LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091516\
Data File : BF090094.D
Acq On : 15 Sep 2016 16:22
Operator : UM/SJ
Sample : H4780-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-61-SW

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-BF091516.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	1.701	8	10	37	rVB	540438	1390038	31.14%	4.278%
2	4.650	266	268	275	rBV	193278	250958	5.62%	0.772%
3	5.119	306	309	311	rBV	1956088	2048360	45.89%	6.305%
4	6.193	401	403	406	rBV	1285985	1384719	31.02%	4.262%
5	6.319	411	414	416	rBV	2976934	3494726	78.30%	10.756%
6	6.547	431	434	436	rBV	1037781	925592	20.74%	2.849%
7	6.707	445	448	450	rBV	3064800	3285765	73.62%	10.113%
8	7.119	481	484	486	rBV	2257313	2387588	53.49%	7.349%
9	7.599	523	526	531	rBV2	36253	67166	1.50%	0.207%
10	7.839	544	547	549	rBV	1064515	1242153	27.83%	3.823%
11	8.205	577	579	582	rBV	25827	45934	1.03%	0.141%
12	8.799	626	631	633	rBV2	27312	50354	1.13%	0.155%
13	8.913	638	641	644	rBV	3523276	4463277	100.00%	13.738%
14	9.313	674	676	678	rBV	195149	165687	3.71%	0.510%
15	9.576	697	699	702	rBV	1657058	1443365	32.34%	4.443%
16	9.816	717	720	725	rBV	38424	61780	1.38%	0.190%
17	10.010	735	737	742	rVB2	44049	55402	1.24%	0.171%
18	10.365	765	768	770	rBV	2182083	2339809	52.42%	7.202%
19	10.639	790	792	796	rVB2	29436	66559	1.49%	0.205%
20	11.051	825	828	830	rBV	1119565	1250185	28.01%	3.848%
21	11.302	848	850	855	rBV	75866	85725	1.92%	0.264%
22	11.611	874	877	881	rBV2	114478	224249	5.02%	0.690%
23	12.331	934	940	943	rBV4	16066	57565	1.29%	0.177%
24	12.388	943	945	951	rVV	76690	101216	2.27%	0.312%
25	12.628	964	966	969	rBV	2375899	3020896	67.68%	9.298%
26	13.542	1044	1046	1053	rBV	80625	101911	2.28%	0.314%
27	13.657	1053	1056	1065	rBV	940692	1027188	23.01%	3.162%
28	14.125	1095	1097	1100	rBV2	32196	59361	1.33%	0.183%
29	14.982	1170	1172	1175	rBV	657066	803394	18.00%	2.473%
30	15.280	1193	1198	1202	rBV4	47159	217427	4.87%	0.669%
31	16.628	1314	1316	1322	rVB7	19440	54966	1.23%	0.169%
32	18.537	1477	1483	1494	rVB5	49214	316282	7.09%	0.973%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H4780-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-61-SW

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-BF091516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

