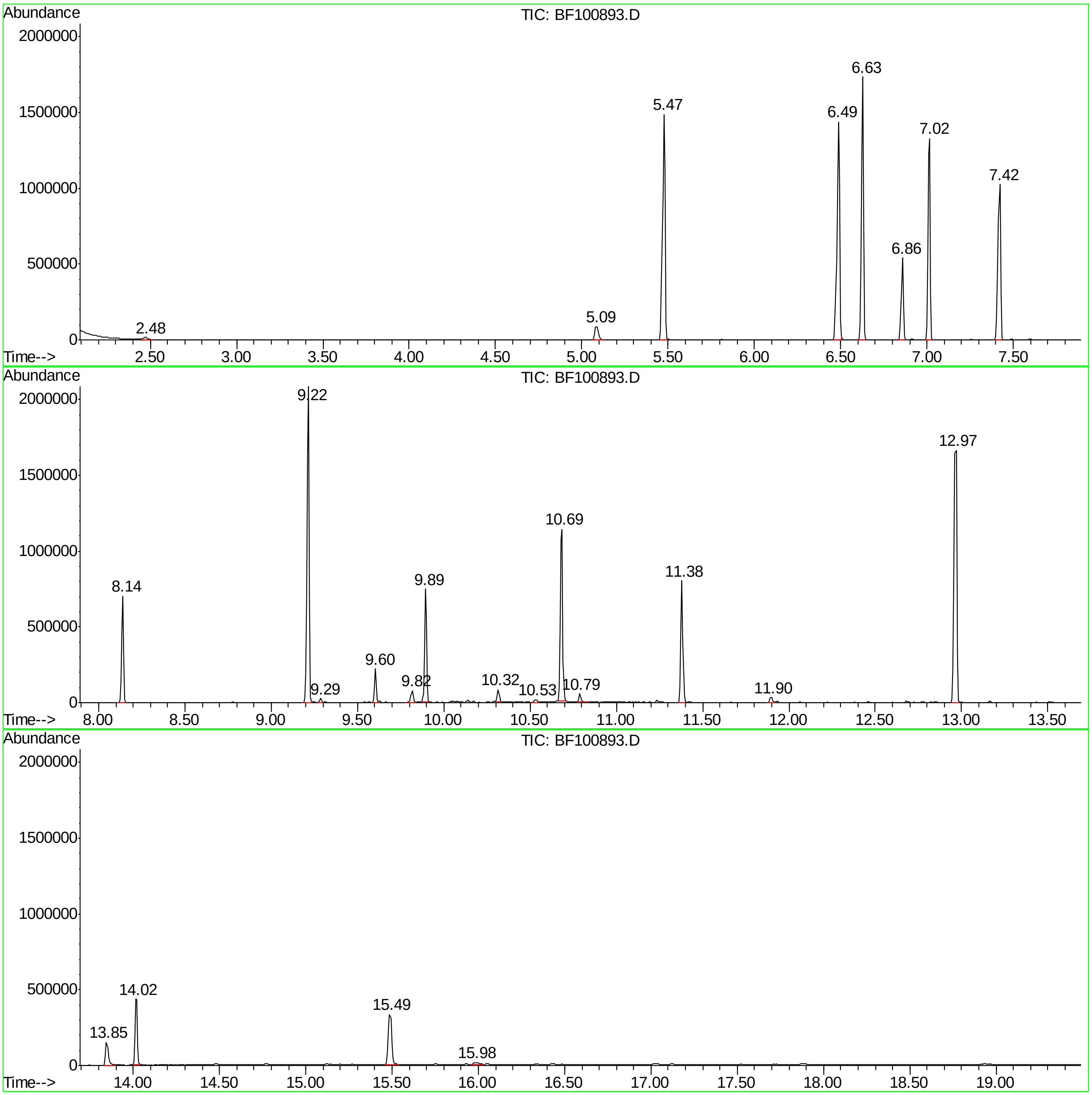
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Instrument :
BNA_F
ClientSampleId :
P003-S003-0001-01



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

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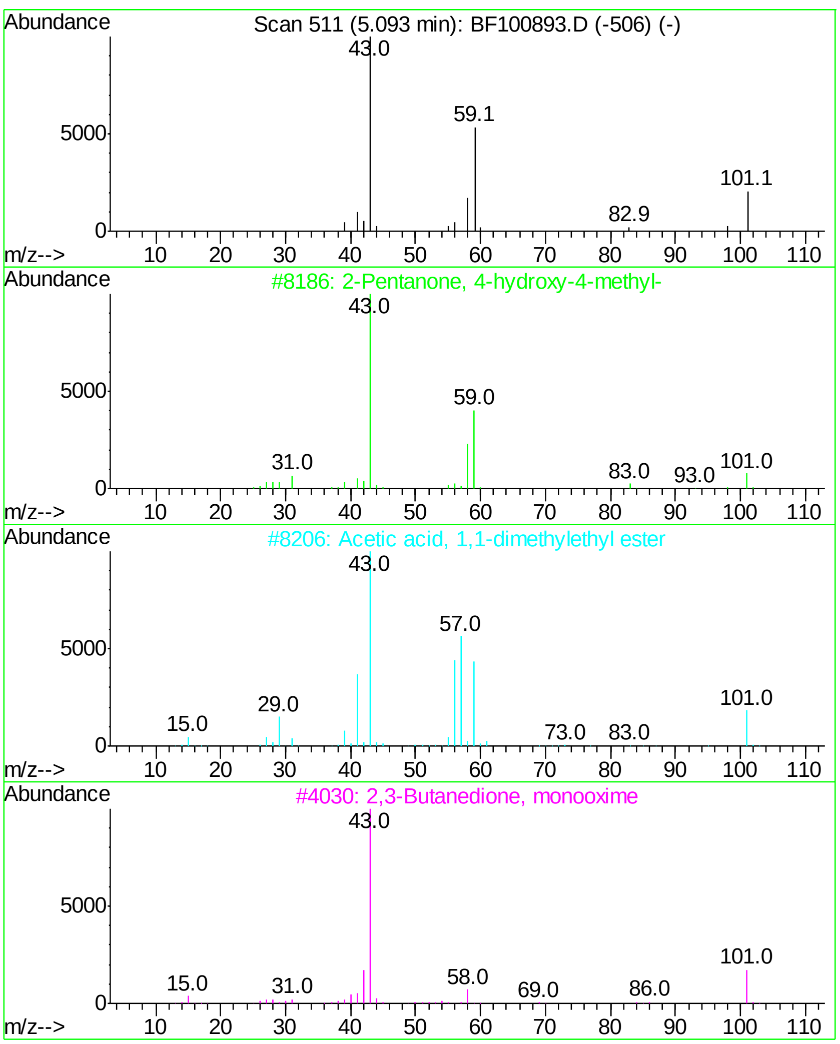
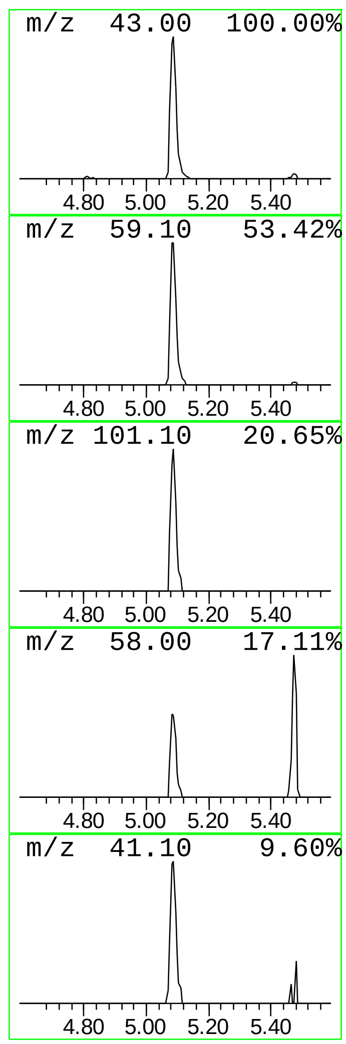
