LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
Data File : BF082021.D
Acq On : 3 Oct 2015 14:58
Operator : UM/IZ
Sample : G3857-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A3-COMP

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-BF092815.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	5.074	253	257	268	rBV	863141	1280944	37.78%	4.831%
2	5.486	290	293	295	rBV	2213257	2584000	76.22%	9.746%
3	6.514	380	383	385	rBV	2147481	2315737	68.31%	8.734%
4	6.652	392	395	398	rBV	2511281	2485112	73.30%	9.373%
5	6.880	414	415	424	rVB	319392	470294	13.87%	1.774%
6	7.040	427	429	432	rBV	2200197	1981748	58.46%	7.475%
7	7.452	462	465	471	rBV	1400559	1508920	44.51%	5.691%
8	8.172	525	528	530	rBV	678390	613652	18.10%	2.314%
9	9.258	620	623	625	rBV	2261129	3164843	93.35%	11.937%
10	9.646	655	657	660	rBV	559426	508092	14.99%	1.916%
11	9.932	679	682	684	rBV	871829	793544	23.41%	2.993%
12	10.366	715	720	721	rBV2	23760	46258	1.36%	0.174%
13	10.721	749	751	754	rBV2	1516823	1910810	56.36%	7.207%
14	10.835	759	761	766	rVB	57126	75082	2.21%	0.283%
15	11.281	798	800	806	rVB2	32737	53606	1.58%	0.202%
16	11.418	810	812	821	rBV	611113	819406	24.17%	3.091%
17	12.732	925	927	929	rVB	83094	90415	2.67%	0.341%
18	12.835	933	936	938	rBV	241224	278065	8.20%	1.049%
19	12.869	938	939	941	rVB2	88408	113304	3.34%	0.427%
20	13.018	949	952	955	rBV	3109360	3390180	100.00%	12.787%
21	13.475	990	992	995	rBV	30066	44910	1.32%	0.169%
22	13.544	995	998	1000	rVV	93613	84360	2.49%	0.318%
23	13.921	1029	1031	1041	rBV	56424	147884	4.36%	0.558%
24	14.069	1041	1044	1053	rVV	719471	831737	24.53%	3.137%
25	14.835	1108	1111	1117	rBV	258422	341820	10.08%	1.289%
26	15.532	1168	1172	1182	rBV	332362	578691	17.07%	2.183%

