LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051817\
Data File : BF095244.D
Acq On : 19 May 2017 2:54
Operator : SJ/MA
Sample : I3200-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-20170517

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-BF050217.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	5.119	537	541	562	rBV	126865	301747	9.87%	1.478%
2	5.760	646	650	683	rBV	260808	812009	26.55%	3.976%
3	7.336	915	918	931	rBV	152572	416524	13.62%	2.040%
4	7.436	931	935	956	rVB	1070613	1966440	64.30%	9.629%
5	7.772	988	992	1009	rVB	431514	551929	18.05%	2.703%
6	8.007	1027	1032	1050	rBV	1344298	1756717	57.44%	8.602%
7	8.666	1140	1144	1174	rBV	789376	1349338	44.12%	6.607%
8	9.789	1331	1335	1356	rBV	440084	778755	25.46%	3.813%
9	11.554	1630	1635	1660	rBV	2085873	3058178	100.00%	14.975%
10	11.907	1691	1695	1710	rBV4	25581	70596	2.31%	0.346%
11	12.618	1811	1816	1838	rBV2	543989	912758	29.85%	4.469%
12	13.912	2031	2036	2051	rBV	1064405	1834078	59.97%	8.981%
13	14.154	2072	2077	2104	rBV	140705	386785	12.65%	1.894%
14	15.024	2220	2225	2243	rBV2	510712	862554	28.20%	4.224%
15	16.012	2389	2393	2411	rVB	251001	469606	15.36%	2.299%
16	17.342	2613	2619	2634	rBV2	2381625	2998289	98.04%	14.681%
17	17.453	2634	2638	2661	rVV	178142	413144	13.51%	2.023%
18	18.659	2838	2843	2846	rBV	158418	256768	8.40%	1.257%
19	18.695	2846	2849	2855	rVB	393017	538855	17.62%	2.639%
20	19.712	3017	3022	3035	rBV3	69217	196774	6.43%	0.964%
21	20.371	3130	3134	3145	rBV	241421	429403	14.04%	2.103%
22	20.706	3184	3191	3197	rBV5	23057	61113	2.00%	0.299%

Sum of corrected areas: 20422360

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051817\
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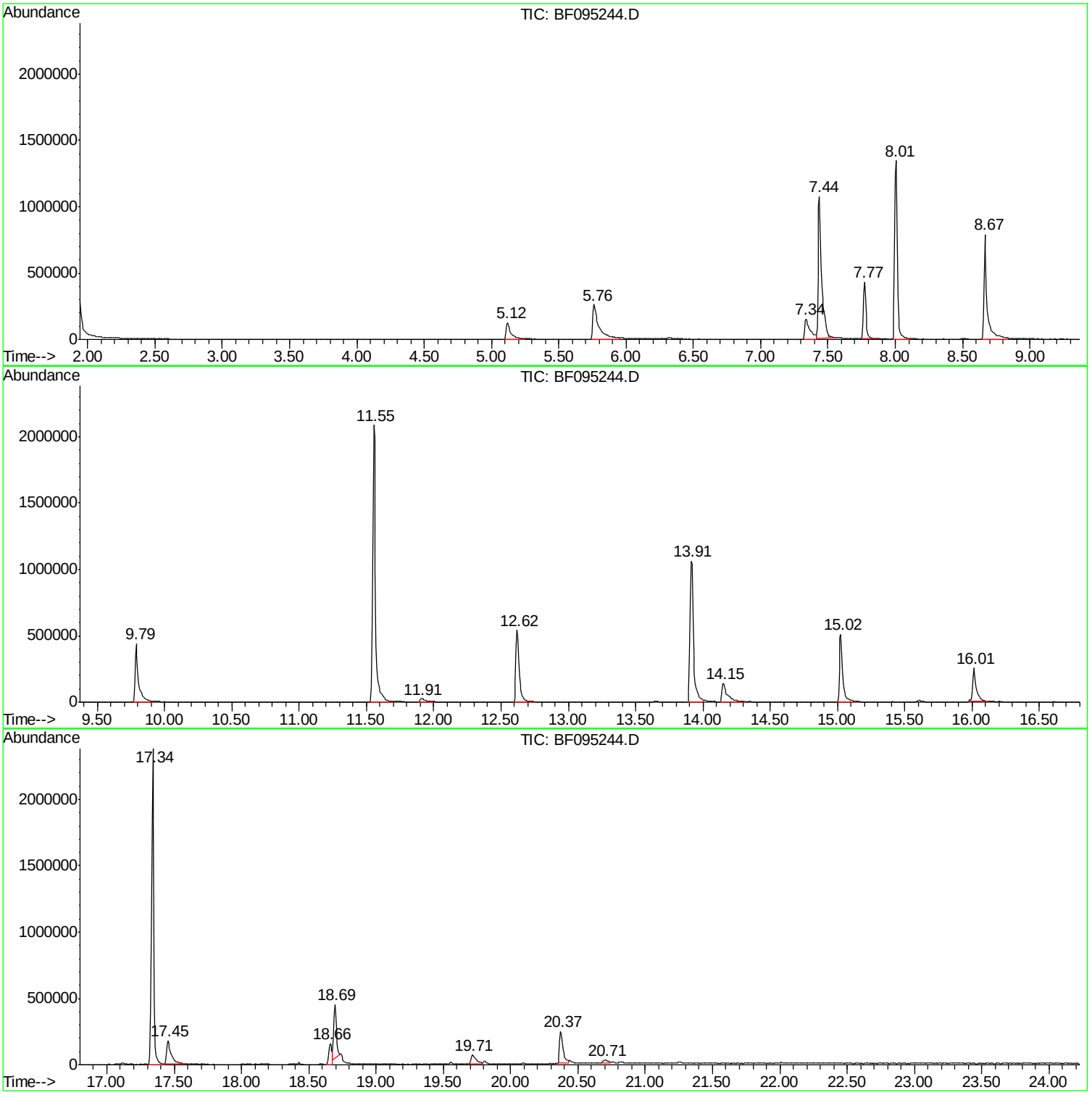
