LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090265.D
Acq On : 27 Sep 2016 21:22
Operator : UM/SJ
Sample : H4949-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-2-LOC-2(10-15)

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-BF092016.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	1.644	4	5	50	rVB	2628226	7319659	100.00%	20.194%
2	4.559	257	260	273	rVB	329651	671701	9.18%	1.853%
3	5.039	299	302	305	rBV	2465269	2813917	38.44%	7.763%
4	6.136	395	398	401	rBV	2485696	2959306	40.43%	8.164%
5	6.239	405	407	410	rVV	2403472	3125253	42.70%	8.622%
6	6.479	426	428	430	rBV	637430	752649	10.28%	2.076%
7	6.627	439	441	444	rBV	2065651	2456075	33.55%	6.776%
8	7.050	475	478	480	rBV	1977654	2028821	27.72%	5.597%
9	7.187	487	490	495	rVB	60508	102182	1.40%	0.282%
10	7.759	538	540	543	rBV	966028	1004100	13.72%	2.770%
11	8.845	632	635	637	rBV	3236834	3486761	47.64%	9.620%
12	9.245	667	670	672	rBV	1241806	1263912	17.27%	3.487%
13	9.496	690	692	695	rVV	1065355	1106791	15.12%	3.054%
14	9.965	731	733	734	rVB	79515	79554	1.09%	0.219%
15	10.285	758	761	763	rBV	1802907	1784664	24.38%	4.924%
16	10.433	770	774	778	rBV2	93146	169925	2.32%	0.469%
17	10.971	818	821	823	rBV	715383	946707	12.93%	2.612%
18	12.159	923	925	929	rVB	99292	104692	1.43%	0.289%
19	12.388	942	945	947	rBV	104972	118532	1.62%	0.327%
20	12.548	957	959	962	rBV	1944457	1922418	26.26%	5.304%
21	13.051	1000	1003	1005	rBV	92727	131809	1.80%	0.364%
22	13.462	1037	1039	1042	rBV	71741	98512	1.35%	0.272%
23	13.577	1046	1049	1055	rBV	843119	955109	13.05%	2.635%
24	14.560	1133	1135	1138	rBV	60687	118230	1.62%	0.326%
25	14.891	1162	1164	1167	rBV	474583	724923	9.90%	2.000%

