LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081470.D
Acq On : 5 Sep 2015 17:52
Operator : UM/IZ
Sample : G3559-04
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP224BR-23-25

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-BF090115.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	4.399	243	246	263	rVB	504489	1075001	51.64%	6.114%
2	4.902	288	290	293	rBV	1285106	1816425	87.26%	10.332%
3	6.033	386	389	391	rBV	1571573	2081712	100.00%	11.840%
4	6.125	395	397	399	rBV	1988719	1808381	86.87%	10.286%
5	6.353	415	417	420	rVB	404847	350658	16.84%	1.994%
6	6.513	429	431	433	rBV	1509897	1354047	65.04%	7.702%
7	6.936	465	468	470	rBV	1217410	1216047	58.42%	6.917%
8	7.645	528	530	532	rBV	543554	451453	21.69%	2.568%
9	8.730	622	625	627	rBV	2190709	1974629	94.86%	11.231%
10	9.131	658	660	663	rBV	465706	416141	19.99%	2.367%
11	9.382	680	682	685	rVB	491138	452526	21.74%	2.574%
12	10.171	748	751	753	rBV	1300968	1262895	60.67%	7.183%
13	10.319	762	764	770	rVB	32513	36458	1.75%	0.207%
14	10.765	801	803	804	rBV	25799	21821	1.05%	0.124%
15	10.845	808	810	813	rVV	466189	454114	21.81%	2.583%
16	11.428	859	861	866	rBV	140707	146533	7.04%	0.833%
17	12.297	934	937	939	rBV	49647	56616	2.72%	0.322%
18	12.434	946	949	952	rBV	1616183	1631130	78.36%	9.278%
19	12.994	996	998	1000	rBV	41229	40068	1.92%	0.228%
20	13.360	1027	1030	1036	rBV	118229	240523	11.55%	1.368%
21	13.451	1036	1038	1041	rBV	355635	359161	17.25%	2.043%
22	13.977	1082	1084	1086	rBV	19603	22447	1.08%	0.128%
23	14.331	1113	1115	1117	rBV	55006	46704	2.24%	0.266%
24	14.765	1150	1153	1155	rBV	234004	265850	12.77%	1.512%