Sum of corrected areas: 26513414

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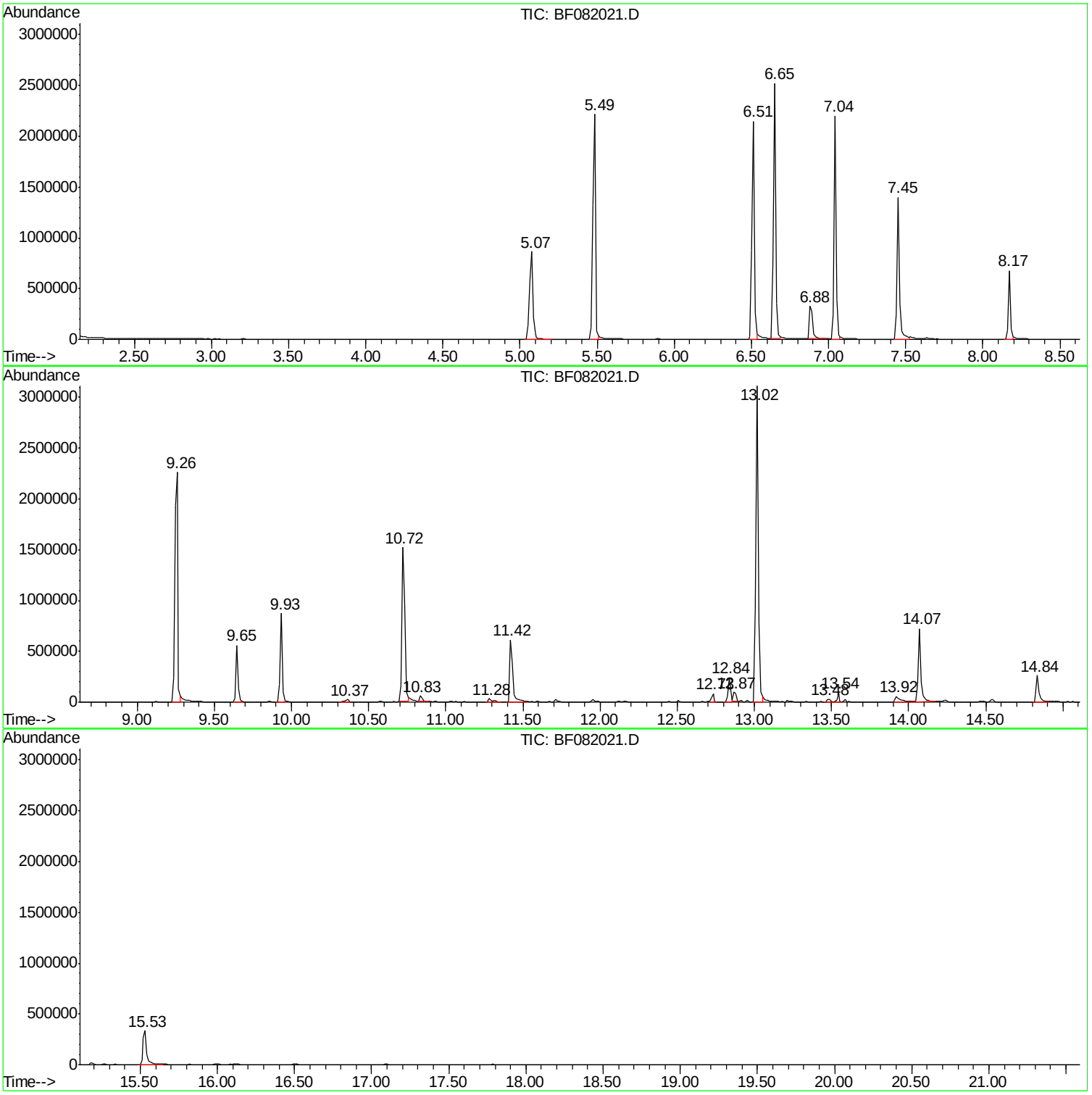
BNA_F
ClientSampleId :
A3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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TIC Library : C:\DATABASE\NIST02.L
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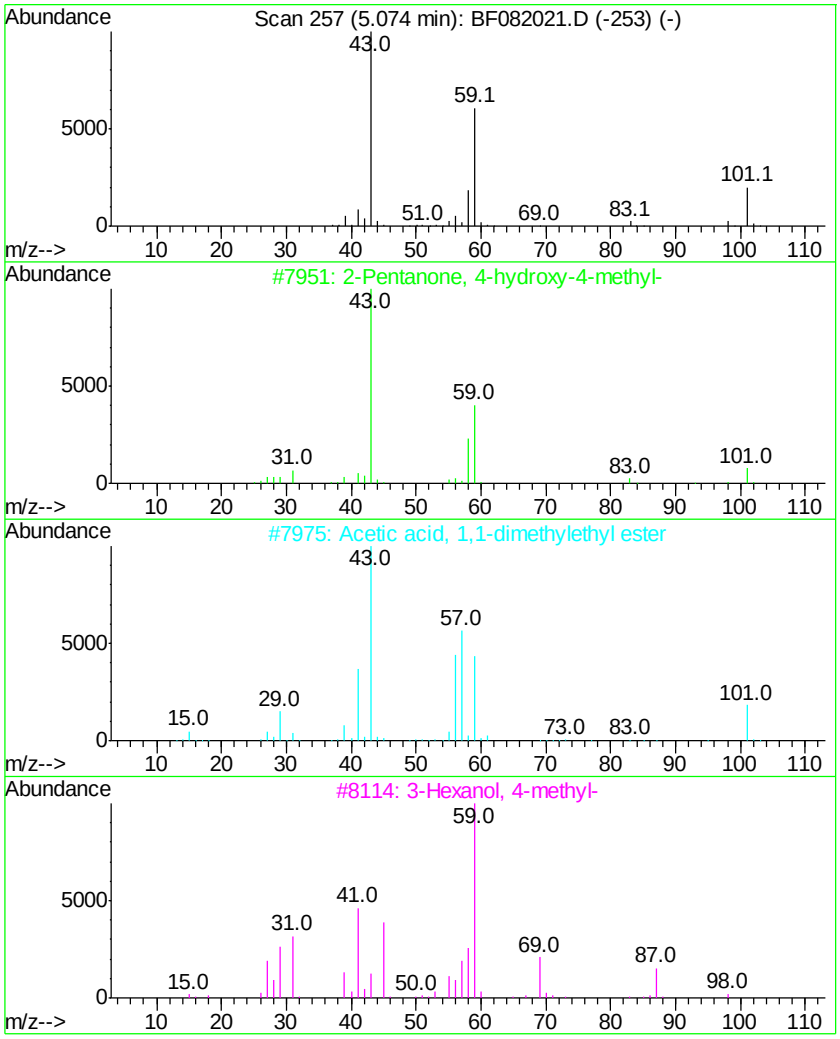
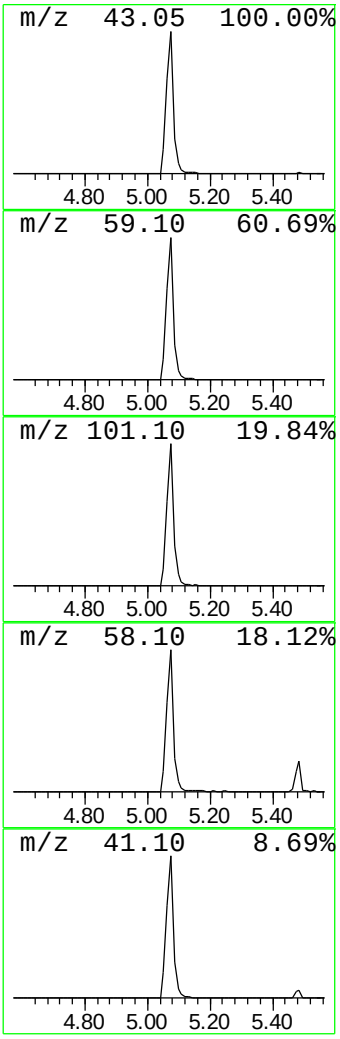
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	54.47 ng	1280940	1,4-Dichlorobenzene-d4	6.89

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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	9





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Acq On : 3 Oct 2015 14:58
Operator : UM/IZ
Sample : G3857-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