Sum of corrected areas: 36246202

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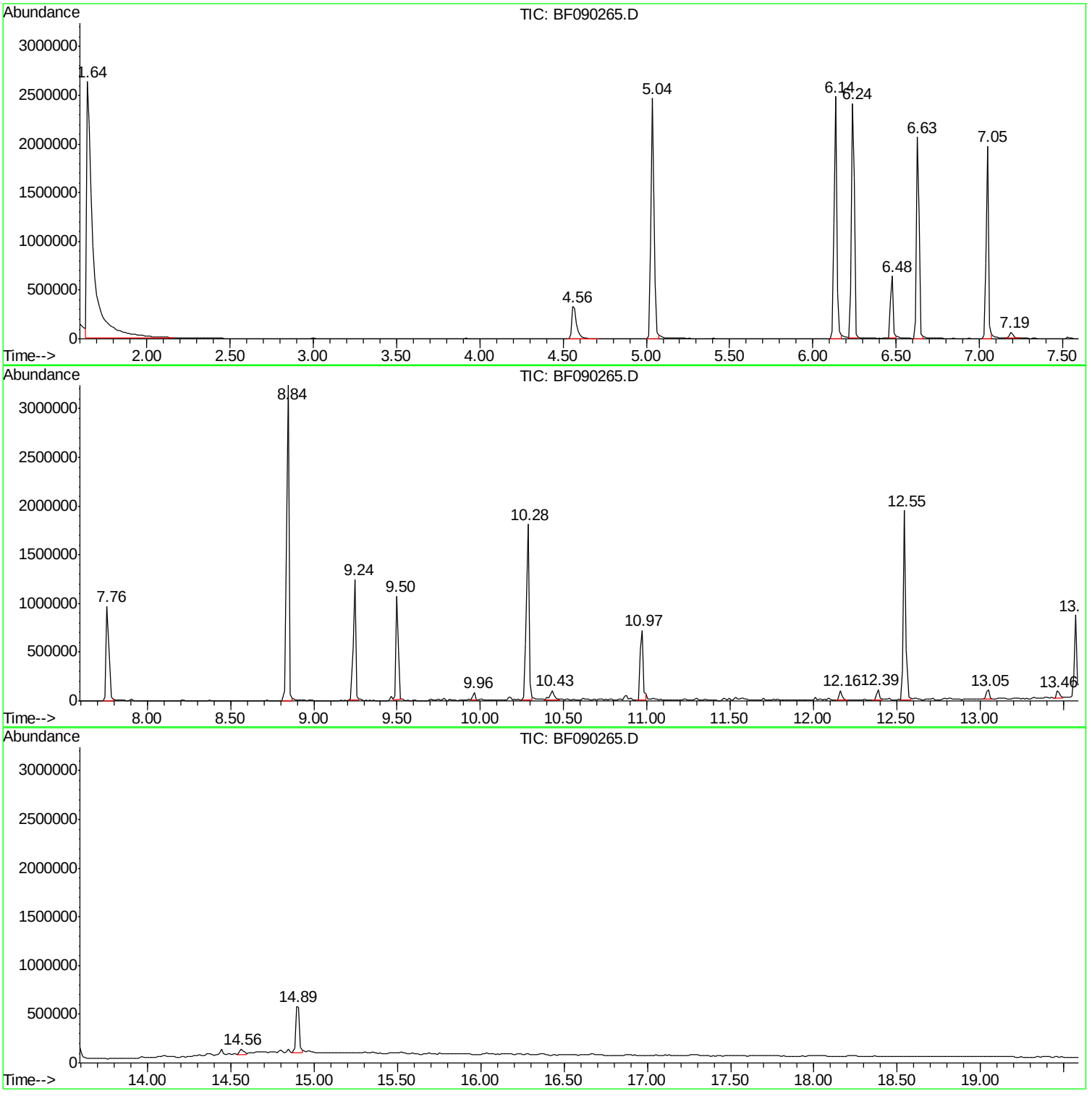
Instrument :
BNA_F
ClientSampleId :
S-2-2-LOC-2(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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Data File : BF090265.D
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Operator : UM/SJ
Sample : H4949-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-2-LOC-2(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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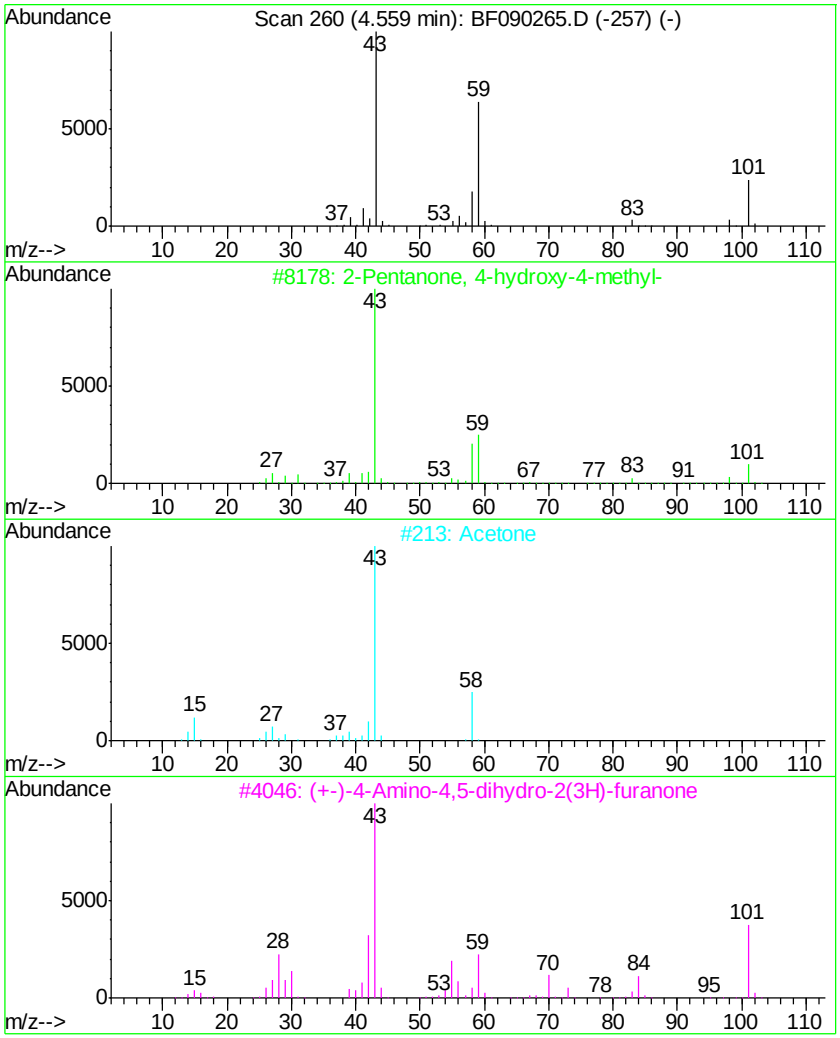
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