Sum of corrected areas: 17581340

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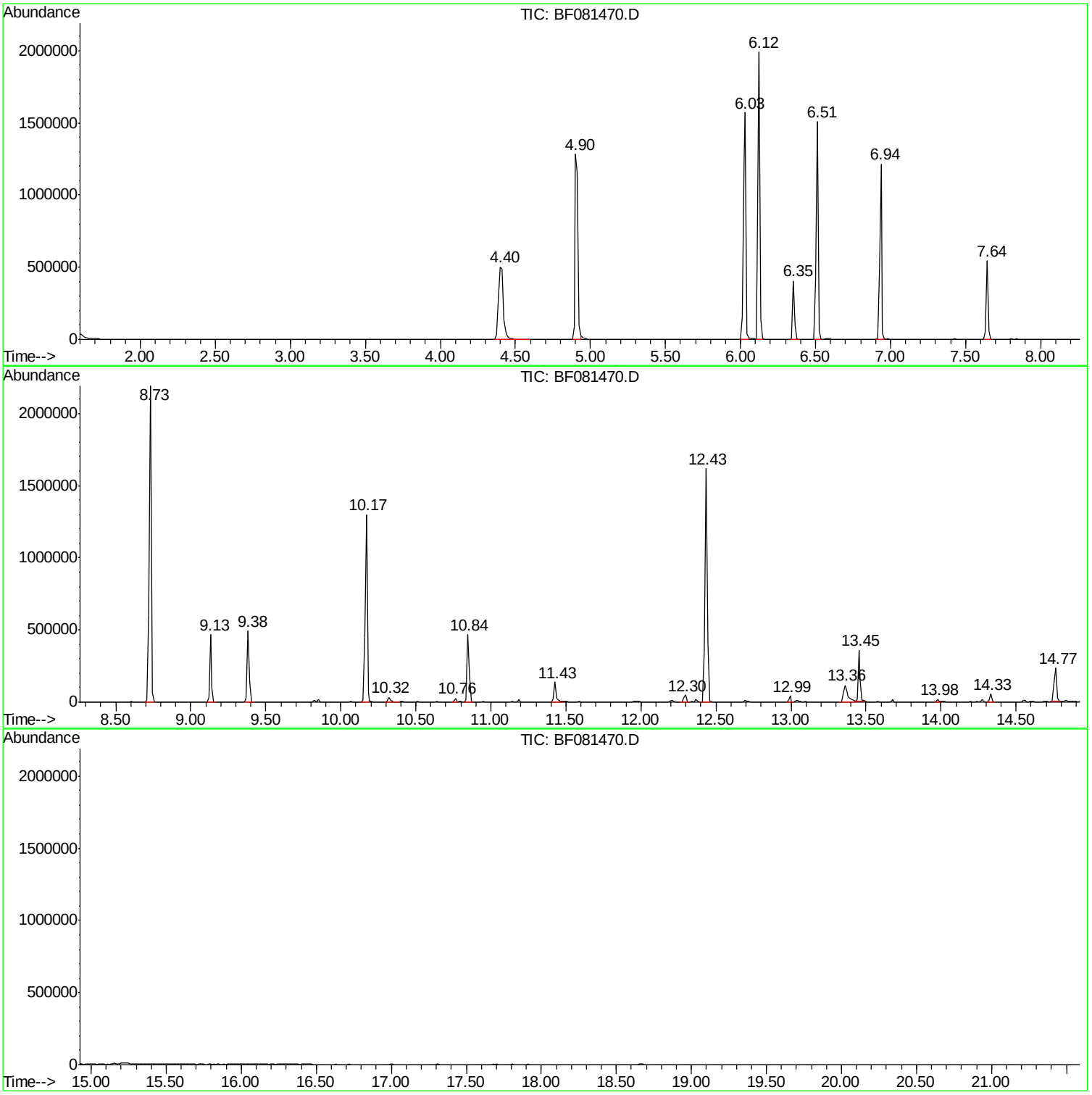
Instrument :
BNA_F
ClientSampleId :
MGP224BR-23-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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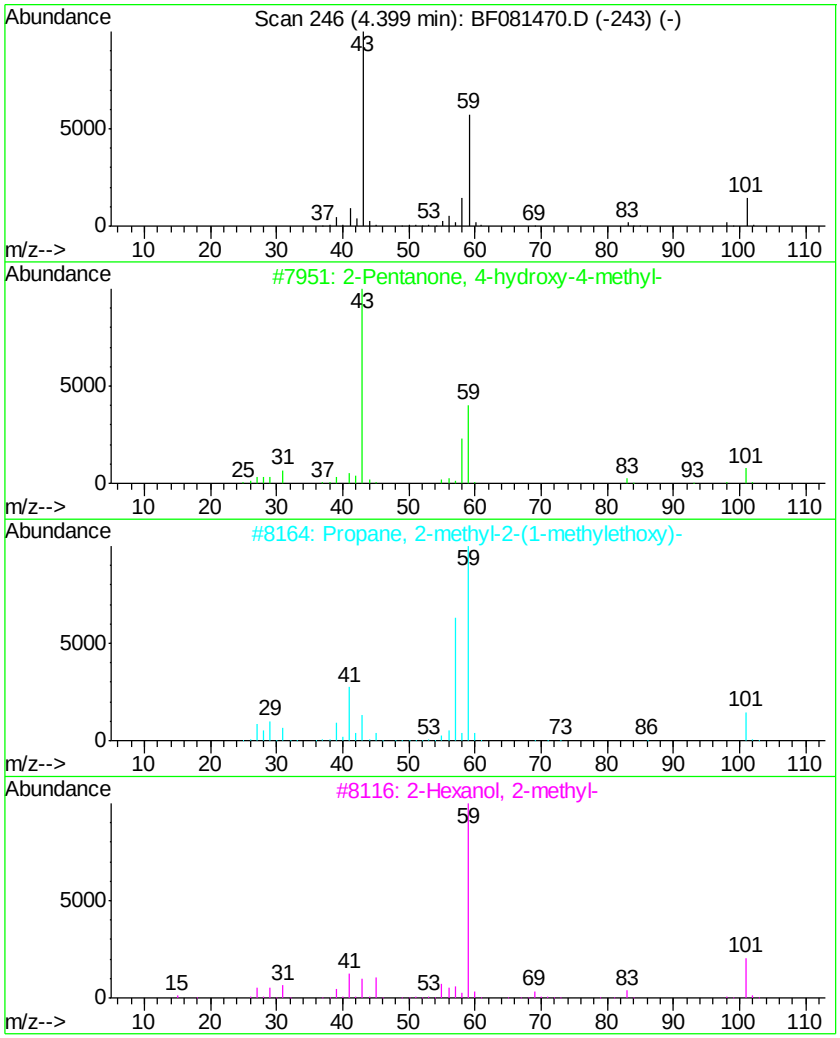
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