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.20 ng	112890	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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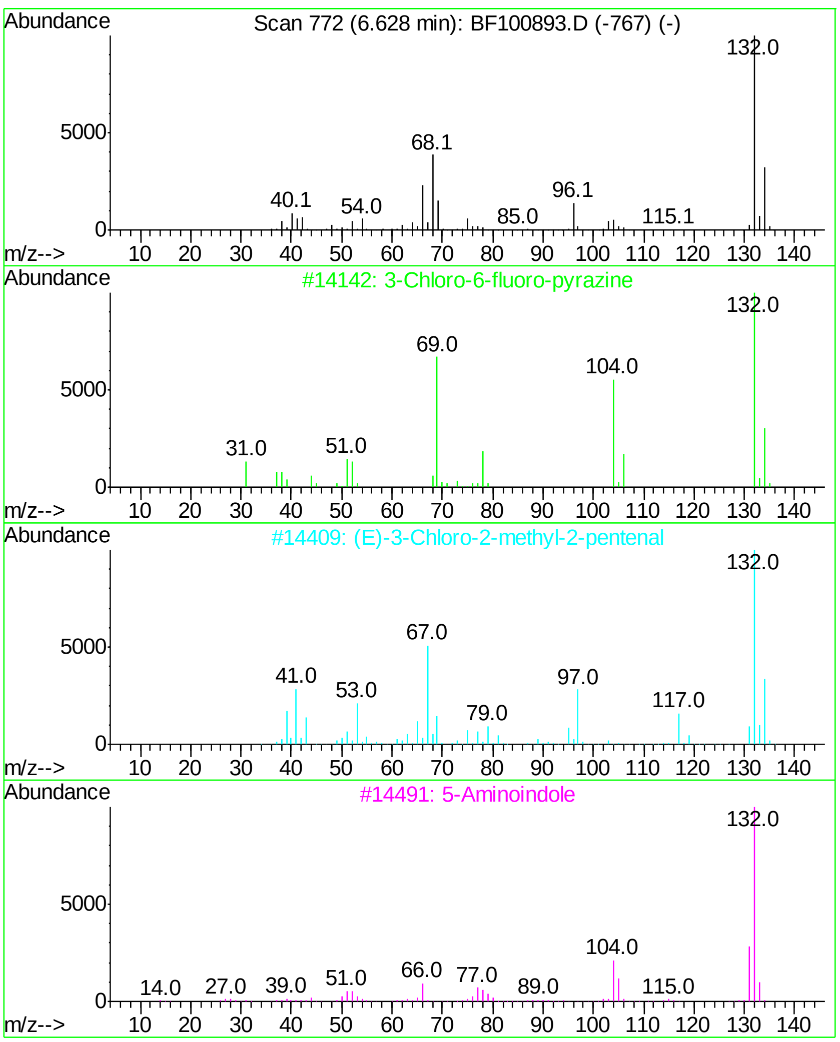
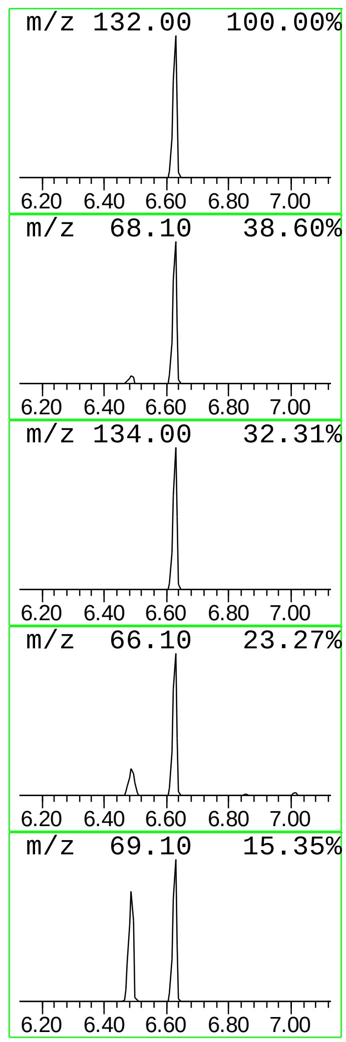
Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	71.79 ng	1558310	1,4-Dichlorobenzene-d4	6.86