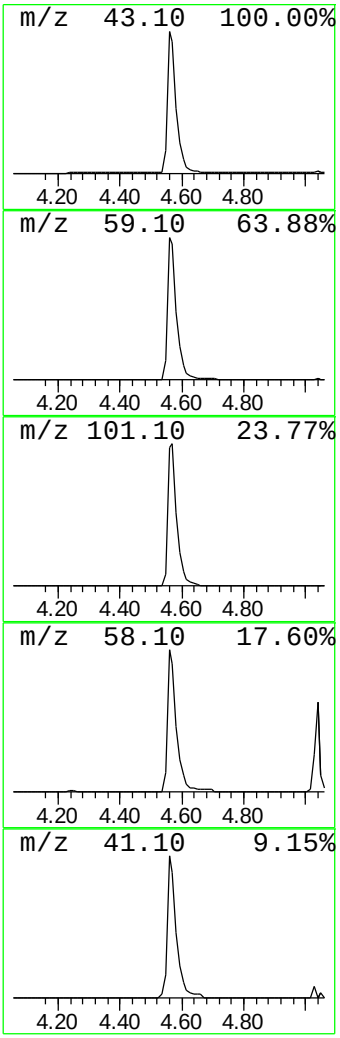
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	17.85 ng	671701	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetone	58	C3H6O	000067-64-1	9
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