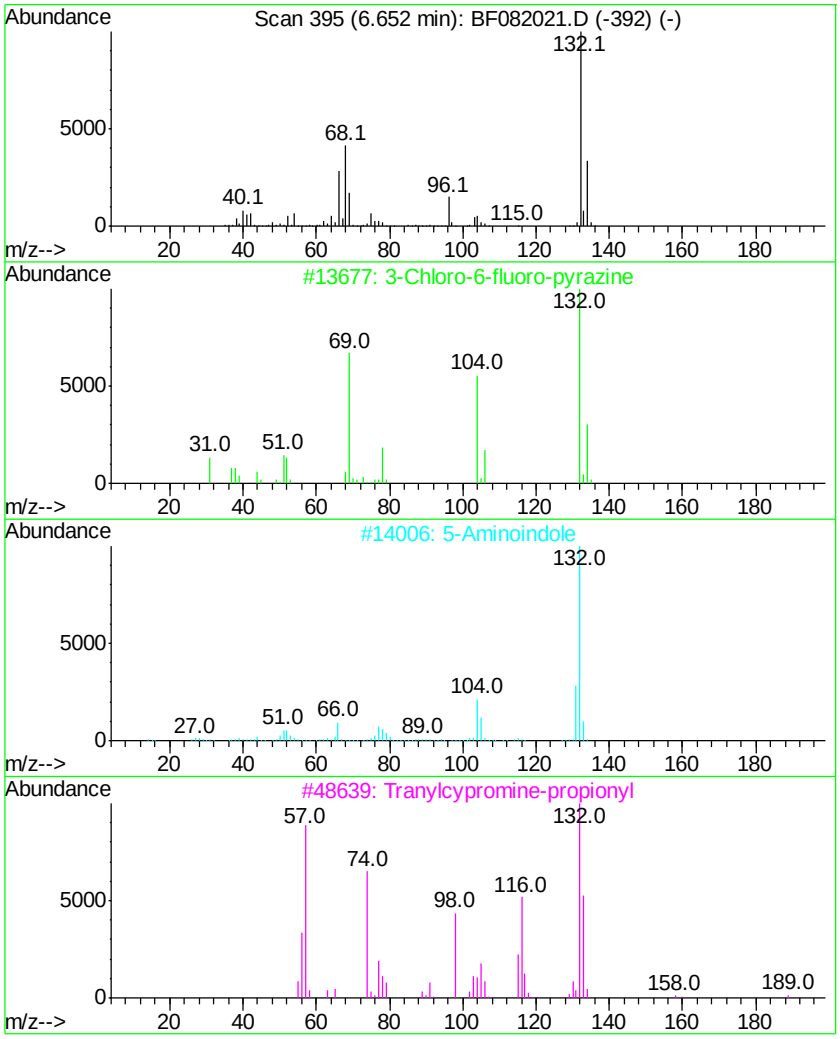
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