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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BNA_F
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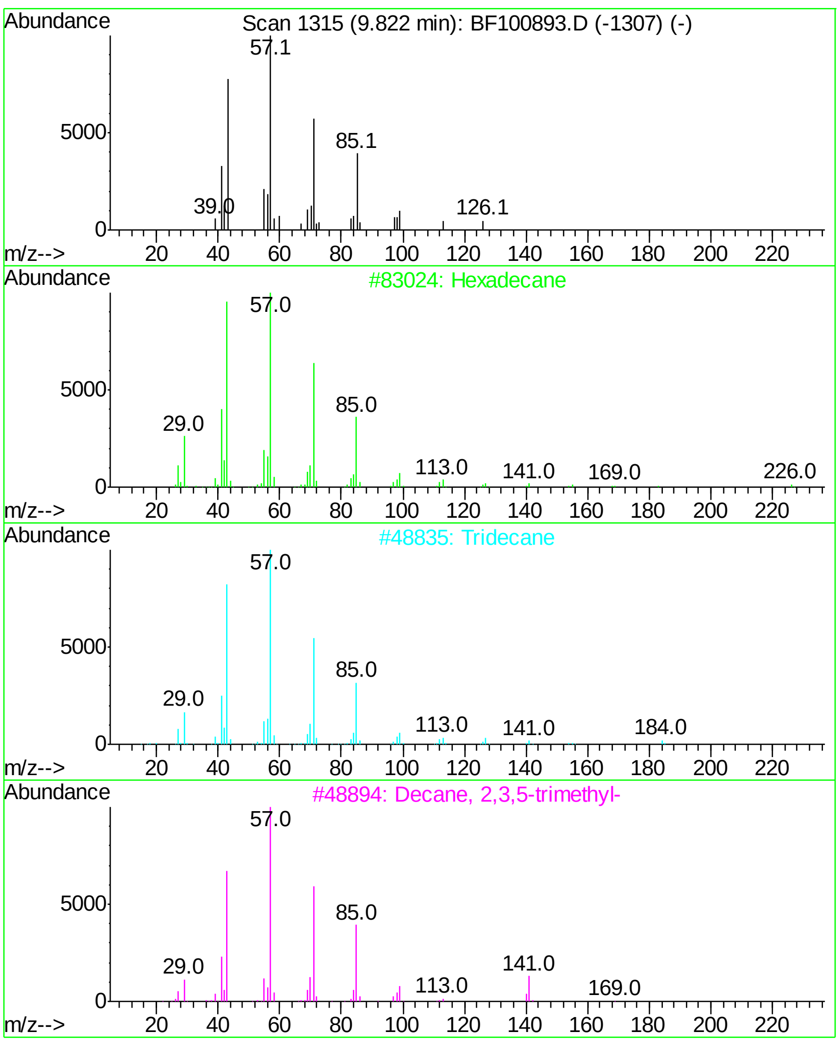
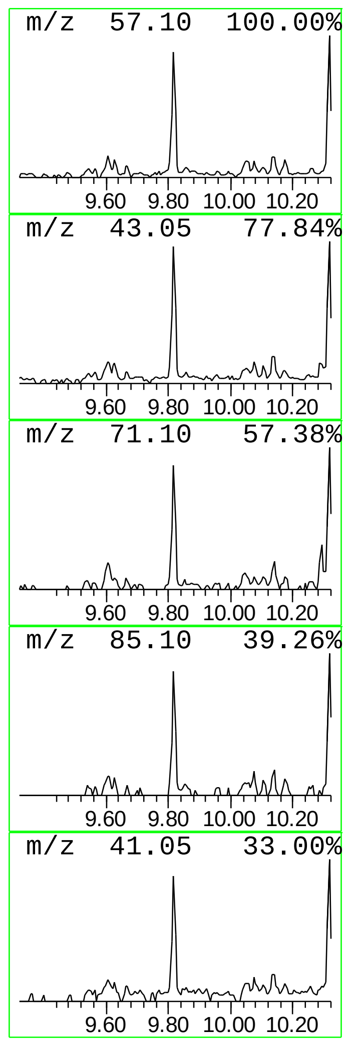
Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	2.08 ng	67074	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Tridecane	184	C13H28	000629-50-5	86