Operator : SJ/MA
Sample : I3200-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-20170517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF051817\
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Acq On : 19 May 2017 2:54
Operator : SJ/MA
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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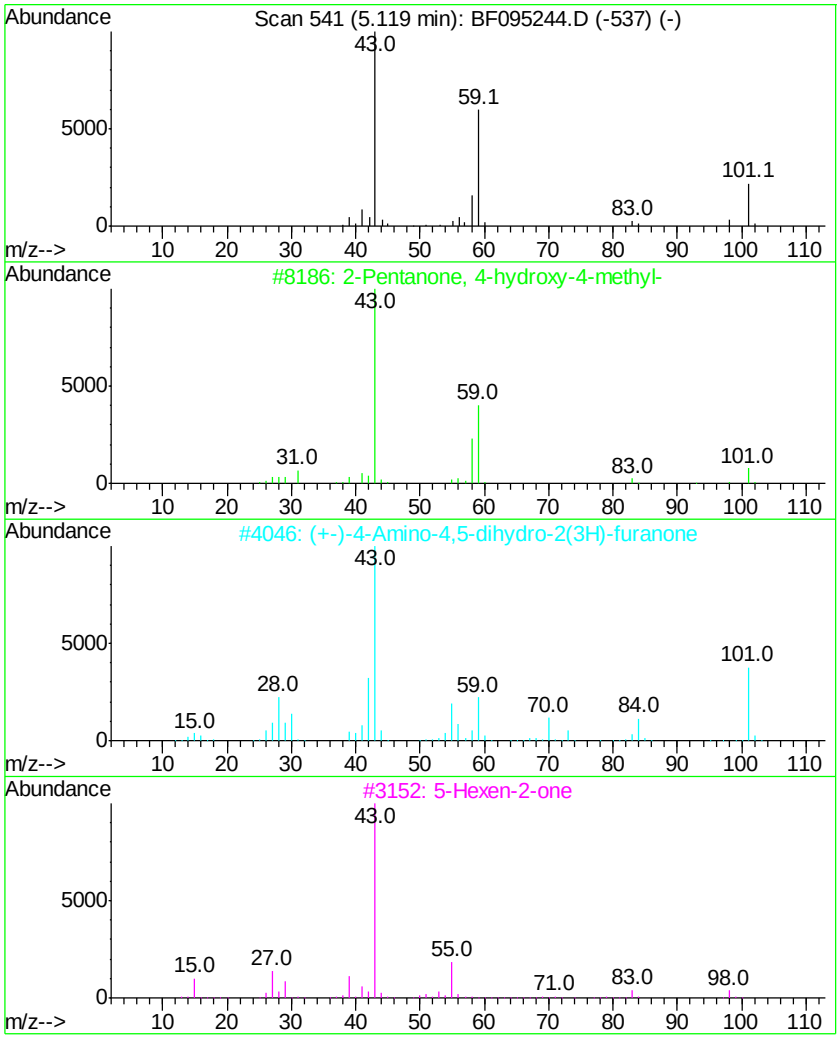
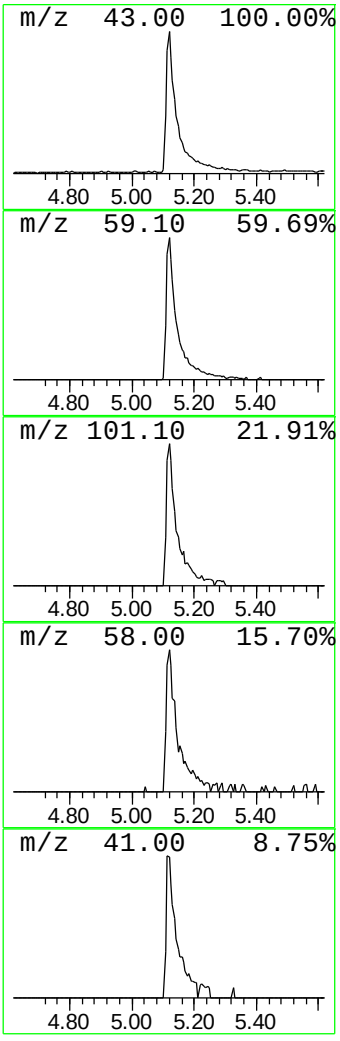
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	10.93 ng	301747	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051817\
Data File : BF095244.D
Acq On : 19 May 2017 2:54
Operator : SJ/MA
Sample : I3200-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-20170517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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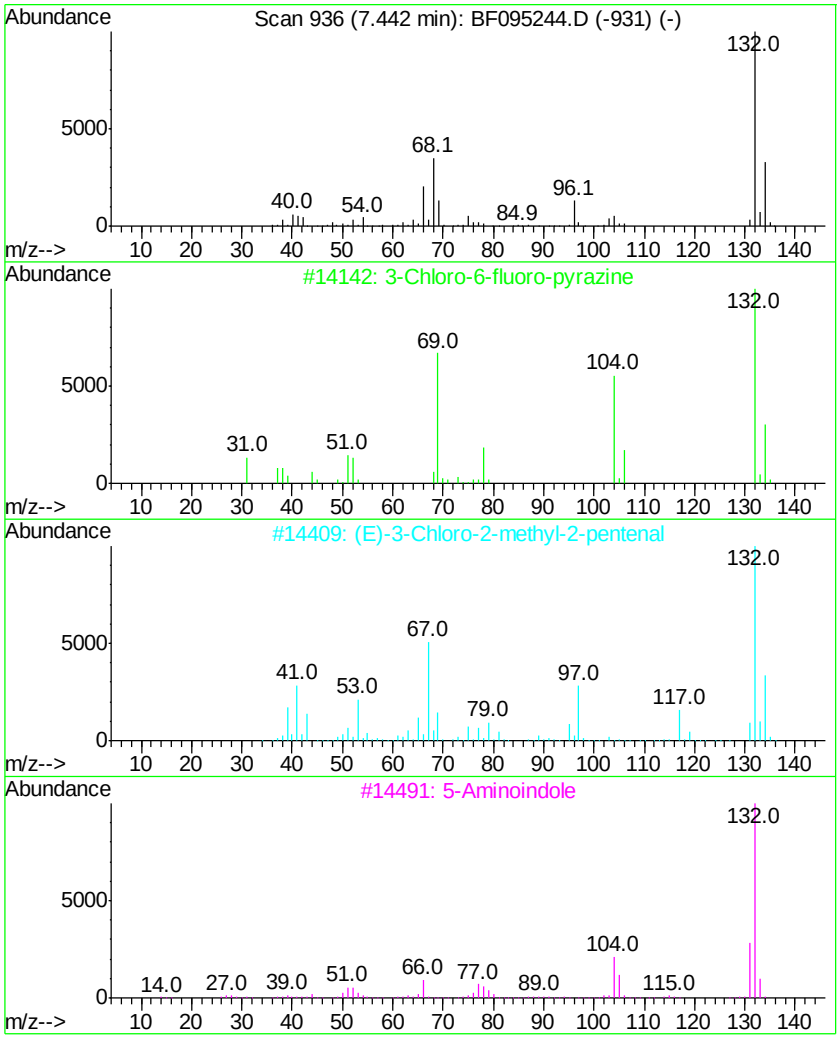