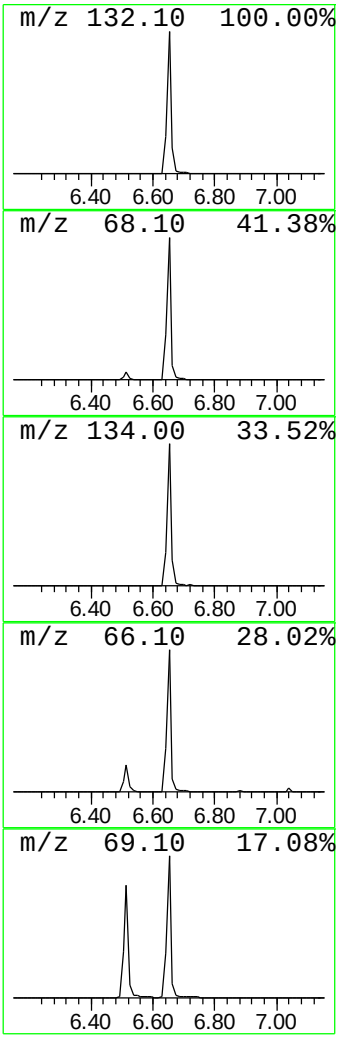
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	105.68 ng	2485110	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
ClientSampleId : A3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
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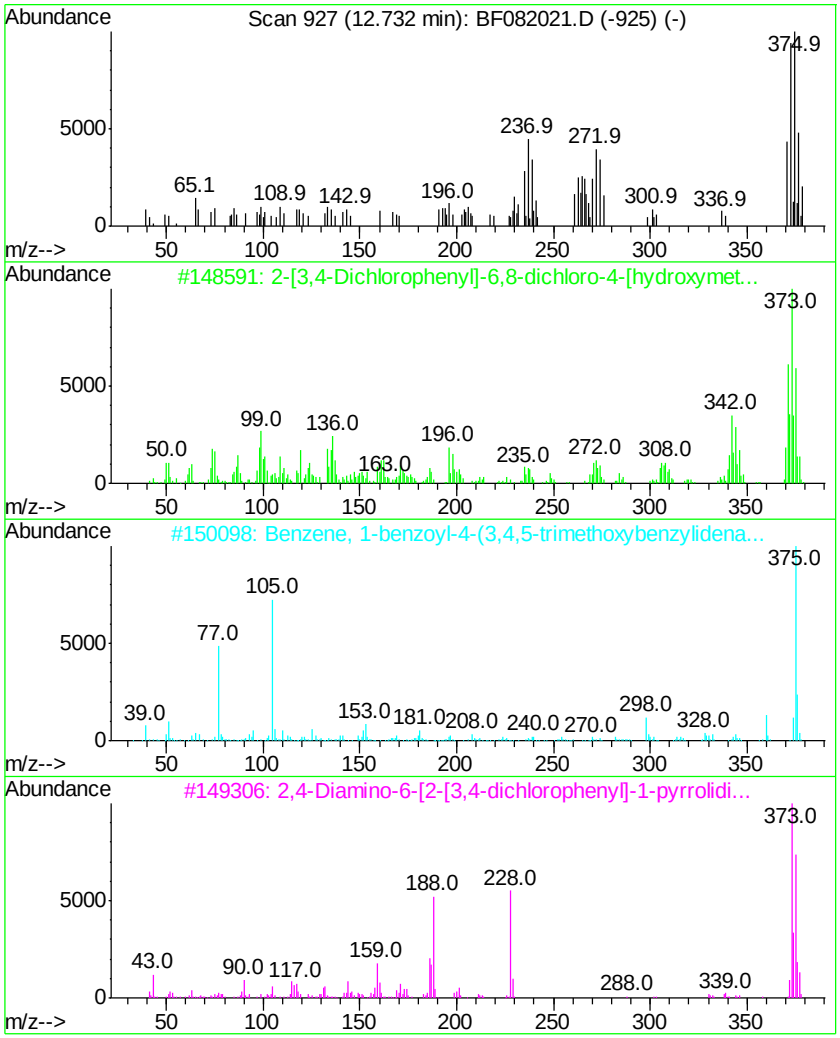
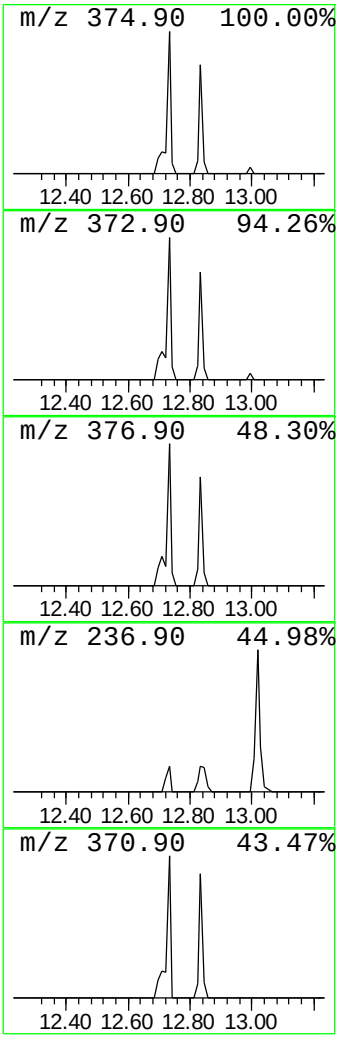
Peak Number 4 unknown12.73 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.21 ng	90415	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[3,4-Dichlorophenyl]-6,8-dichl...	371	C16H9Cl4NO	038599-01-8	25
2	Benzene, 1-benzoyl-4-(3,4,5-trim...	375	C23H21NO4	304668-83-5	9
3	2,4-Diamino-6-[2-[3,4-dichloroph...	373	C18H17Cl2N5	038918-48-8	9
4	4-Pyridinol, 3,5-diiodo-2,6-dime...	375	C7H7I2NO	004563-30-8	9
5	Quinoline, N-oxy-4-[2-[3-[p-chlo...	373	C23H16ClNO2	1000211-32-6	9





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Operator : UM/IZ
Sample : G3857-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

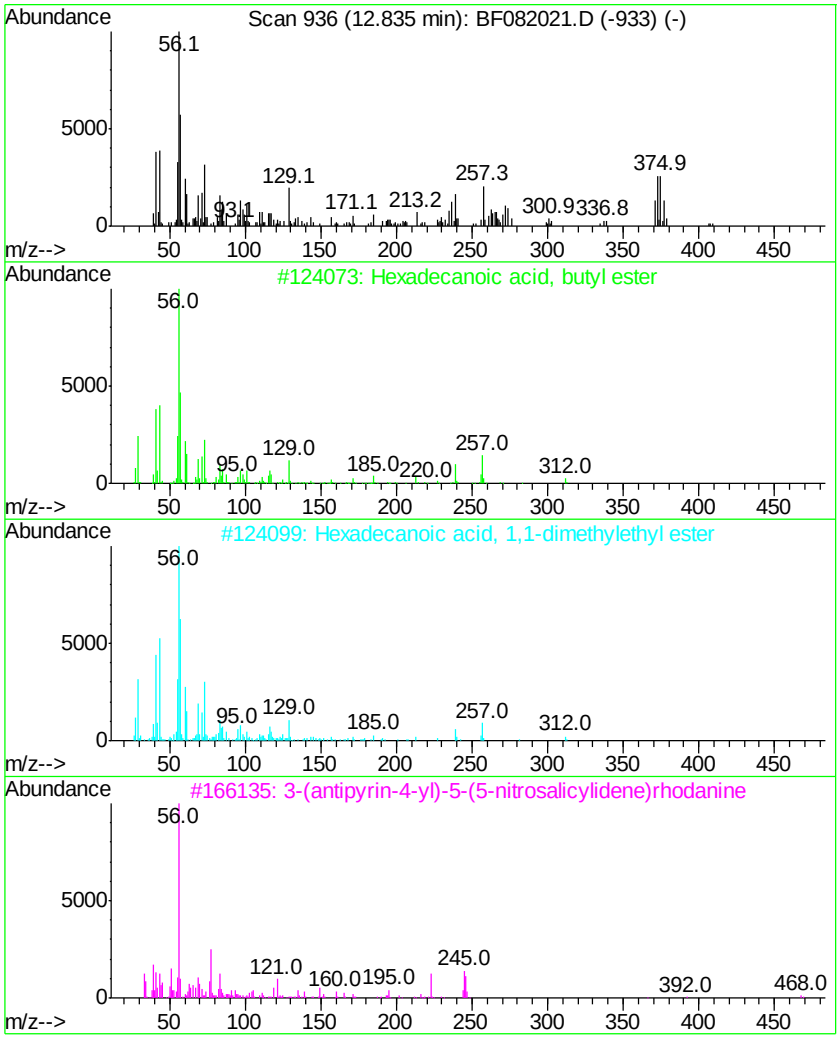
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

