LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096611.D
Acq On : 10 Jul 2017 19:58
Operator : SJ/JU
Sample : I4104-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : I4104-04

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-BF070117.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	4.875	469	474	488	rVB	411731	578615	21.48%	2.409%
2	5.298	541	546	549	rBV	2514150	2479350	92.02%	10.324%
3	6.322	715	720	723	rBV	2381714	2551233	94.69%	10.624%
4	6.451	737	742	745	rBV	2532902	2488965	92.38%	10.364%
5	6.681	777	781	785	rBV	829186	668312	24.80%	2.783%
6	6.839	803	808	811	rBV	2106695	1894751	70.32%	7.890%
7	7.239	871	876	880	rBV	1429696	1595011	59.20%	6.642%
8	7.963	994	999	1002	rBV	1023292	911614	33.84%	3.796%
9	9.039	1176	1182	1186	rBV	2574073	2694290	100.00%	11.219%
10	9.433	1245	1249	1252	rBV	351447	280228	10.40%	1.167%
11	9.716	1291	1297	1301	rBV	923995	965062	35.82%	4.019%
12	10.163	1369	1373	1376	rVB	37498	32680	1.21%	0.136%
13	10.498	1425	1430	1441	rVB	1571504	1573258	58.39%	6.551%
14	10.633	1450	1453	1461	rVB	50685	60219	2.24%	0.251%
15	11.192	1543	1548	1551	rBV	1050870	915366	33.97%	3.812%
16	11.733	1636	1640	1643	rBV	44375	41438	1.54%	0.173%
17	12.780	1812	1818	1821	rBV	2153799	2313436	85.86%	9.633%
18	13.474	1931	1936	1940	rBV	48819	49624	1.84%	0.207%
19	13.680	1962	1971	1977	rBV	201162	250255	9.29%	1.042%
20	13.733	1977	1980	1986	rVB	46888	48464	1.80%	0.202%