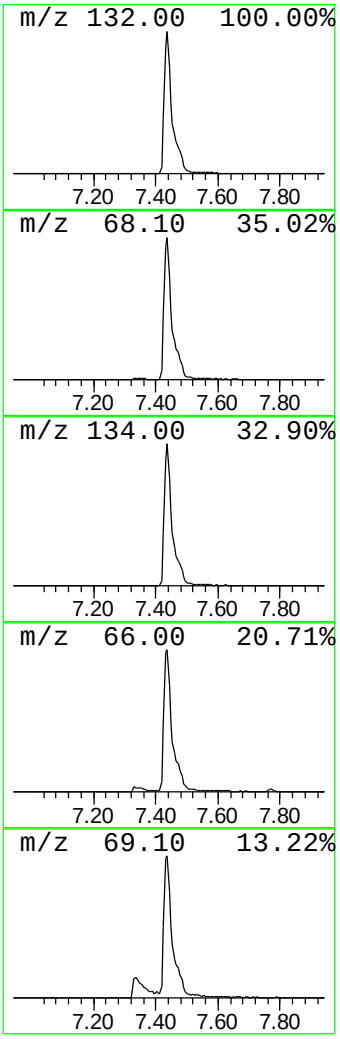
Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	71.26 ng	1966440	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051817\
Data File : BF095244.D
Acq On : 19 May 2017 2:54
Operator : SJ/MA
Sample : I3200-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-20170517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

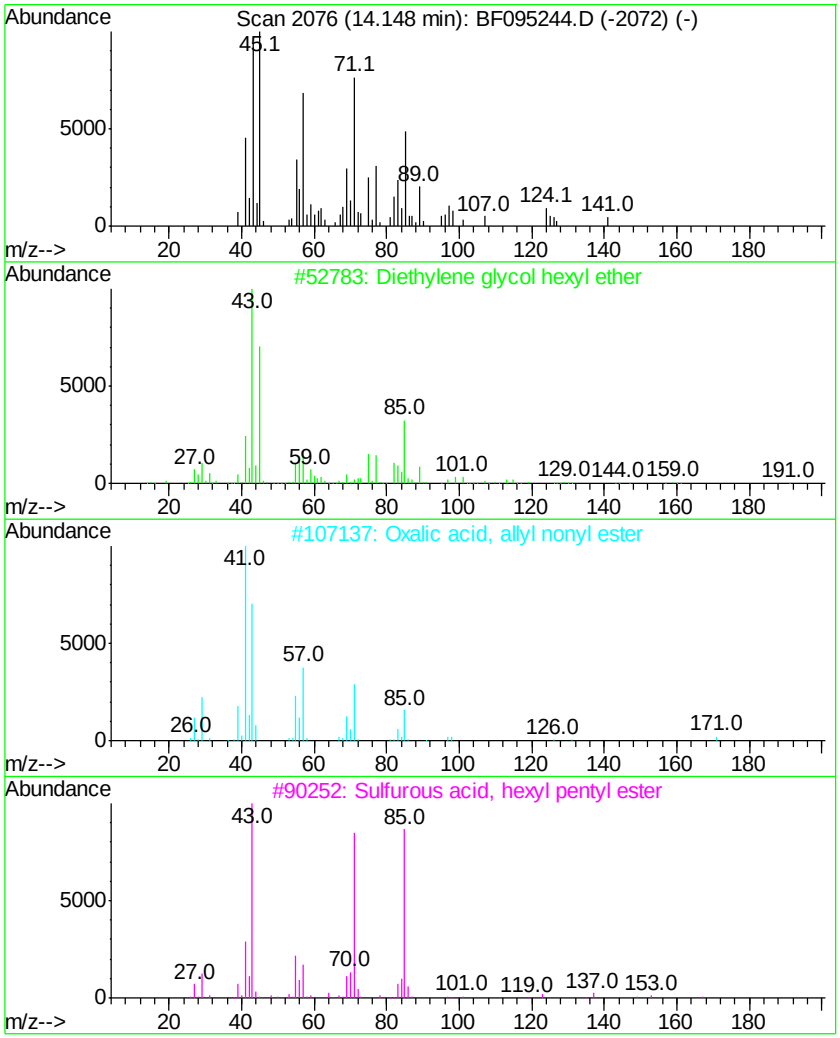
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

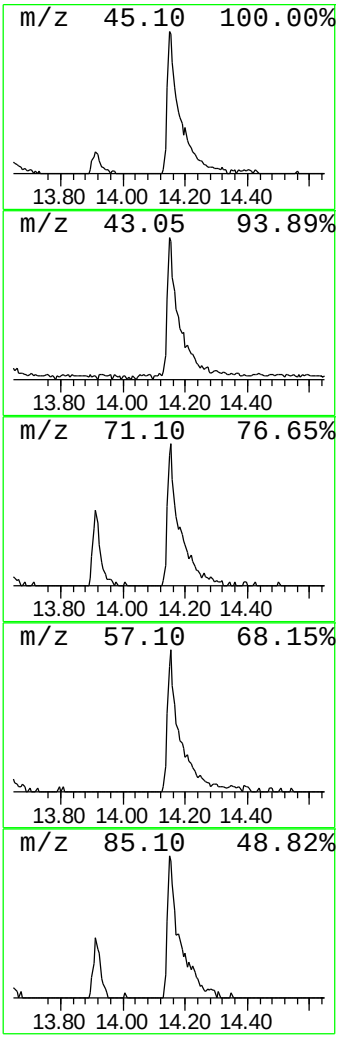
****

Peak Number 4 unknown14.15 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.15	8.97 ng	386785	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol hexyl ether	190	C10H22O3	000112-59-4	49
2	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	41
3	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	35