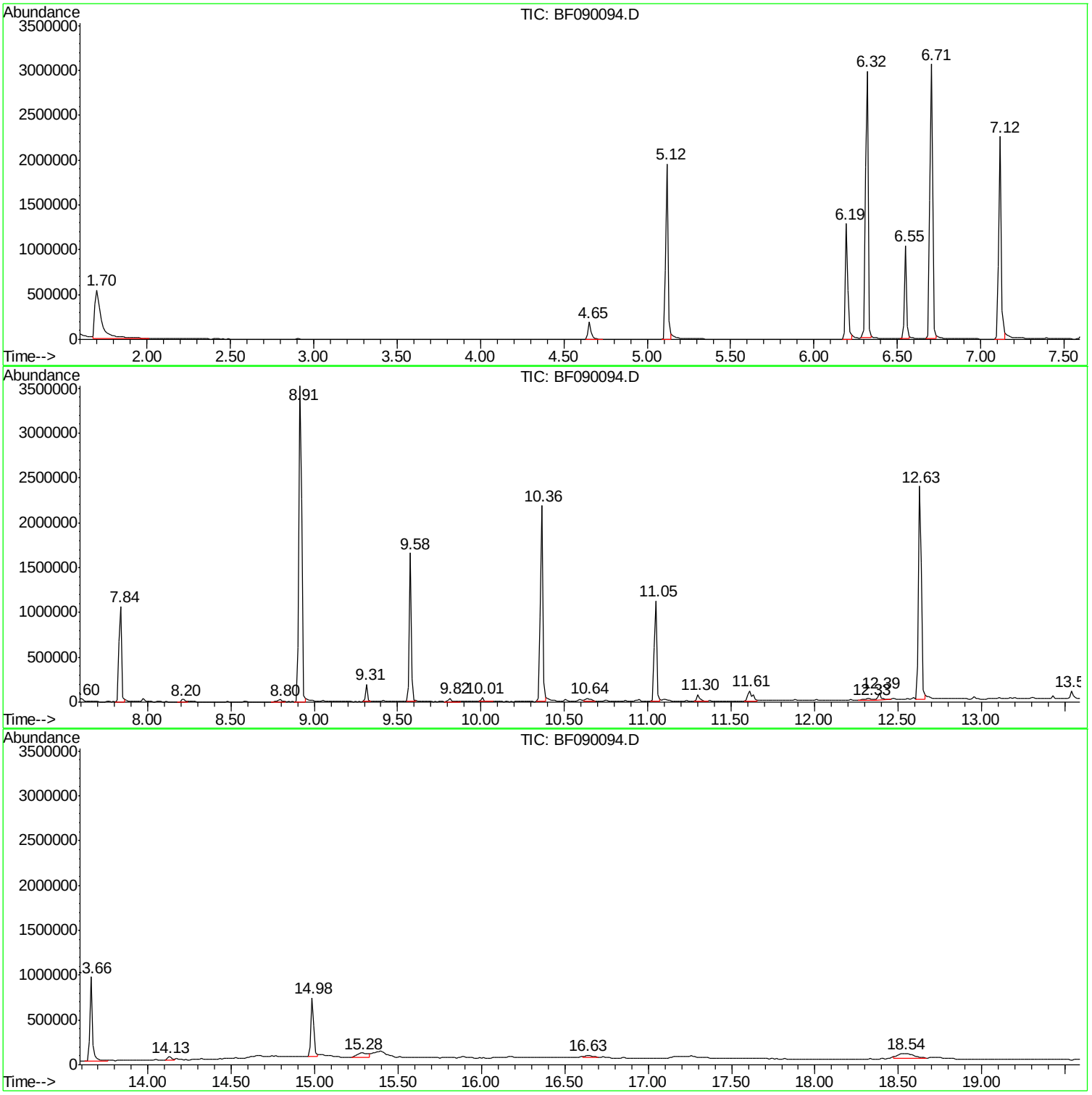
Sum of corrected areas: 32489597

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091516\
Data File : BF090094.D
Acq On : 15 Sep 2016 16:22
Operator : UM/SJ
Sample : H4780-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP-61-SW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.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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Instrument : BNA_F
ClientSampleId : EP-61-SW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.M
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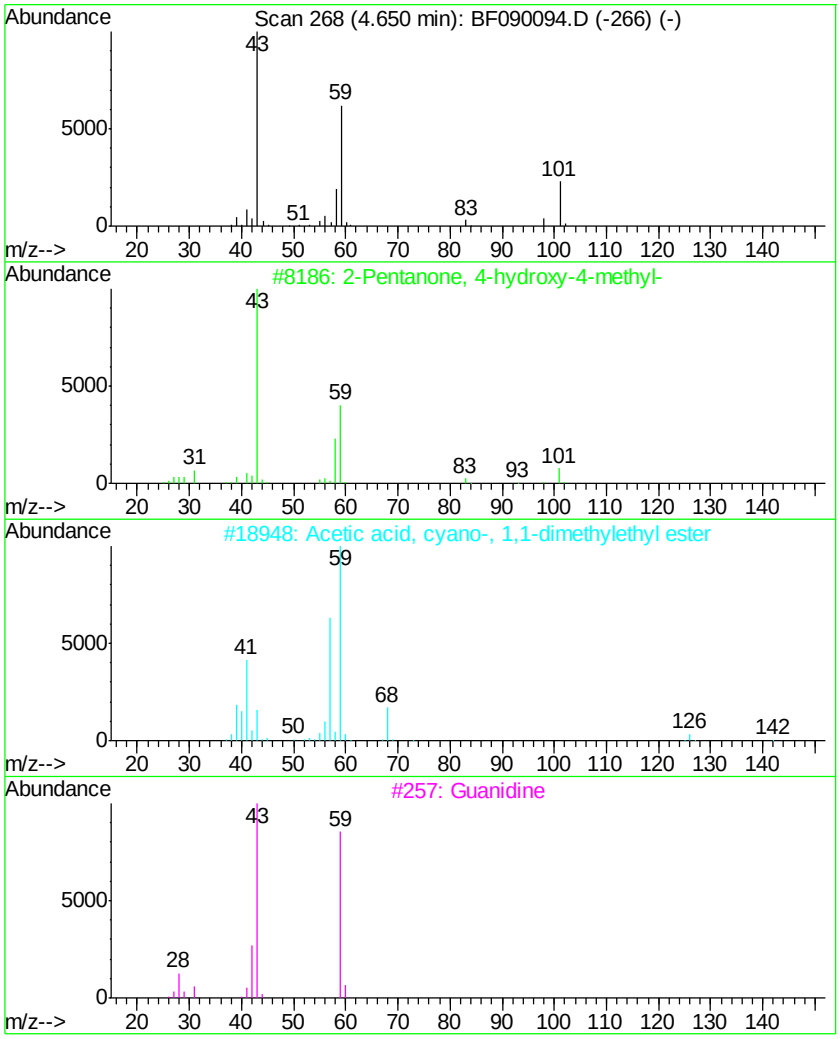
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