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Sample : H4949-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-2-LOC-2(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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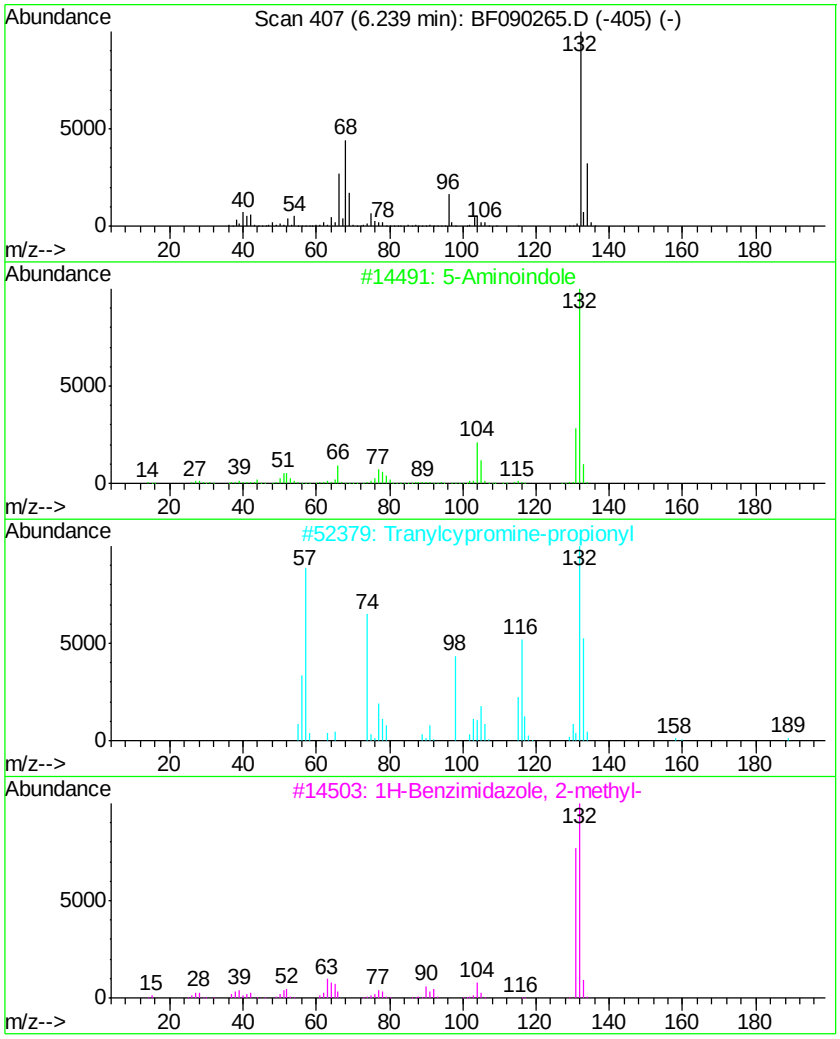
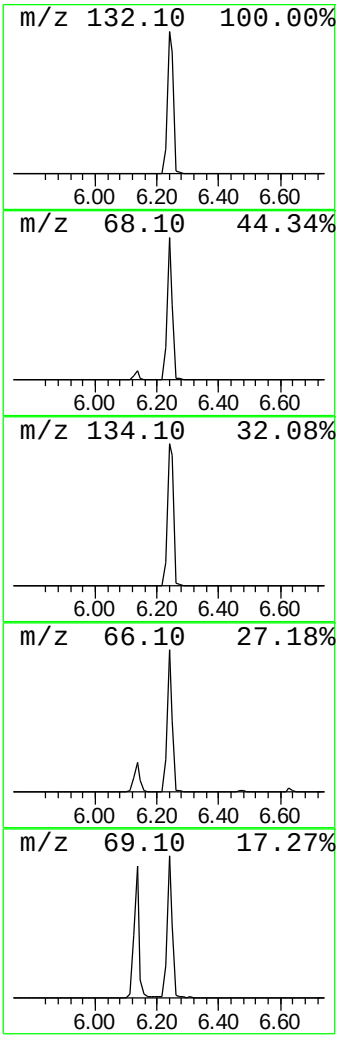
Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	83.05 ng	3125250	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090265.D
Acq On : 27 Sep 2016 21:22
Operator : UM/SJ
Sample : H4949-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-2-LOC-2(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

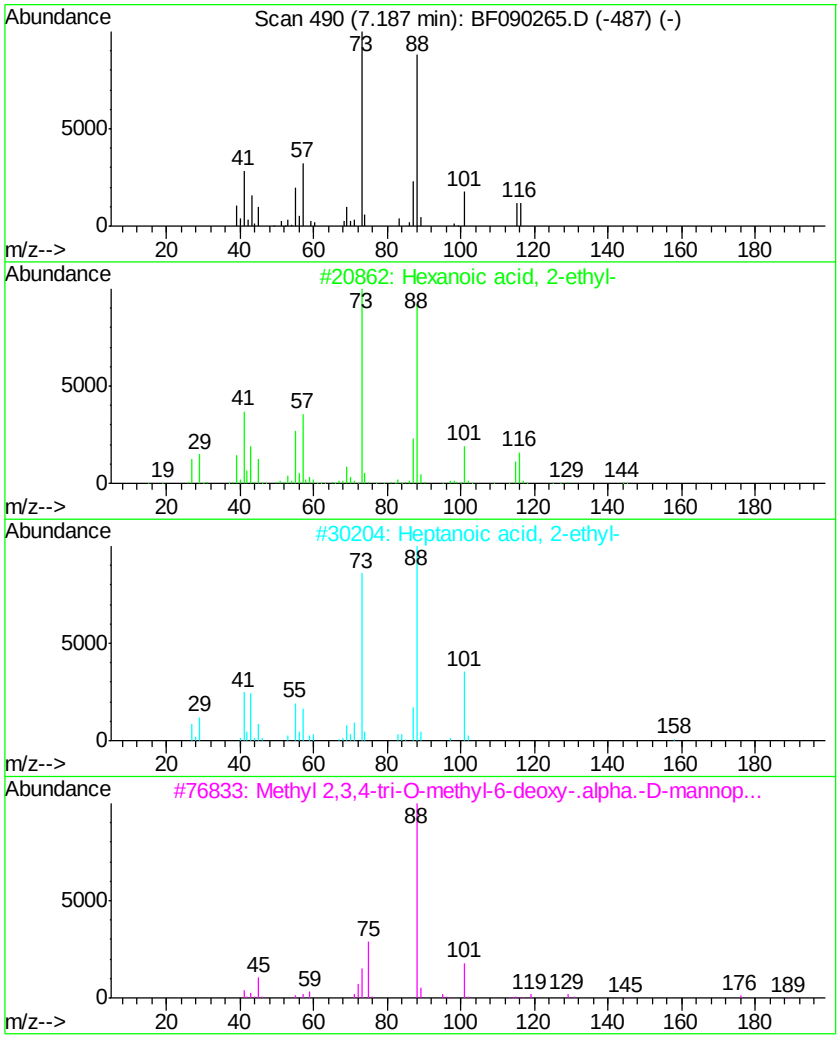
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