4	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	35
5	Heptacosane	380	C27H56	000593-49-7	35





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Data File : BF095244.D
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Operator : SJ/MA
Sample : I3200-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-20170517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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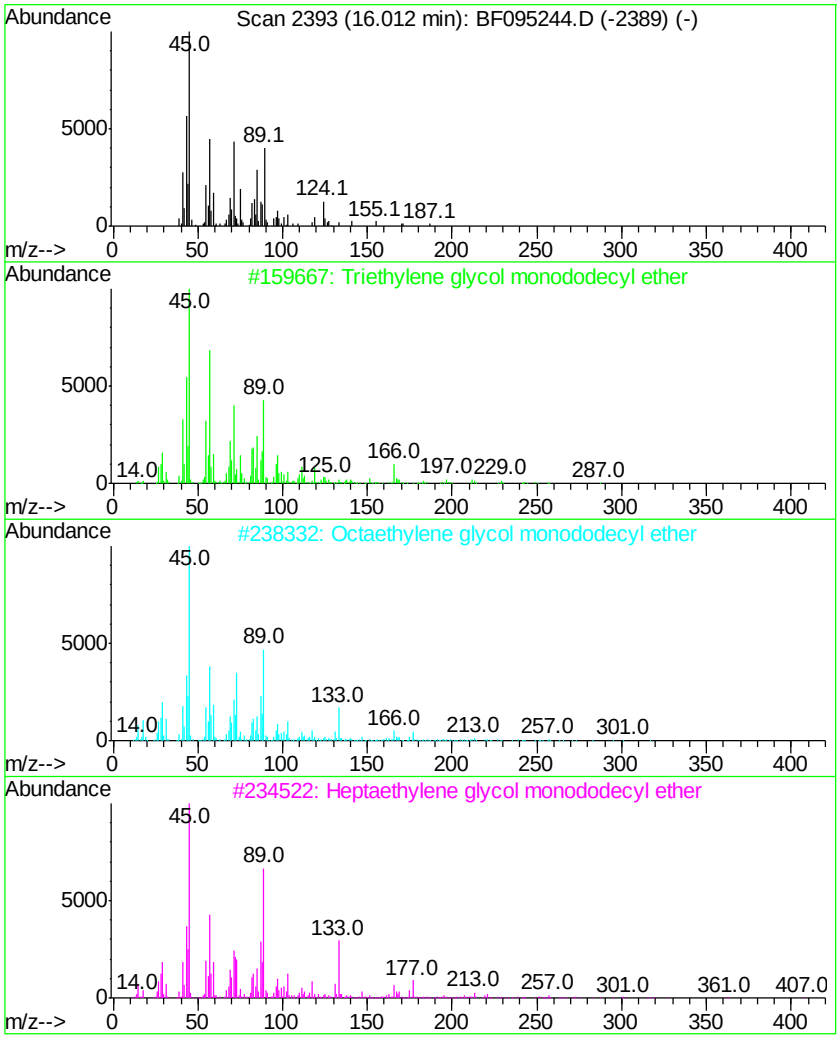
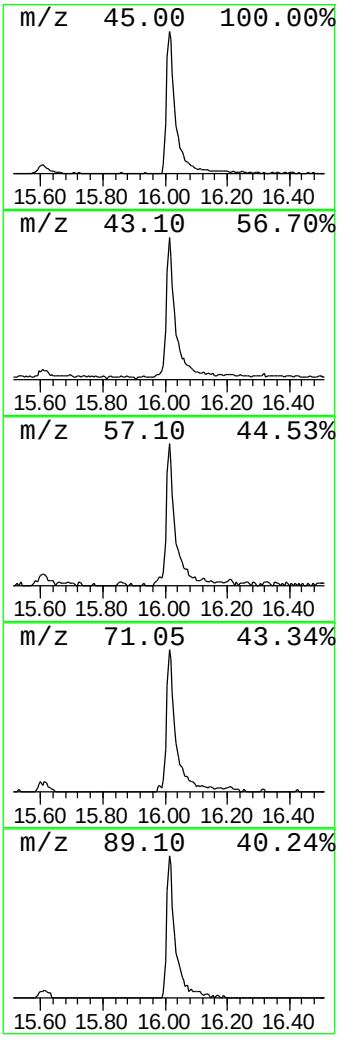
Peak Number 5 Triethylene glycol monodode... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	10.89 ng	469606	Phenanthrene-d10	15.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	72
2	Octaethylene glycol monododecyl ...	538	C28H58O9	003055-98-9	53
3	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	53