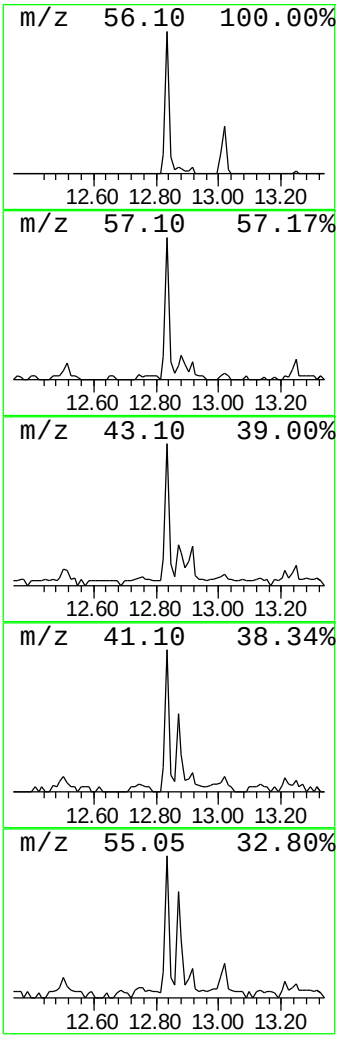
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	6.69 ng	278065	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	50
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	38
3	3-(antipyrin-4-yl)-5-(5-nitrosal...	468	C21H16N4O5S2	314275-32-6	16
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	10
5	2-Propen-1-amine	57	C3H7N	000107-11-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100215\
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Sample : G3857-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

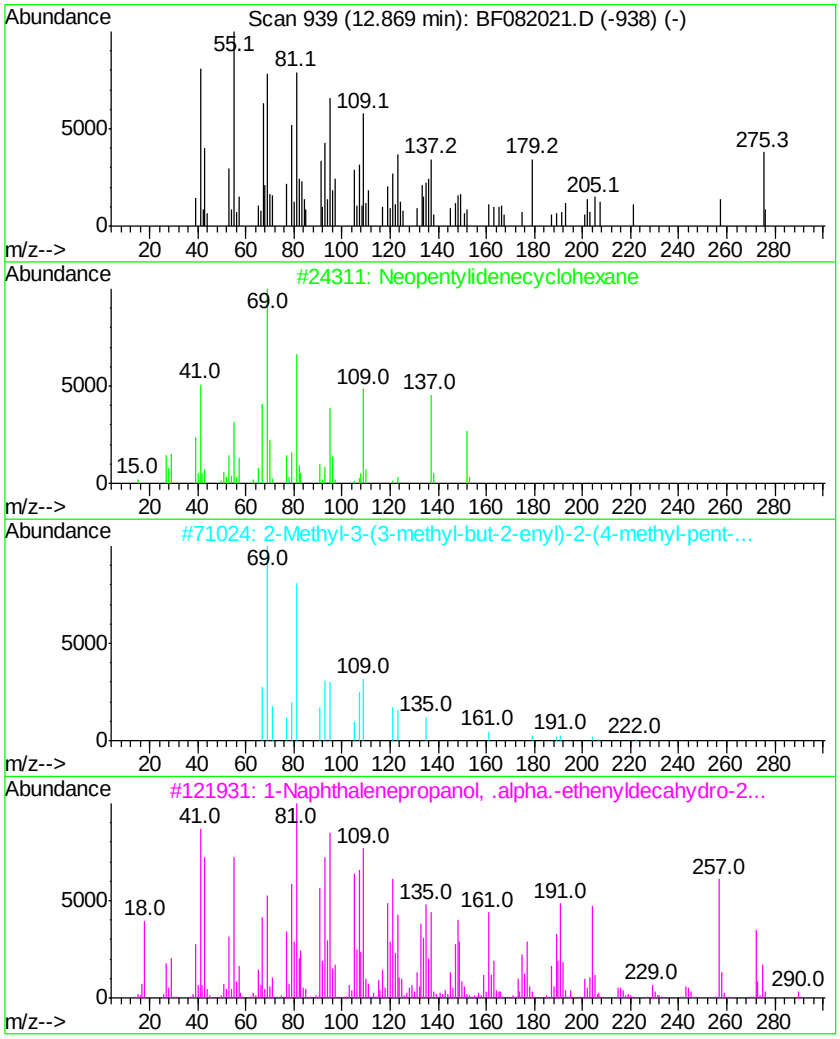
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