21	13.815	1990	1994	1998	rBV	856993	801901	29.76%	3.339%
22	13.968	2011	2020	2022	rBV5	12653	27128	1.01%	0.113%
23	14.315	2074	2079	2085	rBV2	71267	120173	4.46%	0.500%
24	14.915	2177	2181	2183	rBV2	29330	36835	1.37%	0.153%
25	14.939	2183	2185	2191	rVB3	32150	42652	1.58%	0.178%
26	15.210	2226	2231	2237	rBV	441442	548986	20.38%	2.286%
27	15.704	2311	2315	2322	rVB6	25131	45087	1.67%	0.188%

Sum of corrected areas: 24014933

LSC Report - Integrated Chromatogram

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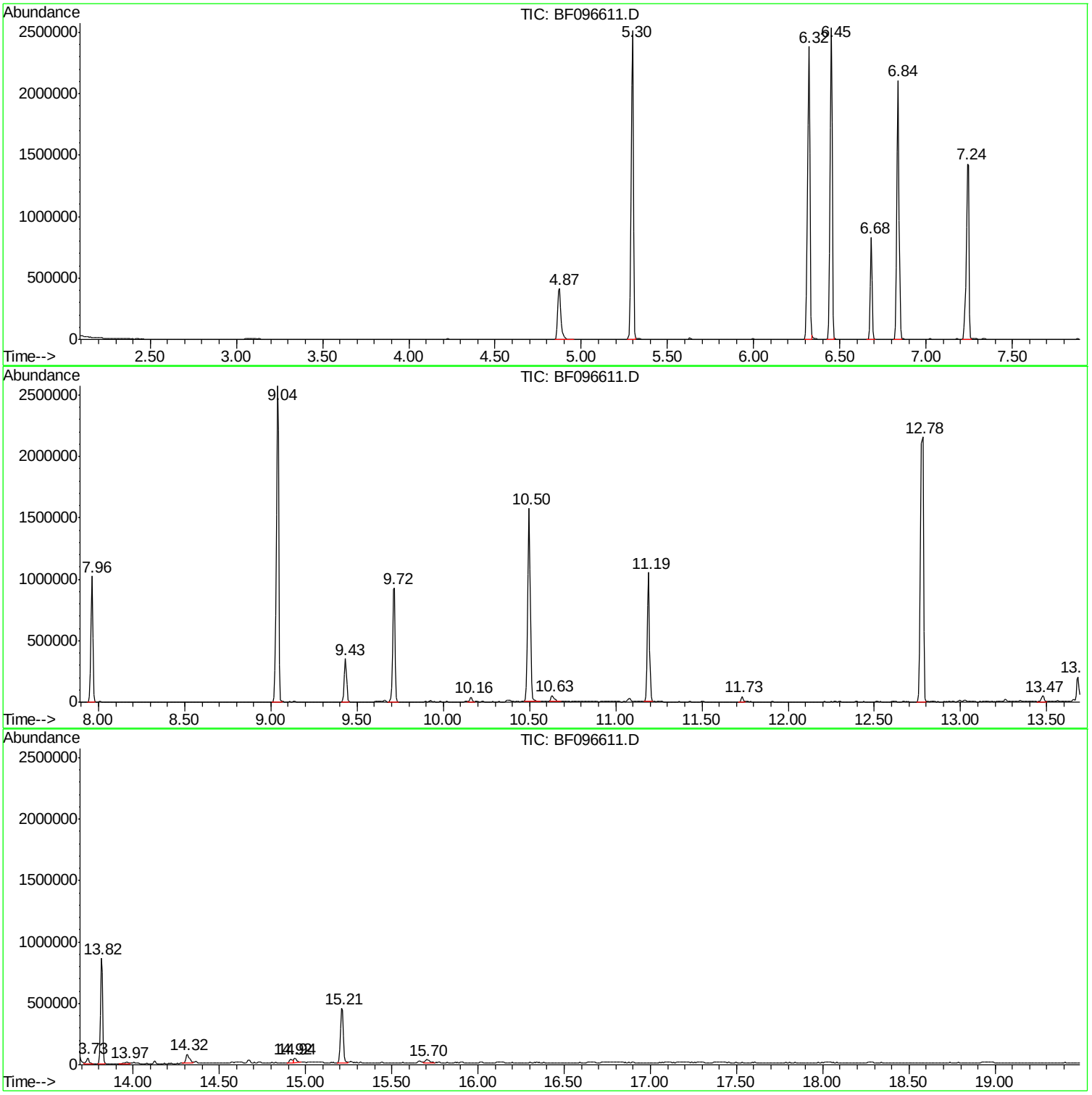
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : I4104-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF071017\
Data File : BF096611.D