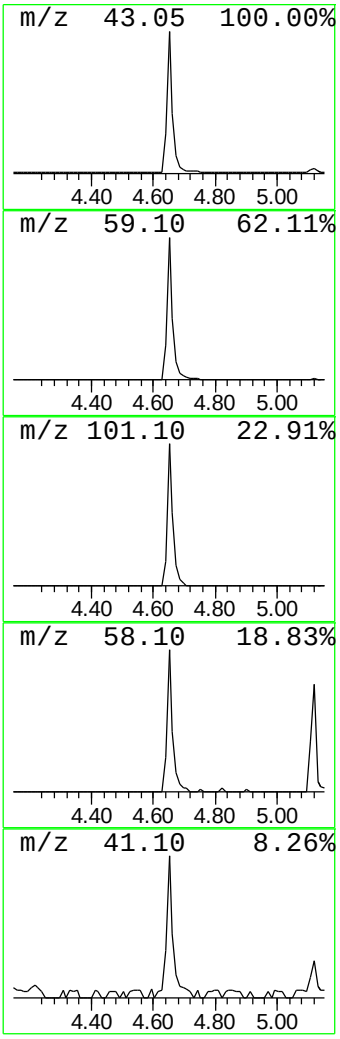
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	5.42 ng	250958	1,4-Dichlorobenzene-d4	6.55

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Guanidine	59	CH5N3	000113-00-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091516\
Data File : BF090094.D
Acq On : 15 Sep 2016 16:22
Operator : UM/SJ
Sample : H4780-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-61-SW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