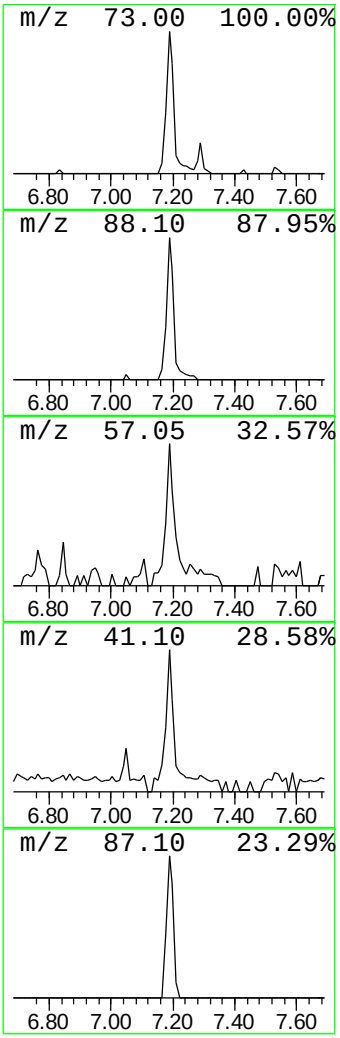
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	2.04 ng	102182	Naphthalene-d8	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
4	1,4-Dioxane	88	C4H8O2	000123-91-1	37
5	Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	36





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092716\
Data File : BF090265.D
Acq On : 27 Sep 2016 21:22
Operator : UM/SJ
Sample : H4949-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-2-LOC-2(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