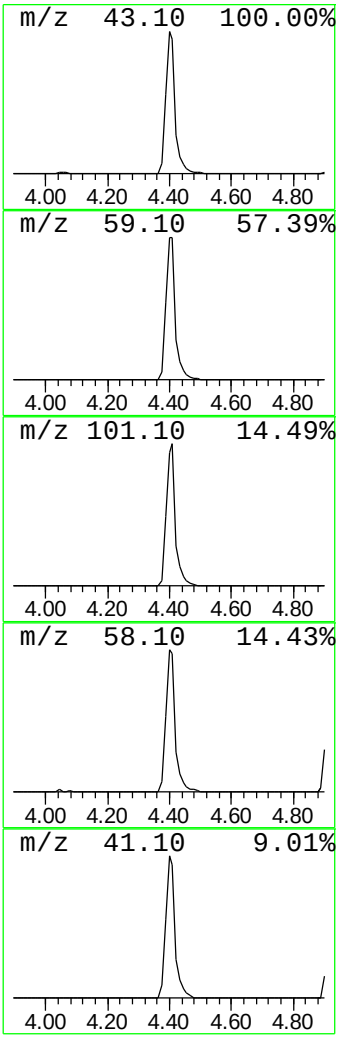
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	61.31 ng	1075000	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Instrument : BNA_F
ClientSampleId : MGP224BR-23-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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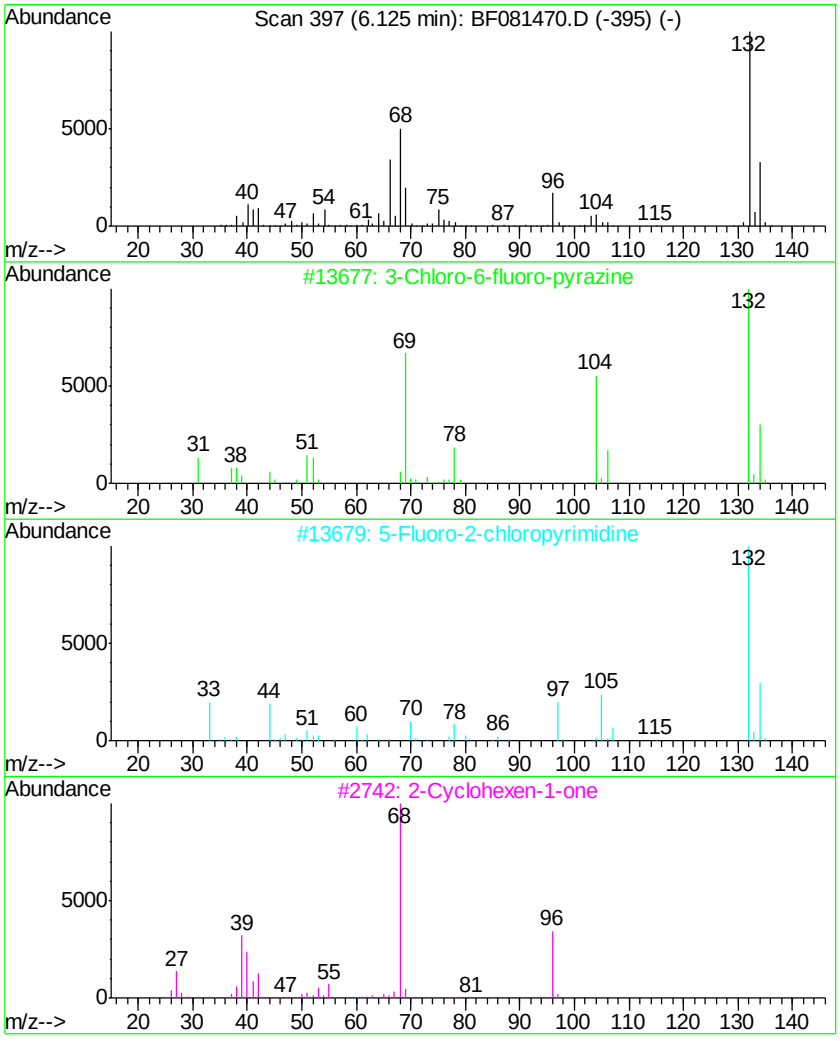
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

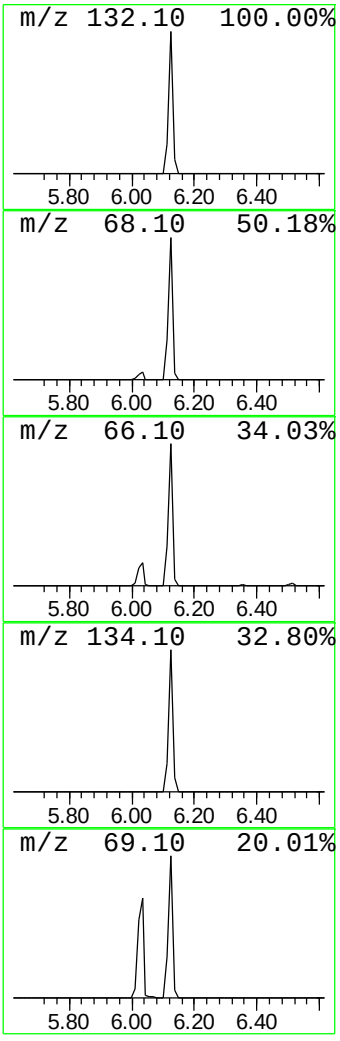
****

Peak Number 2 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	103.14 ng	1808380	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9