Acq On : 10 Jul 2017 19:58
Operator : SJ/JU
Sample : I4104-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : I4104-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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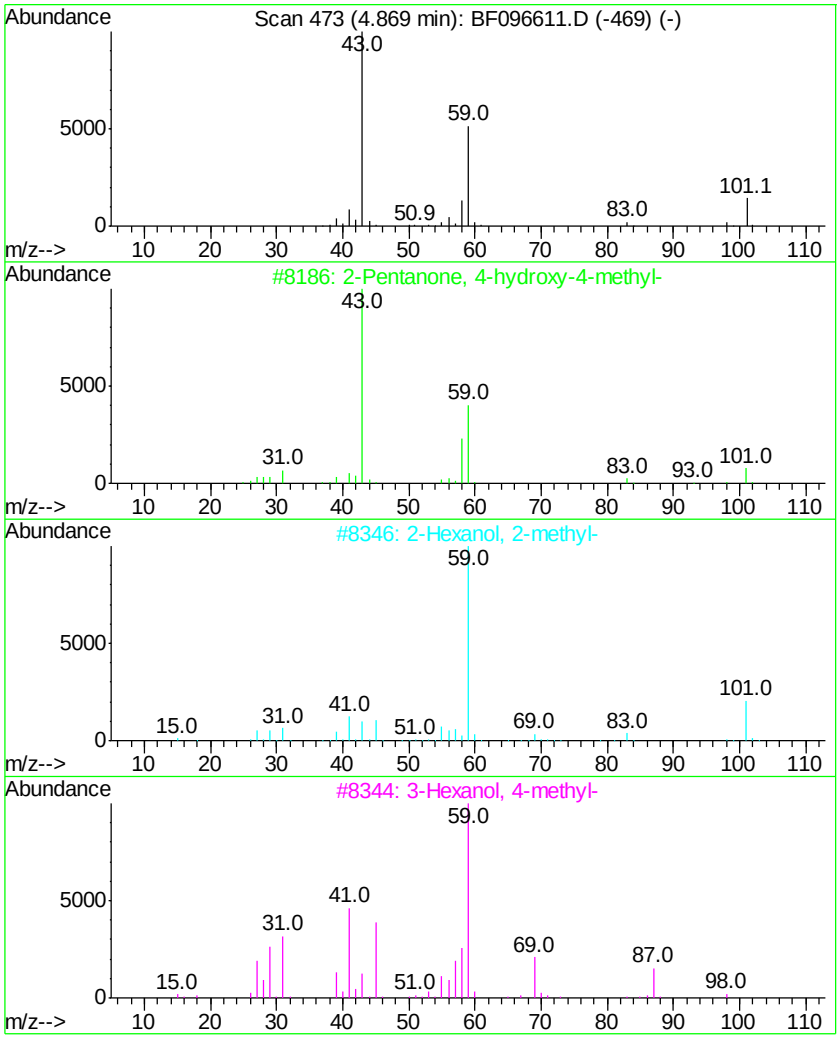
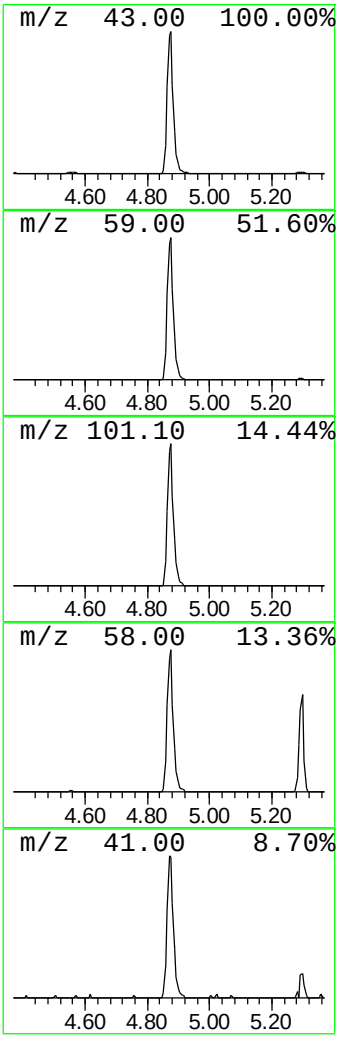
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	17.32 ng	578615	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096611.D
Acq On : 10 Jul 2017 19:58
Operator : SJ/JU
Sample : I4104-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : I4104-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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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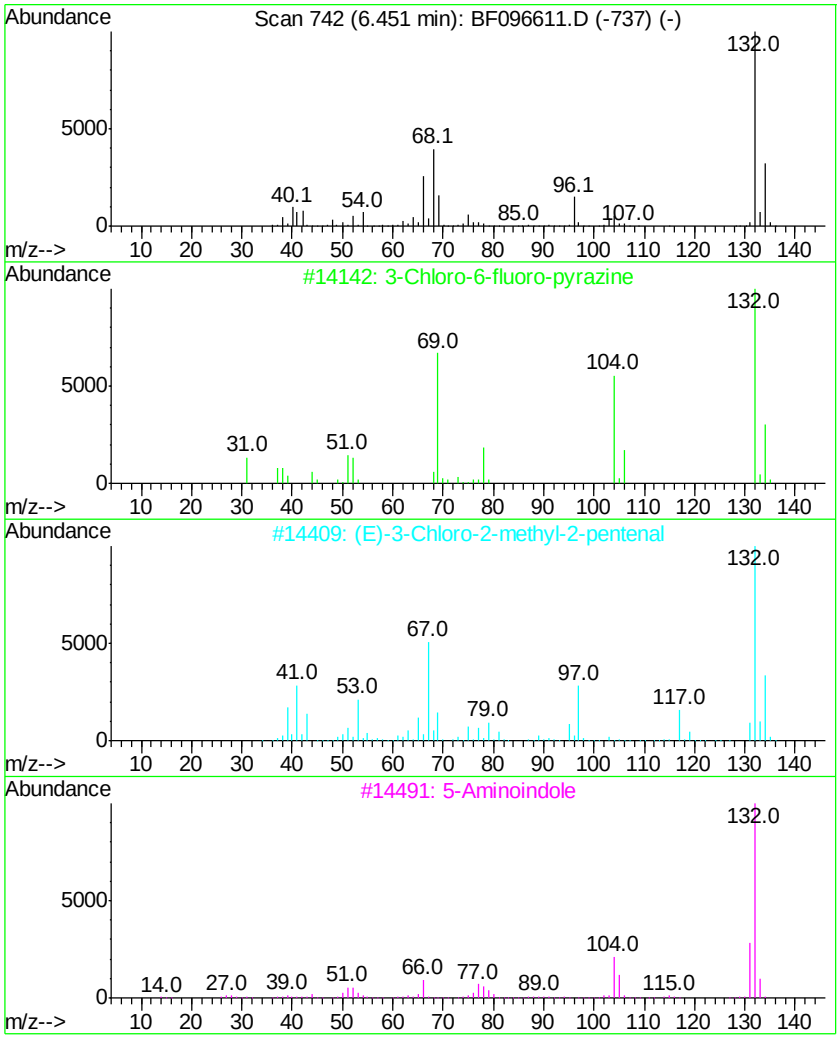