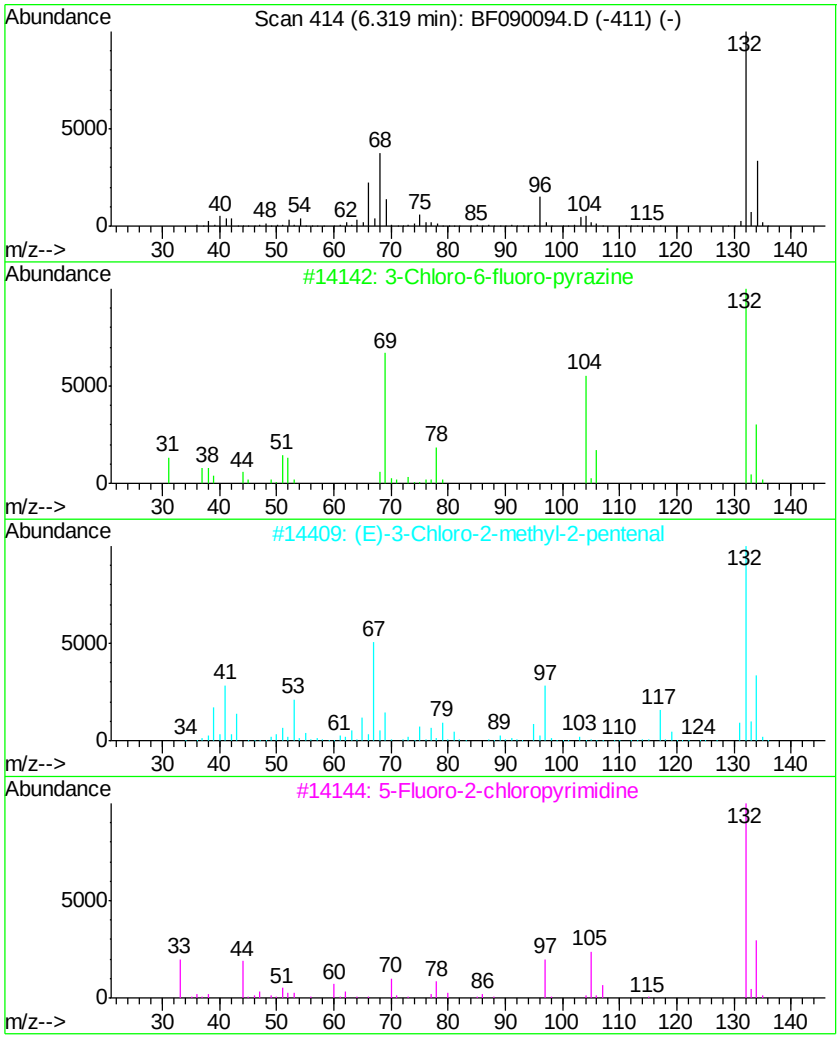
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

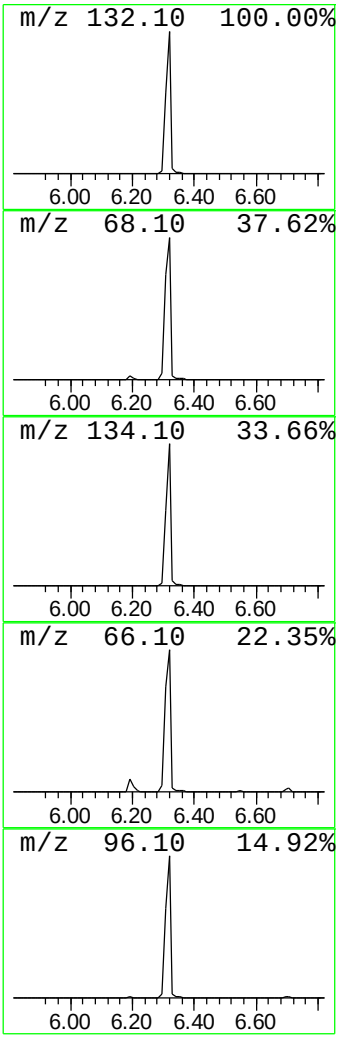
****

Peak Number 3 unknown6.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	75.51 ng	3494730	1,4-Dichlorobenzene-d4	6.55