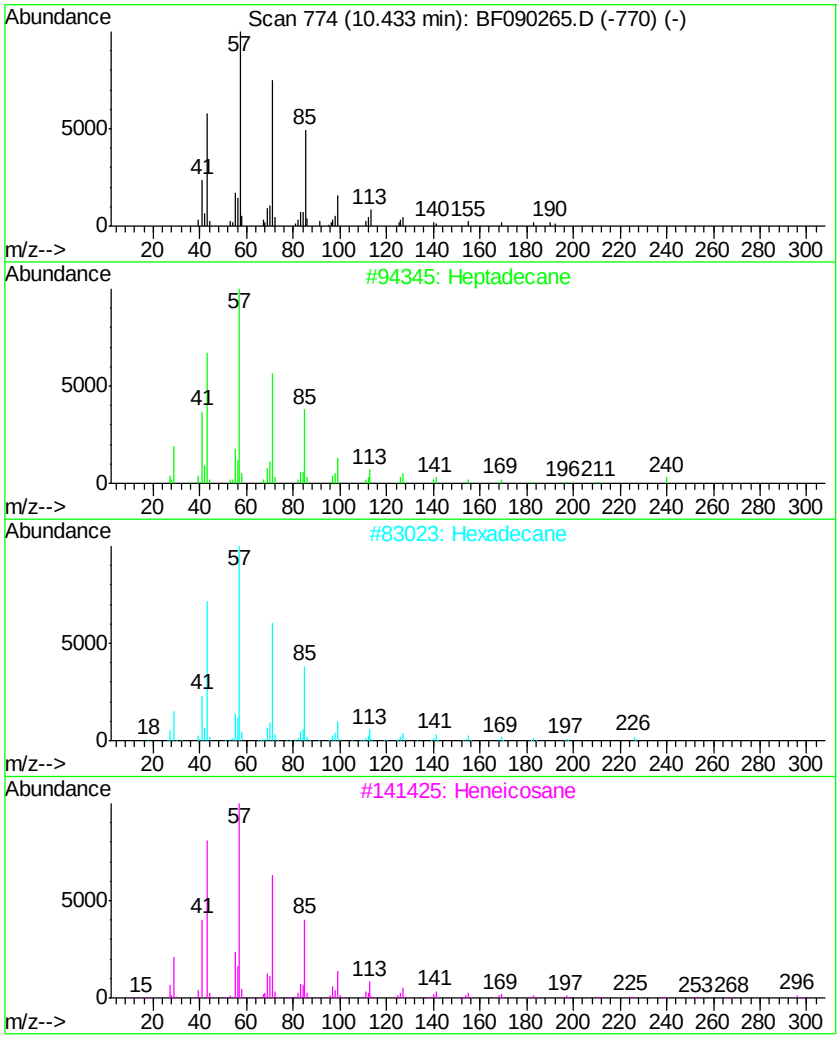
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

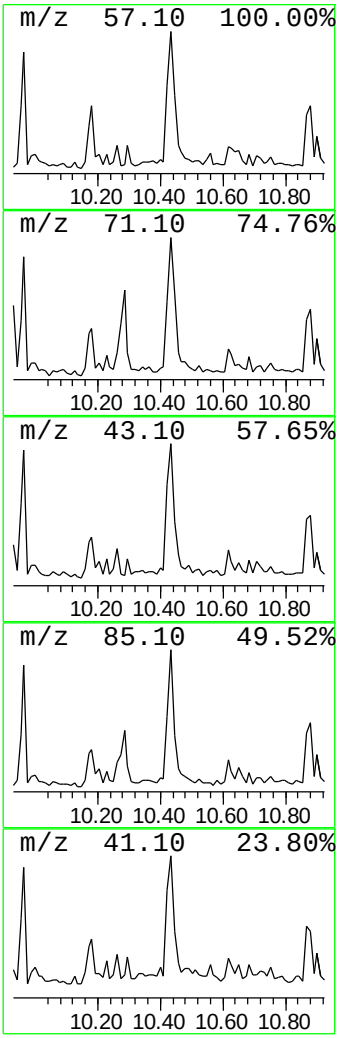
****

Peak Number 6 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	3.59 ng	169925	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Octadecane	254	C18H38	000593-45-3	86





Library Search Compound Report

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Operator : UM/SJ
Sample : H4949-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2-2-LOC-2(10-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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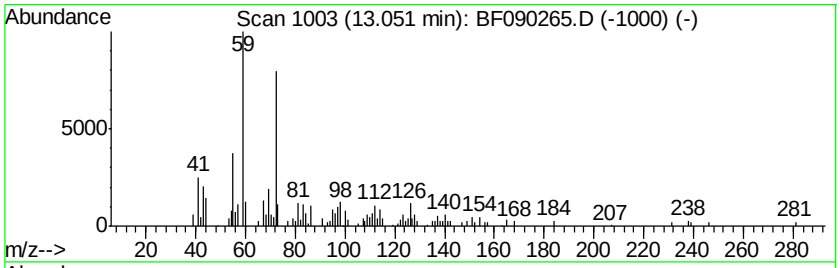
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