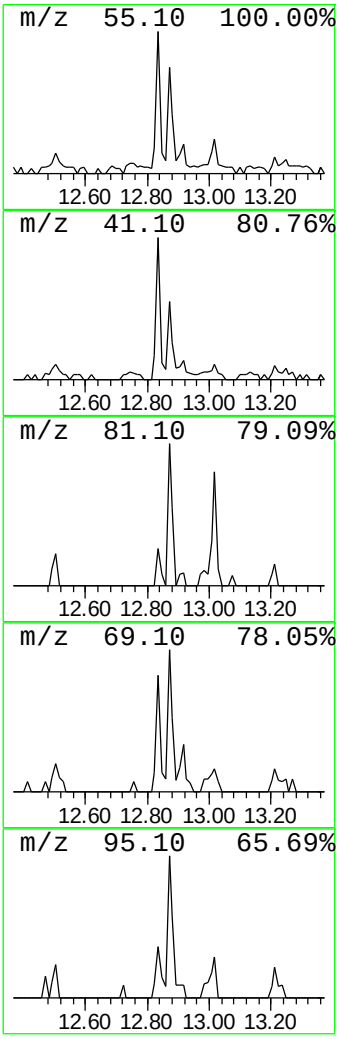
****

Peak Number 6 Neopentylidenecyclohexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.72 ng	113304	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentylidenecyclohexane	152	C11H20	039546-80-0	64
2	2-Methyl-3-(3-methyl-but-2-enyl)...	222	C15H26O	1000144-10-2	47
3	1-Naphthalenepropanol, .alpha.-e...	308	C20H36O2	000515-03-7	35
4	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	30
5	2,2,4-Trimethyl-3-(3,8,12,16-tet...	428	C30H52O	1000194-01-4	25





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Sample : G3857-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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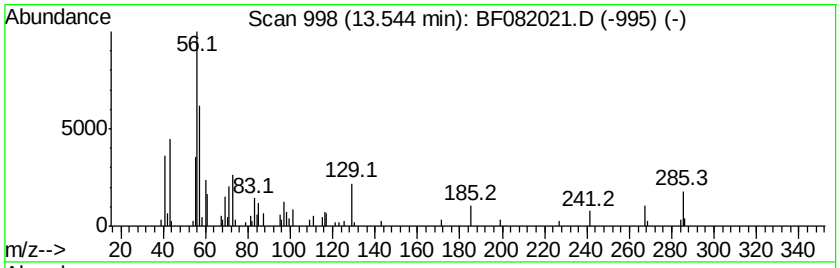
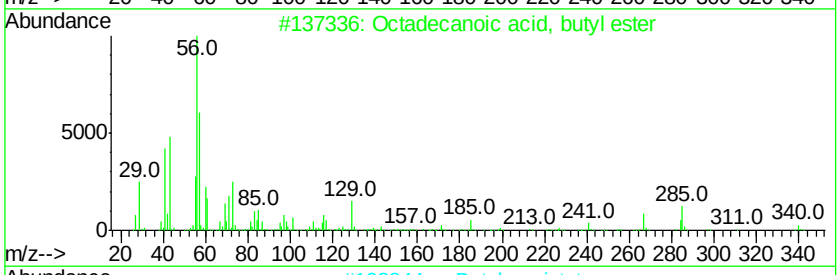
****

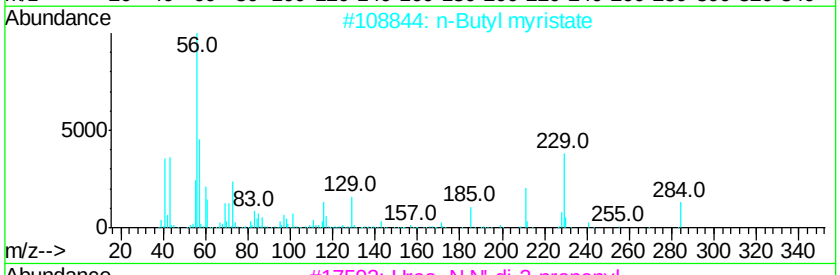
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 9

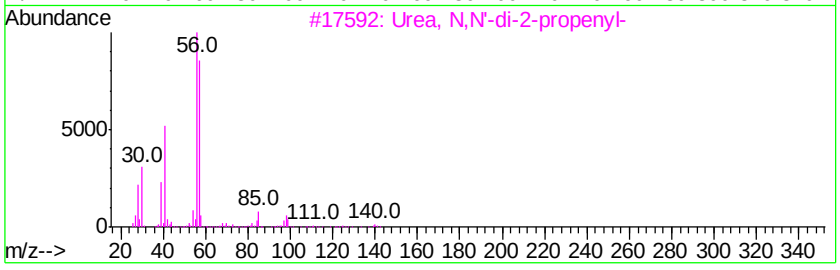
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	2.03 ng	84360	Chrysene-d12	14.07

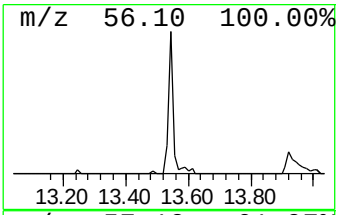
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	n-Butyl myristate	284	C18H36O2	000110-36-1	83
3	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
4	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27