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	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Misc :
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Instrument : BNA_F
ClientSampleId : EP-61-SW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.M
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TIC Library : C:\Database\NIST11.L
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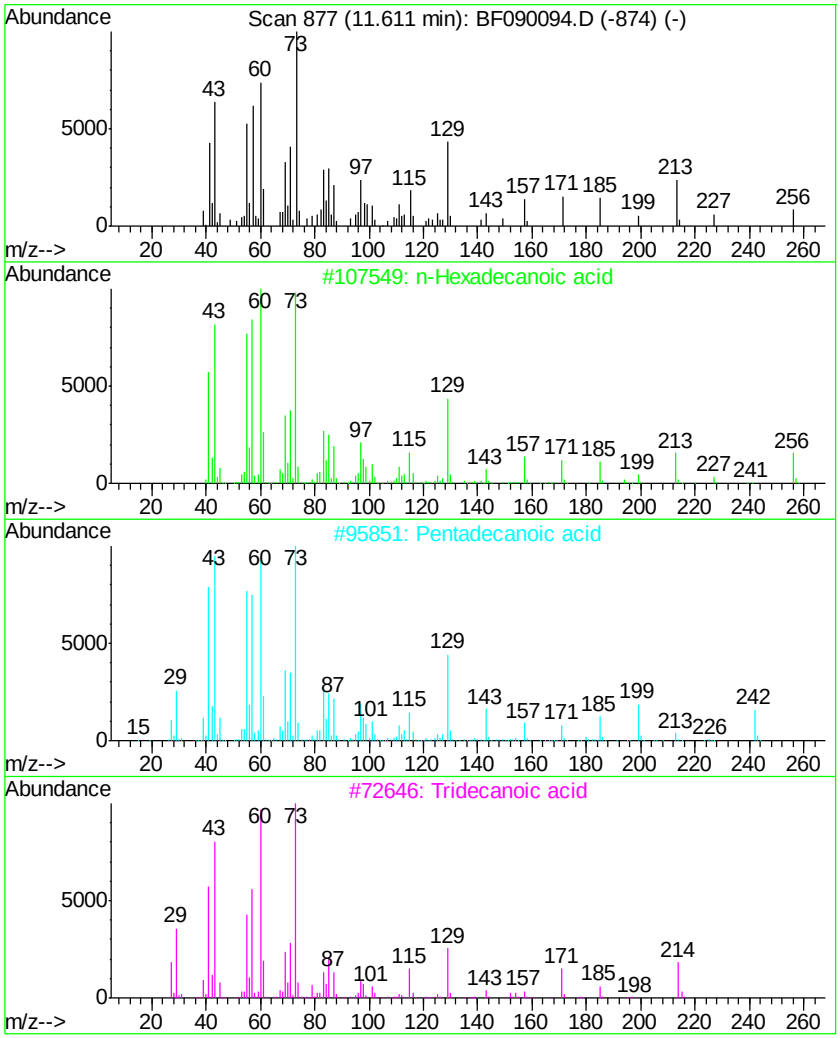
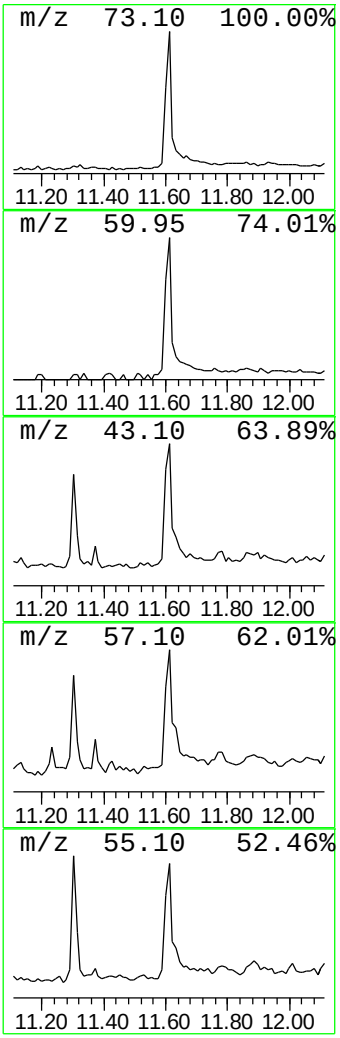
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	3.59 ng	224249	Phenanthrene-d10	11.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	35
5	Nonanoic acid	158	C9H18O2	000112-05-0	30