4	1,4,7,10,13,16-Hexaoxanonadecane...	320	C16H32O6	1000163-65-3	50
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	47





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Sample : I3200-12
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-20170517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
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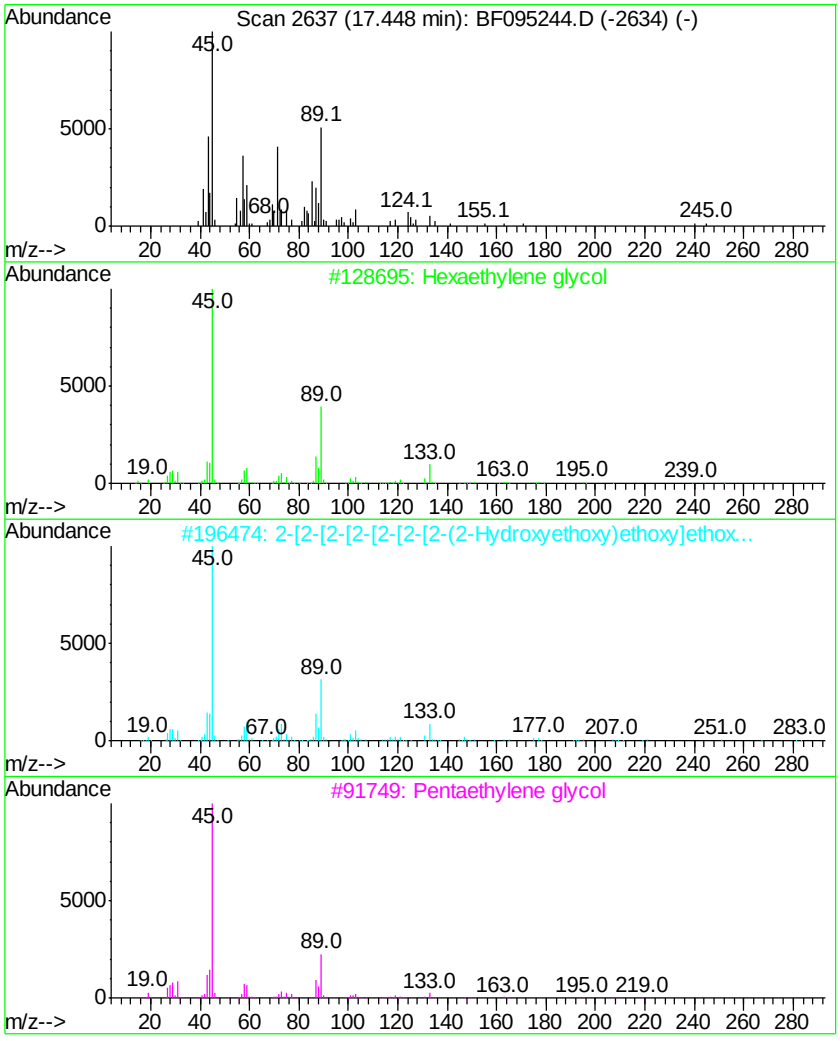
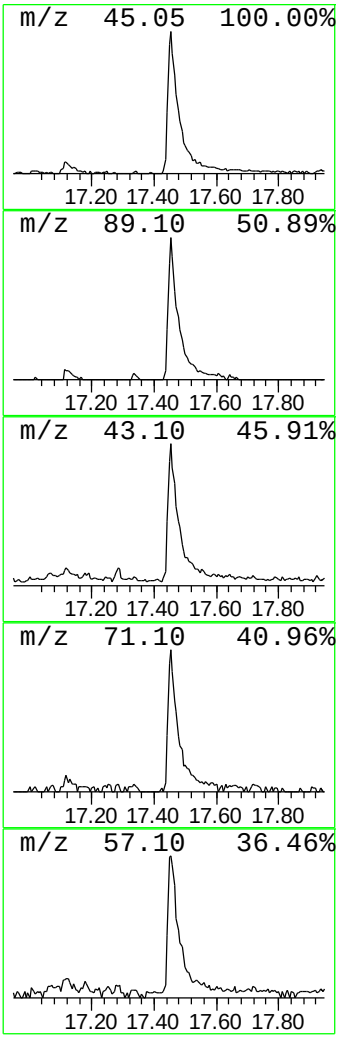
Peak Number 6 Hexaethylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.45	15.33 ng	413144	Chrysene-d12	18.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	58
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	58
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	53
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	53
5	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	47