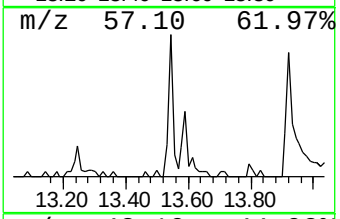


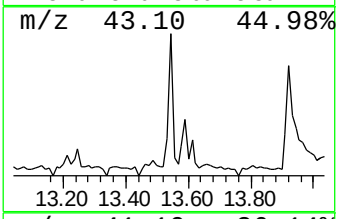


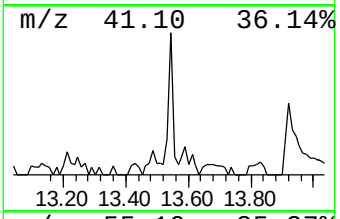


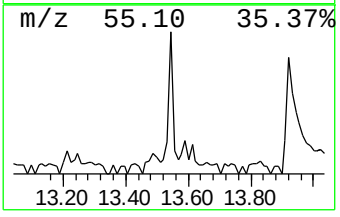












Library Search Compound Report

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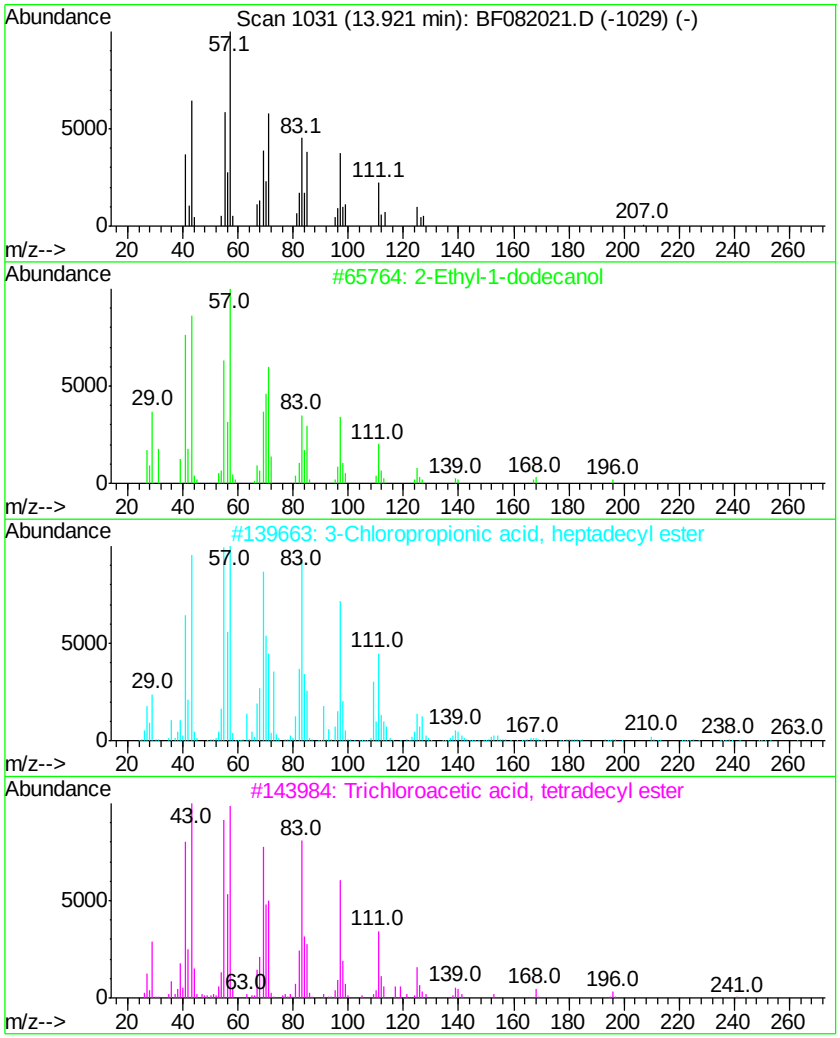
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

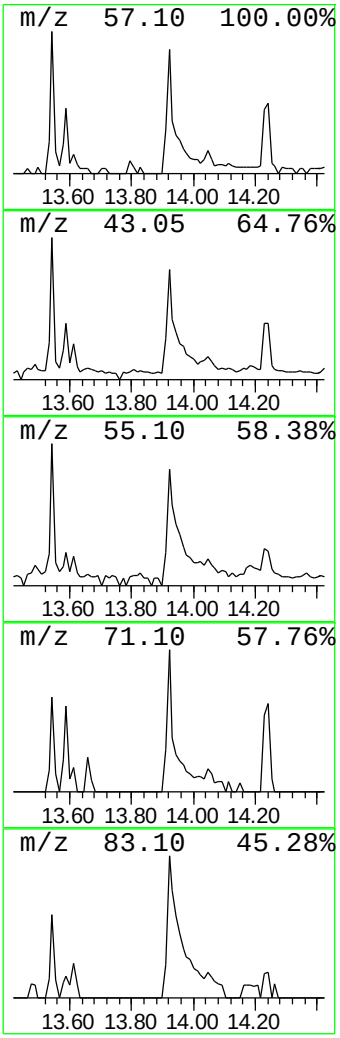
****

Peak Number 8 2-Ethyl-1-dodecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.56 ng	147884	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	90
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	64
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	62
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	58
5	1-Docosene	308	C22H44	001599-67-3	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