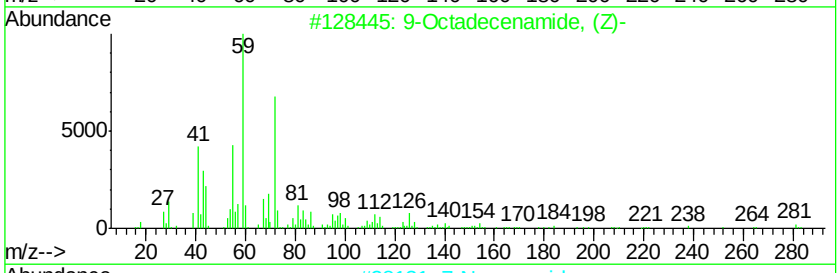
****

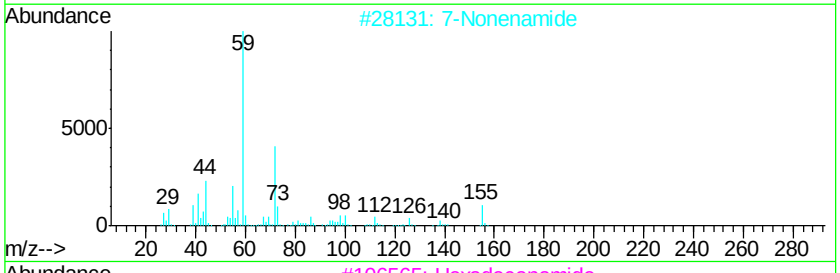
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

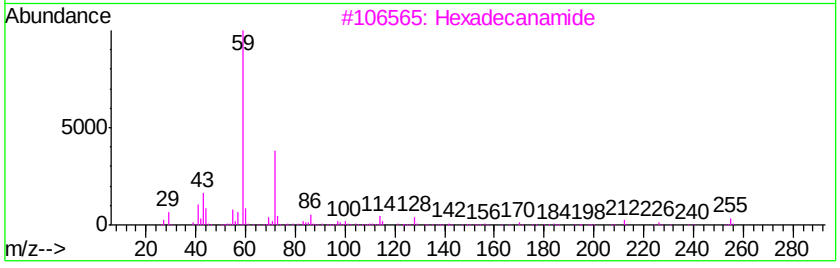
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.05	2.76 ng	131809	Chrysene-d12	13.58

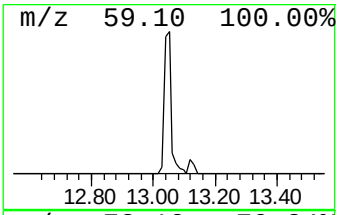
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	7-Nonenamide	155	C9H17NO	090949-53-4	53
3	Hexadecanamide	255	C16H33NO	000629-54-9	50
4	Dodecanamide	199	C12H25NO	001120-16-7	43
5	14-Hydroxy-14-methylpentadecanoi...	272	C16H32O3	091544-39-7	38