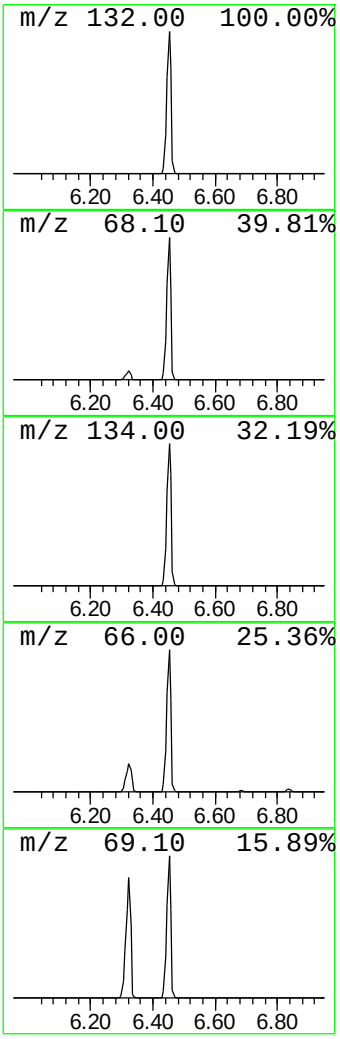
Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	74.49 ng	2488970	1,4-Dichlorobenzene-d4	6.68

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Sample : I4104-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : I4104-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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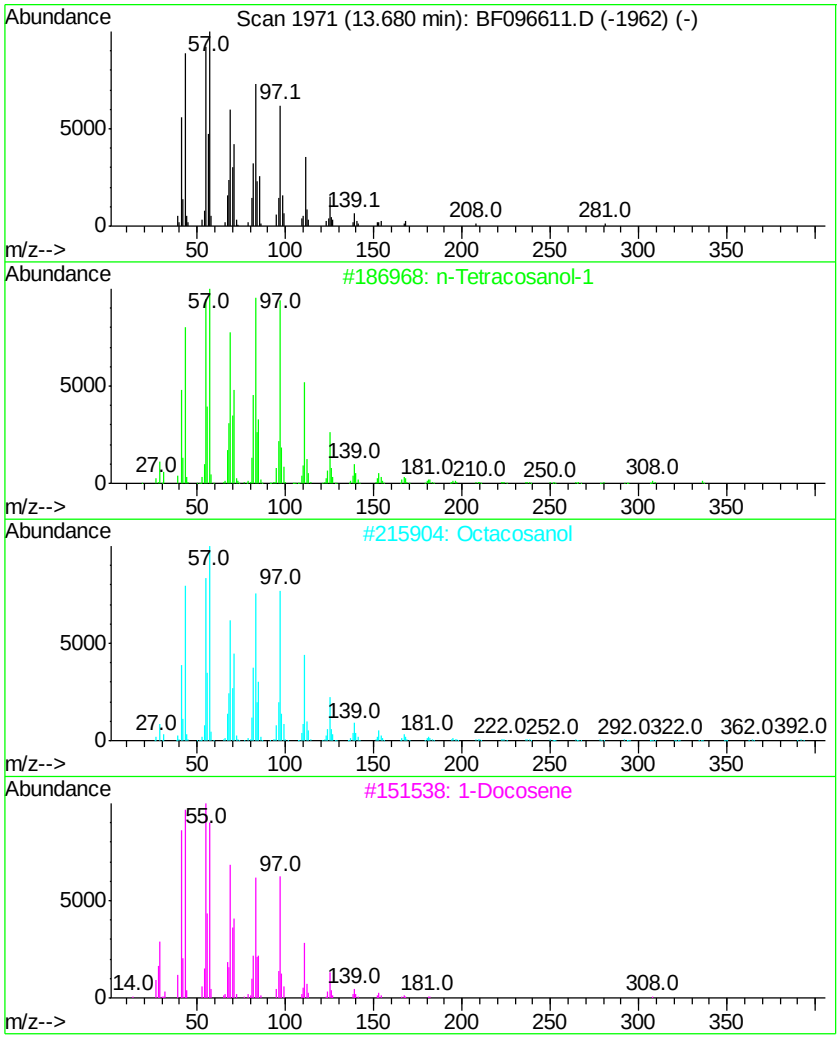
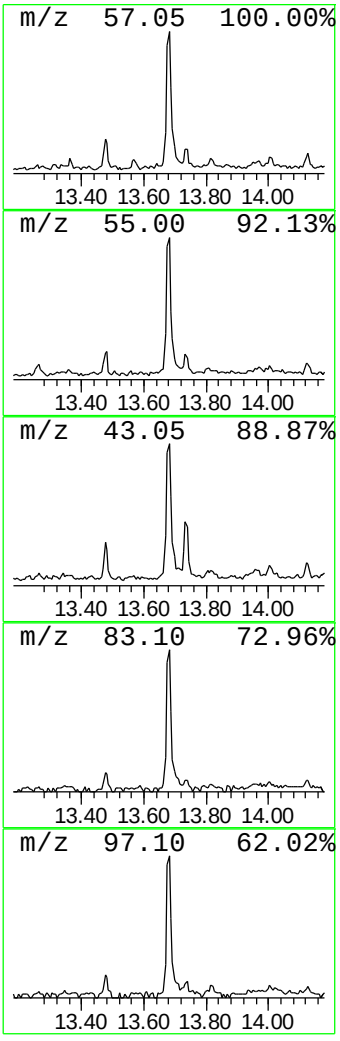
Peak Number 4 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	6.24 ng	250255	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Octacosanol	410	C28H58O	000557-61-9	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