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
4	Tetradecane	198	C14H30	000629-59-4	80
5	Pentadecane	212	C15H32	000629-62-9	78





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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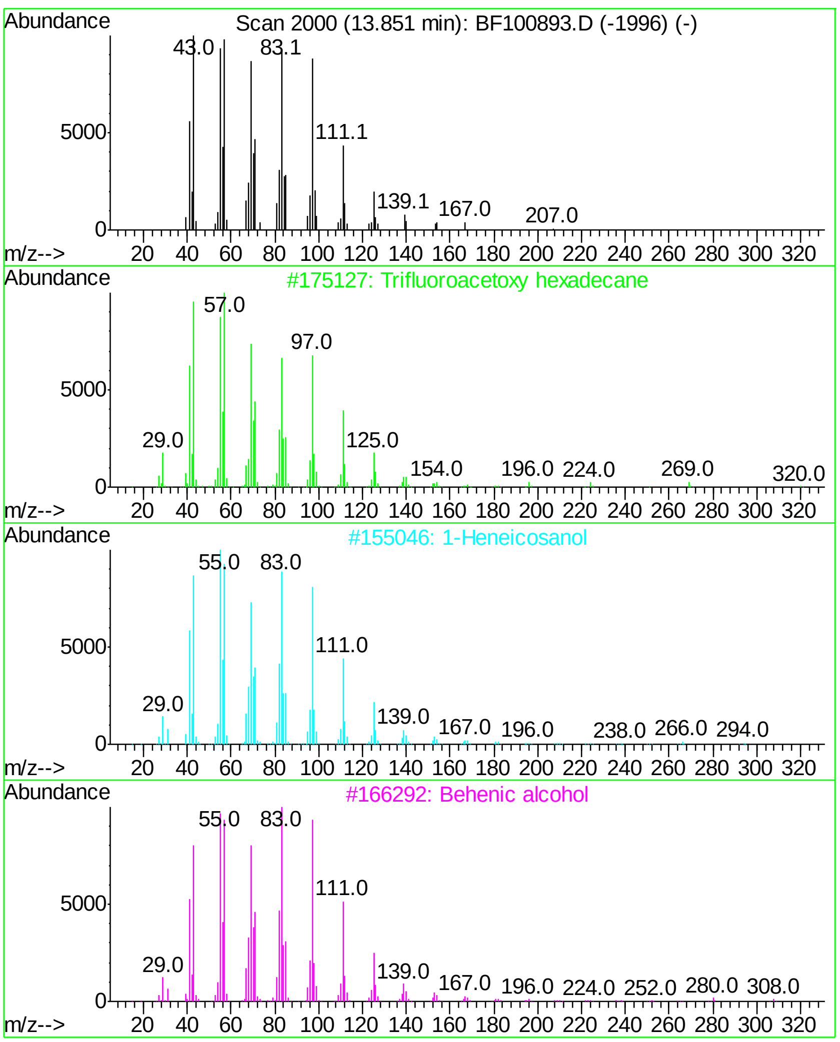
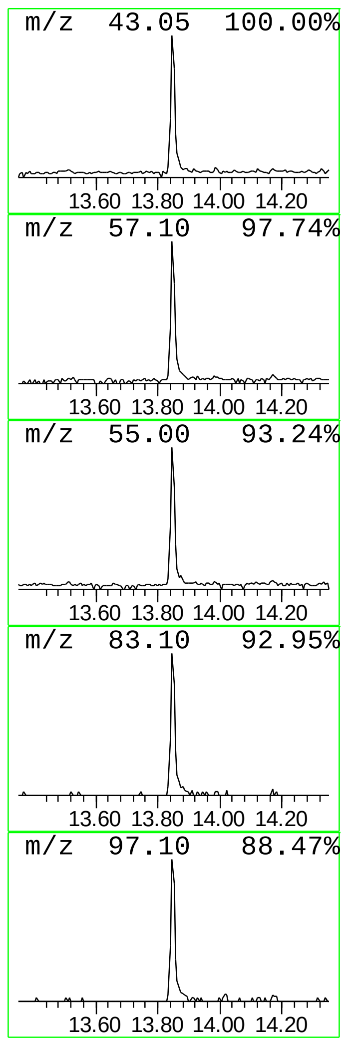
Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	7.12 ng	150780	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	92





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...	5.09	5.2	ng	112890	1	6.86	434102	20.0
unknown6.63	6.63	71.8	ng	1558310	1	6.86	434102	20.0
Hexadecane	9.82	2.1	ng	67074	3	9.89	646357	20.0
Trifluoroacetoxy ...	13.85	7.1	ng	150780	5	14.02	423831	20.0