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091516\
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Sample : H4780-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-61-SW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.M
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TIC Library : C:\Database\NIST11.L
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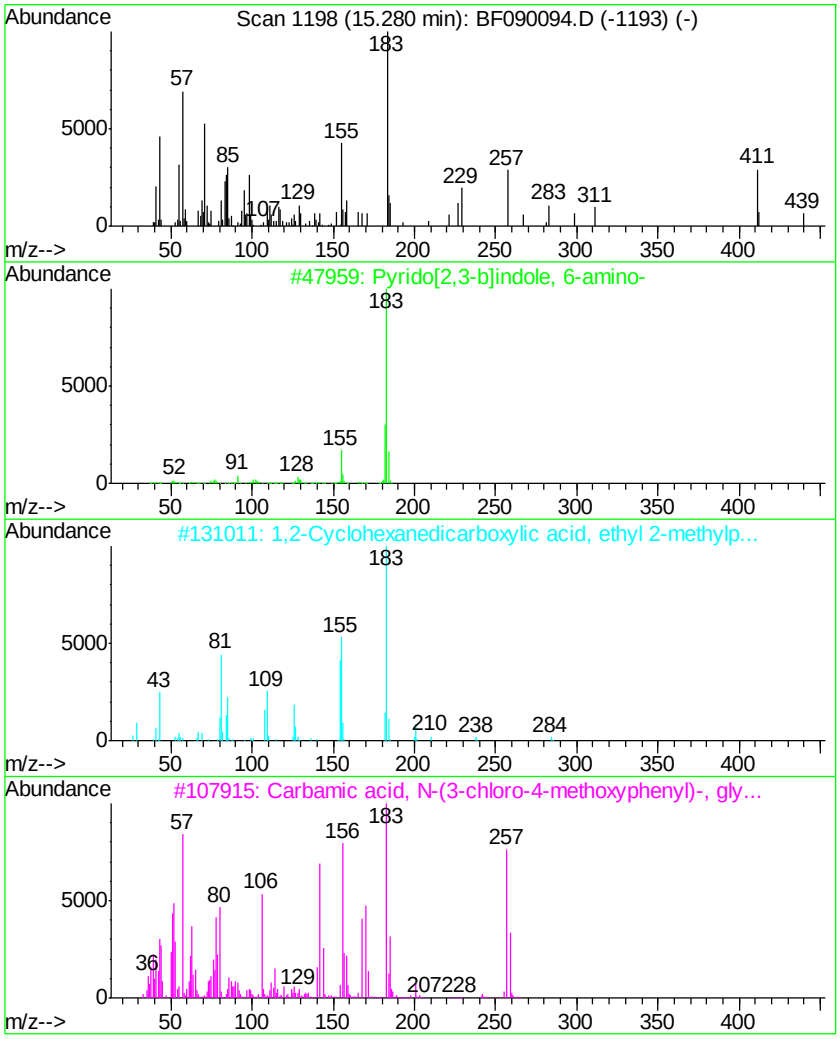
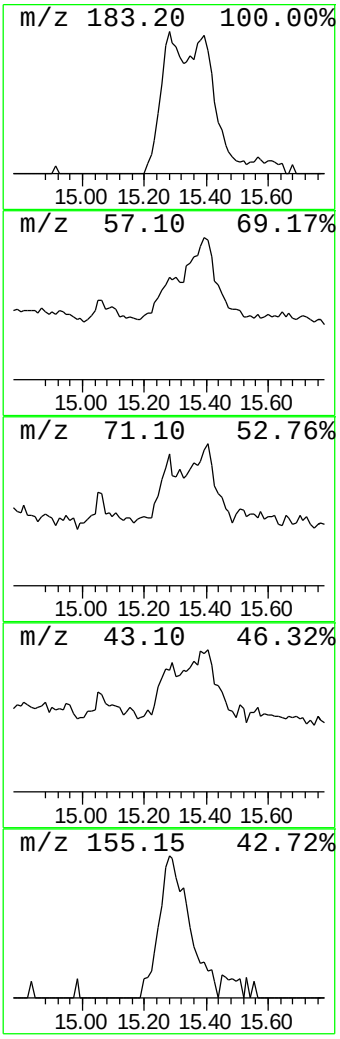
Peak Number 6 unknown15.28 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	5.41 ng	217427	Perylene-d12	14.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrido[2,3-b]indole, 6-amino-	183	C11H9N3	006453-26-5	46
2	1,2-Cyclohexanedicarboxylic acid...	284	C16H28O4	1000339-44-0	43
3	Carbamic acid, N-(3-chloro-4-met...	257	C11H12ClNO4	339273-80-2	30
4	4-Hydroxy-3-nitrobenzoic acid	183	C7H5NO5	000616-82-0	27
5	4-Methoxy-3-nitrobenzyl alcohol	183	C8H9NO4	041870-24-0	27





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Sample : H4780-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-61-SW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