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Instrument : BNA_F
ClientSampleId : I4104-04

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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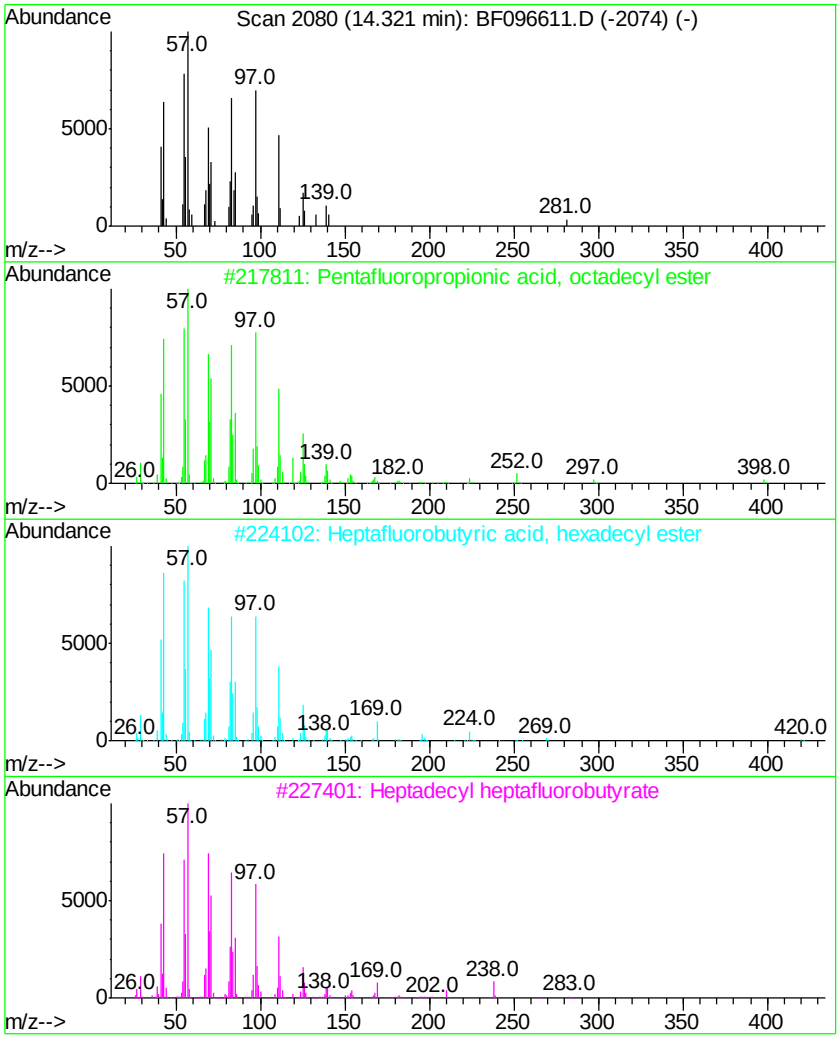
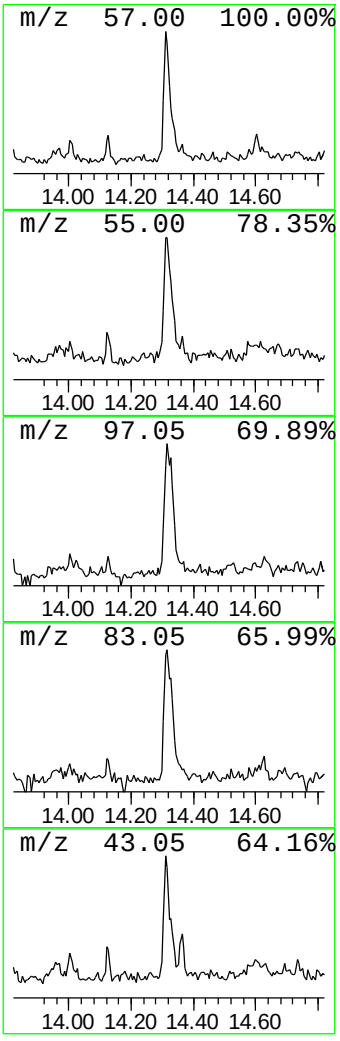
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	3.00 ng	120173	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





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...	4.87	17.3	ng	578615	1	6.68	668312	20.0
unknown6.45	6.45	74.5	ng	2488970	1	6.68	668312	20.0
n-Tetracosanol-1	13.68	6.2	ng	250255	5	13.82	801901	20.0
Pentafluoropropio...	14.32	3.0	ng	120173	5	13.82	801901	20.0