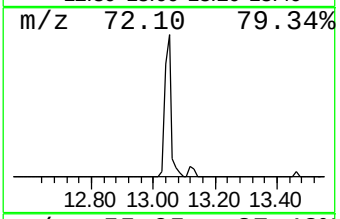


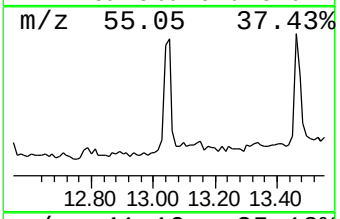


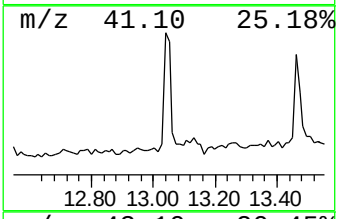


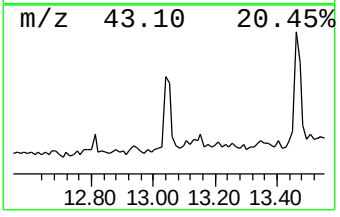












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

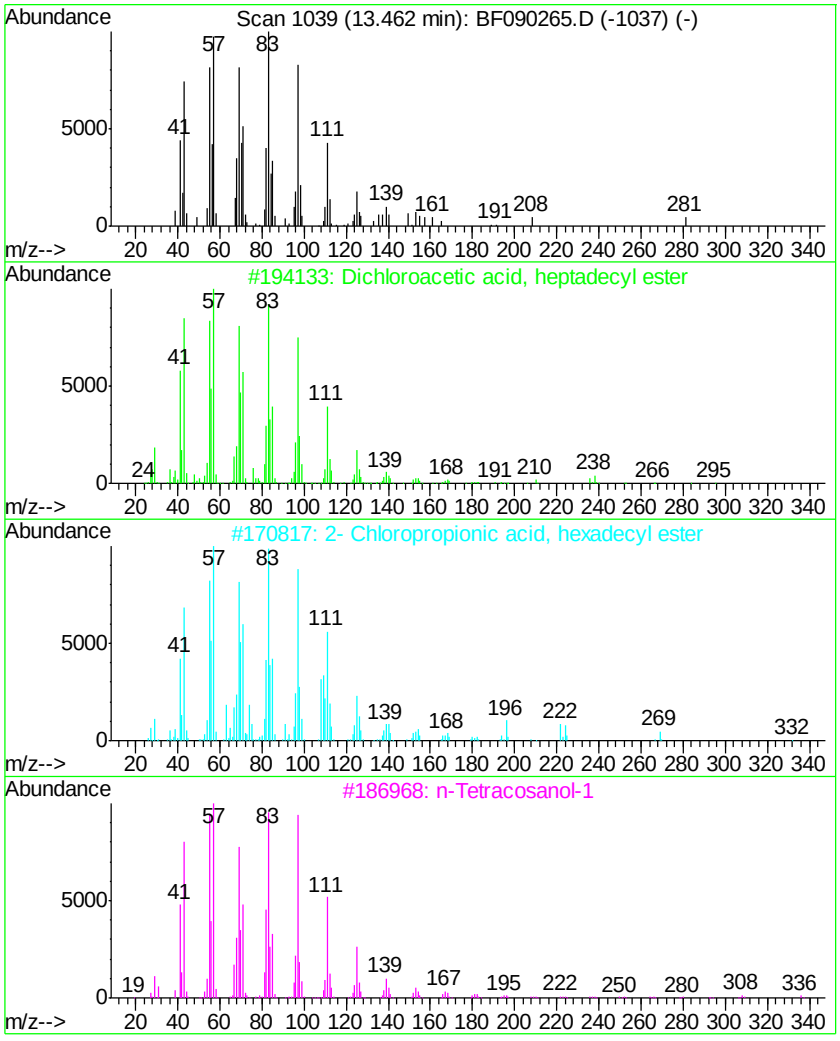
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

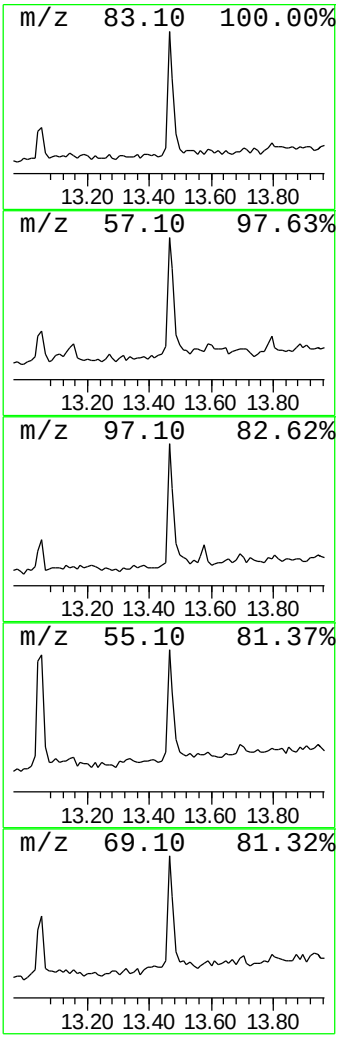
****

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	2.06 ng	98512	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.56	17.9	ng	671701	1	6.48	752649	20.0
unknown6.24	6.24	83.0	ng	3125250	1	6.48	752649	20.0
Hexanoic acid, 2-...	7.19	2.0	ng	102182	2	7.76	1004100	20.0
Heptadecane	10.43	3.6	ng	169925	4	10.97	946707	20.0
9-Octadecenamide,...	13.05	2.8	ng	131809	5	13.58	955109	20.0
Dichloroacetic ac...	13.46	2.1	ng	98512	5	13.58	955109	20.0