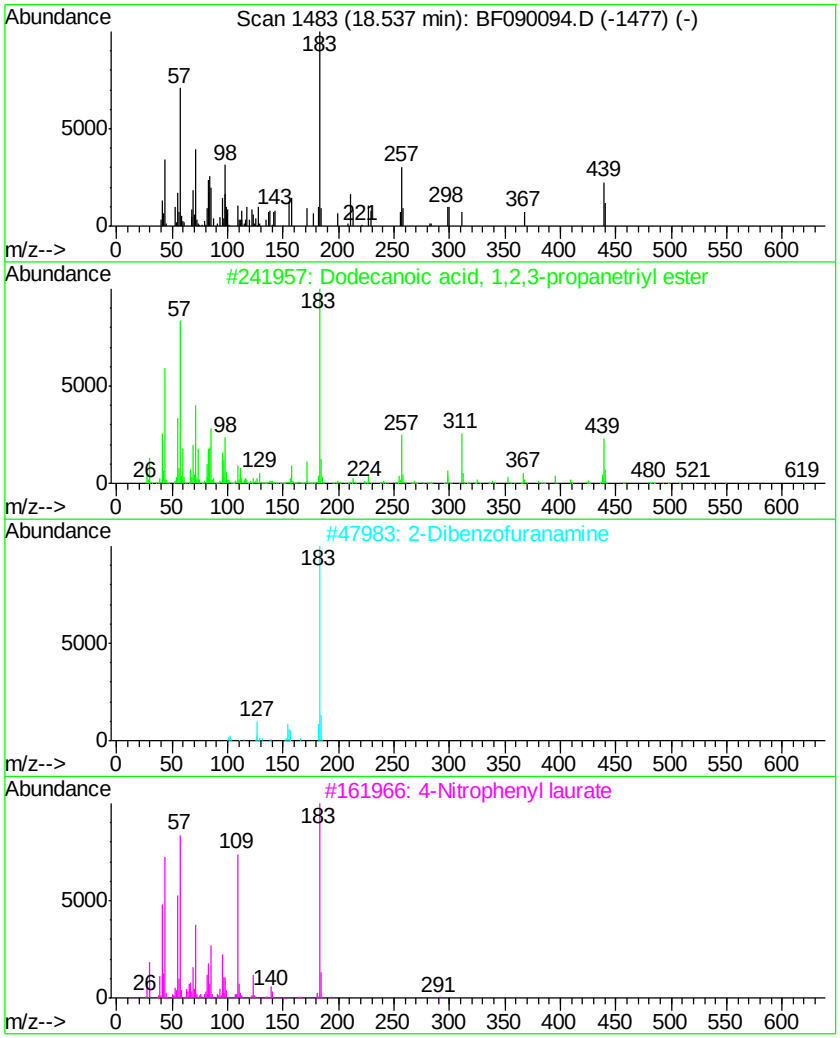
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

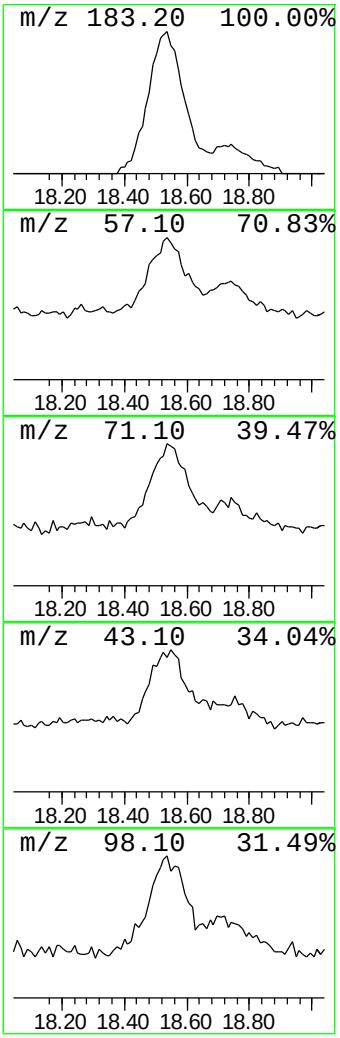
****

Peak Number 7 Dodecanoic acid, 1,2,3-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	7.87 ng	316282	Perylene-d12	14.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, 1,2,3-propanetr...	639	C39H74O6	000538-24-9	72
2	2-Dibenzofuranamine	183	C12H9NO	003693-22-9	38
3	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	32
4	Dodecanoic acid, pentafluorophen...	366	C18H23F5O2	1000360-54-1	32
5	7-Methyl-octadecane	268	C19H40	1000192-63-3	27





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...	4.65	5.4	ng	250958	1	6.55	925592	20.0
unknown6.32	6.32	75.5	ng	3494730	1	6.55	925592	20.0
n-Hexadecanoic acid	11.61	3.6	ng	224249	4	11.05	1250190	20.0
unknown15.28	15.28	5.4	ng	217427	6	14.98	803394	20.0
Dodecanoic acid, ...	18.54	7.9	ng	316282	6	14.98	803394	20.0