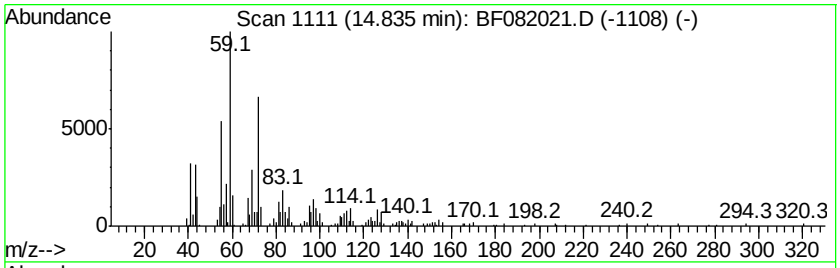
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

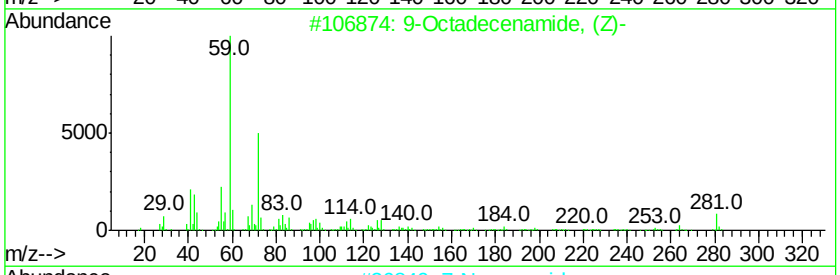
****

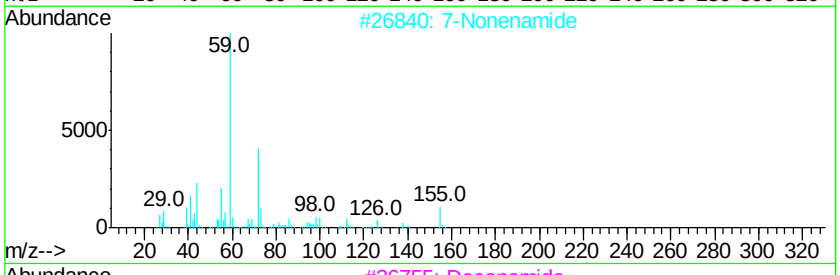
Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 4

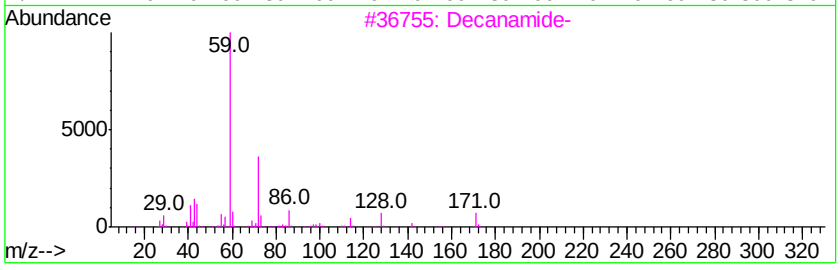
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	11.81 ng	341820	Perylene-d12	15.53

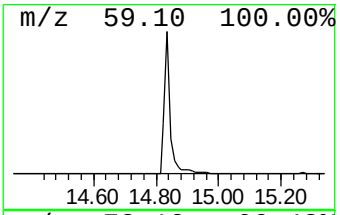
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	7-Nonenamide	155	C9H17NO	090949-53-4	64
3	Decanamide-	171	C10H21NO	002319-29-1	59
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
5	Dodecanamide	199	C12H25NO	001120-16-7	53

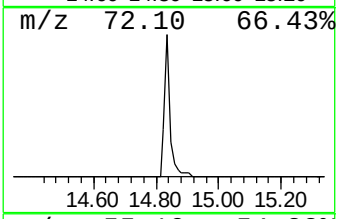


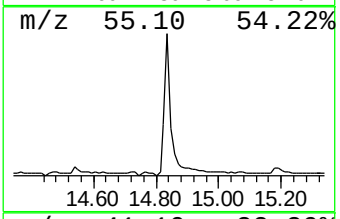


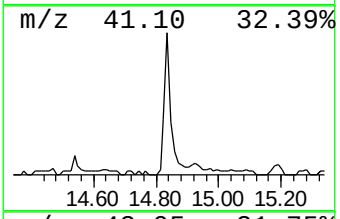


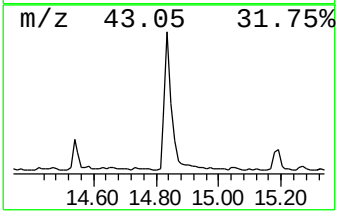












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100215\
Data File : BF082021.D
Acq On : 3 Oct 2015 14:58
Operator : UM/IZ
Sample : G3857-07
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A3-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.07	54.5	ng	1280940	1	6.89	470294	20.0
unknown6.65	6.65	105.7	ng	2485110	1	6.89	470294	20.0
unknown12.73	12.73	2.2	ng	90415	4	11.42	819406	20.0
Hexadecanoic acid...	12.84	6.7	ng	278065	5	14.07	831737	20.0
Neopentylidenecyc...	12.87	2.7	ng	113304	5	14.07	831737	20.0
Octadecanoic acid...	13.54	2.0	ng	84360	5	14.07	831737	20.0
2-Ethyl-1-dodecanol	13.92	3.6	ng	147884	5	14.07	831737	20.0
9-Octadecenamide,...	14.84	11.8	ng	341820	6	15.53	578691	20.0