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Instrument : BNA_F
ClientSampleId : FB-20170517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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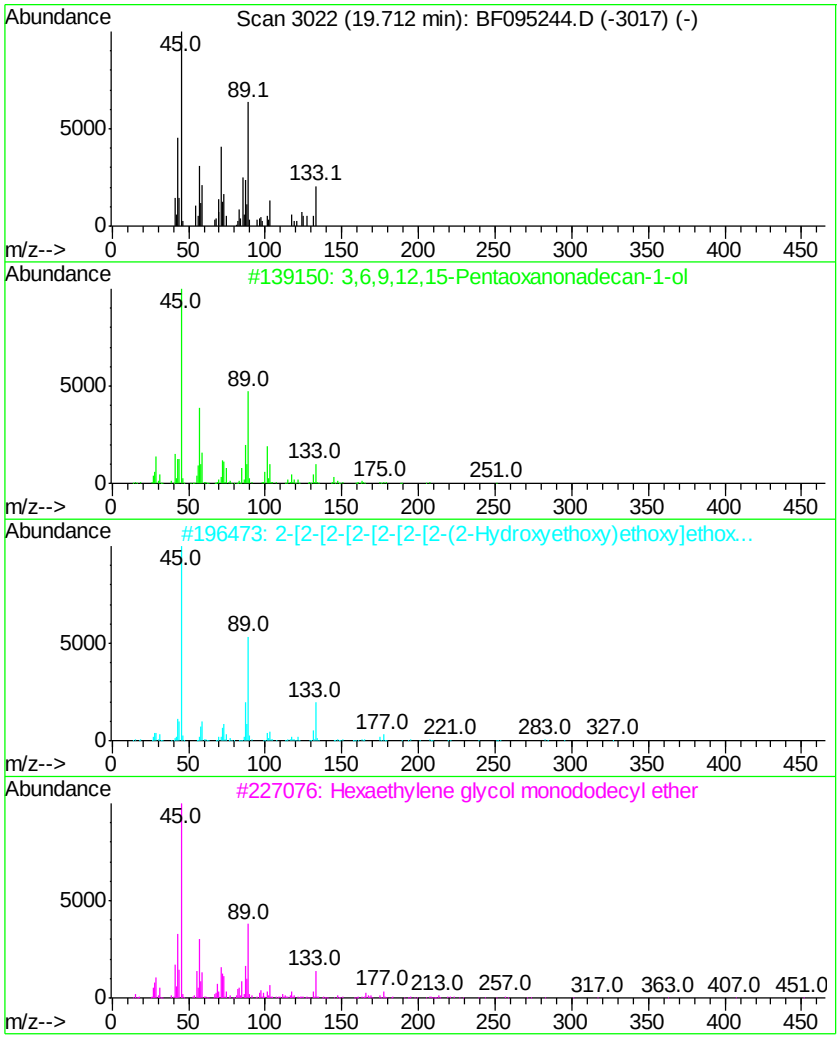
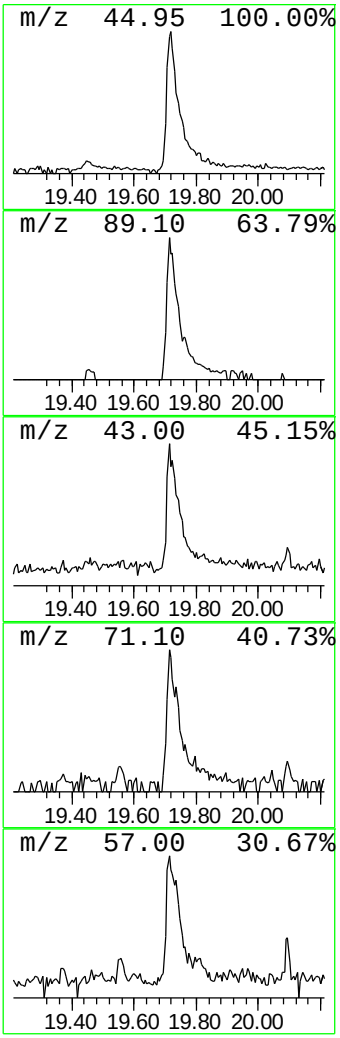
Peak Number 7 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.71	9.17 ng	196774	Perylene-d12	20.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	68
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	62
3	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	58
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	53
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	52





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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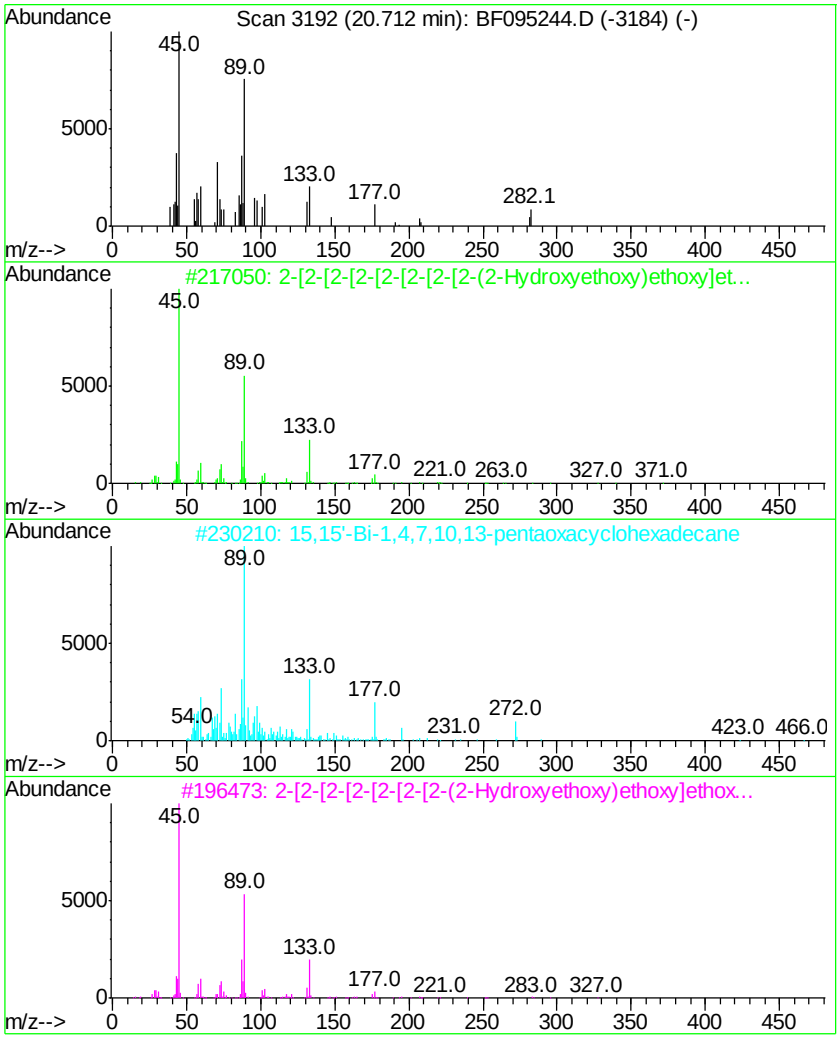
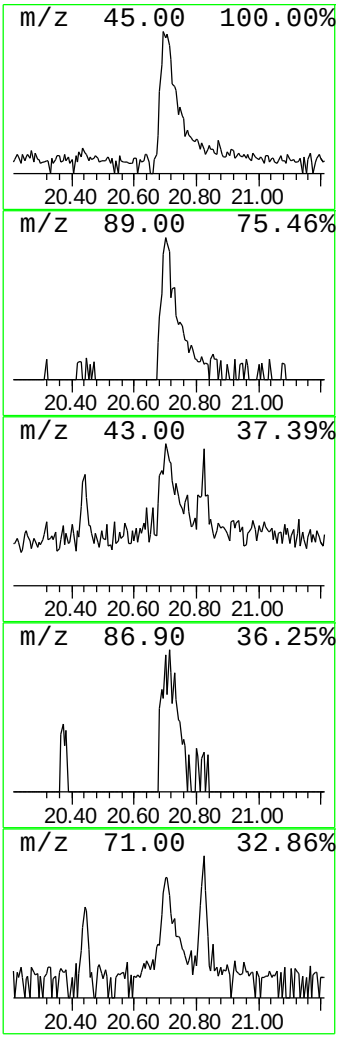
Peak Number 8 2-[2-[2-[2-[2-[2-[2-[2-(2-H... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.71	2.85 ng	61113	Perylene-d12	20.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	86
2	15,15'-Bi-1,4,7,10,13-pentaoxacy...	466	C22H42O10	109773-67-3	78
3	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	78
4	Cyclohexyl-15-crown-5	274	C14H26O5	017454-48-7	78
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	72





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	10.9	ng	301747	1	7.77	551929	20.0
unknown7.44	7.44	71.3	ng	1966440	1	7.77	551929	20.0
unknown14.15	14.15	9.0	ng	386785	4	15.02	862554	20.0
Triethylene glyco...	16.01	10.9	ng	469606	4	15.02	862554	20.0
Hexaethylene glycol	17.45	15.3	ng	413144	5	18.69	538855	20.0
3,6,9,12,15-Penta...	19.71	9.2	ng	196774	6	20.37	429403	20.0
2-[2-[2-[2-[2-[2-...	20.71	2.9	ng	61113	6	20.37	429403	20.0