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Operator : UM/IZ
Sample : G3559-04
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ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP224BR-23-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
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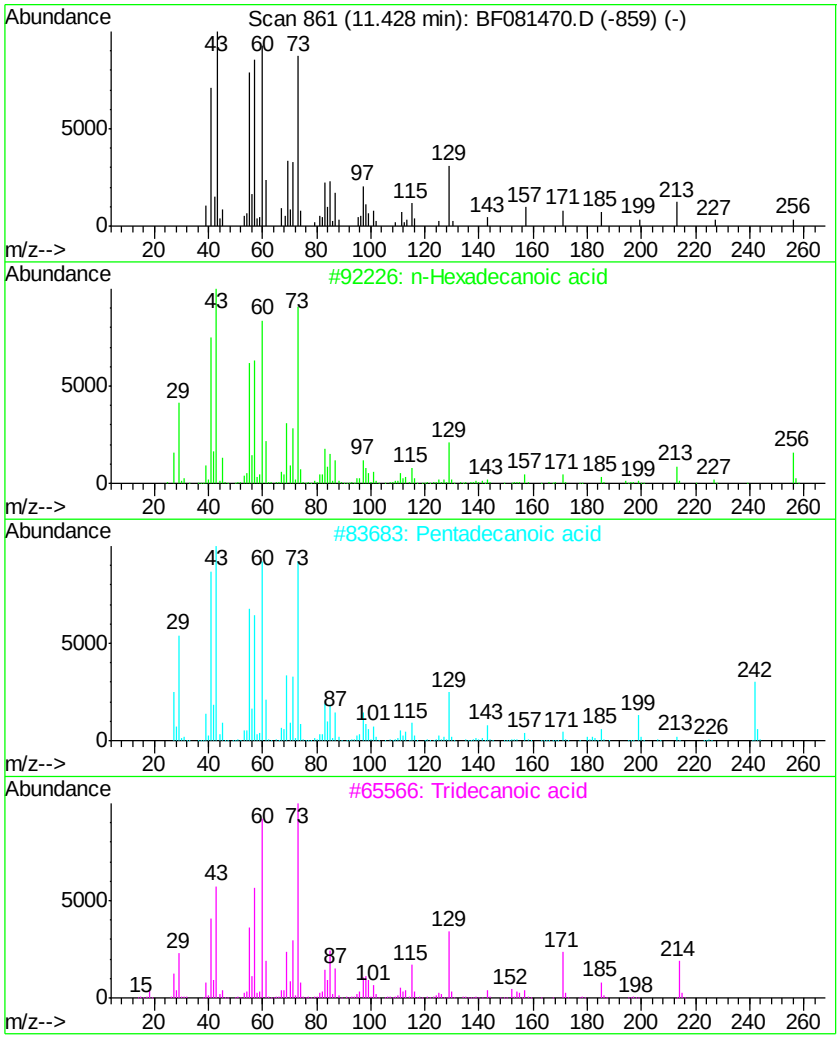
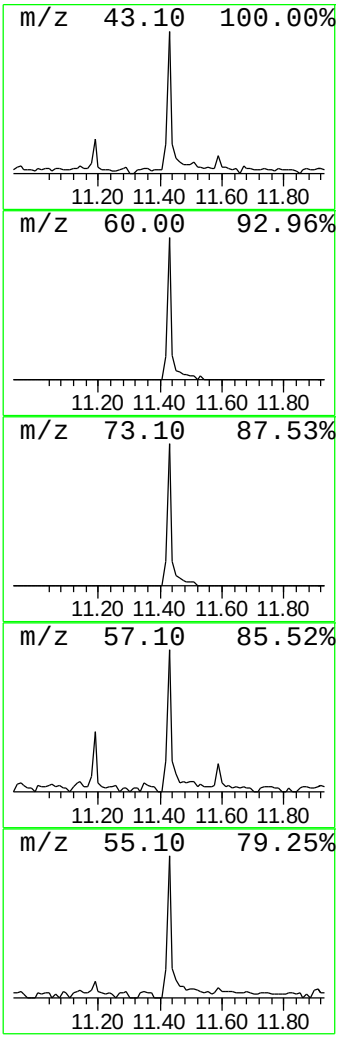
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	6.45 ng	146533	Phenanthrene-d10	10.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	80





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Acq On : 5 Sep 2015 17:52
Operator : UM/IZ
Sample : G3559-04
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP224BR-23-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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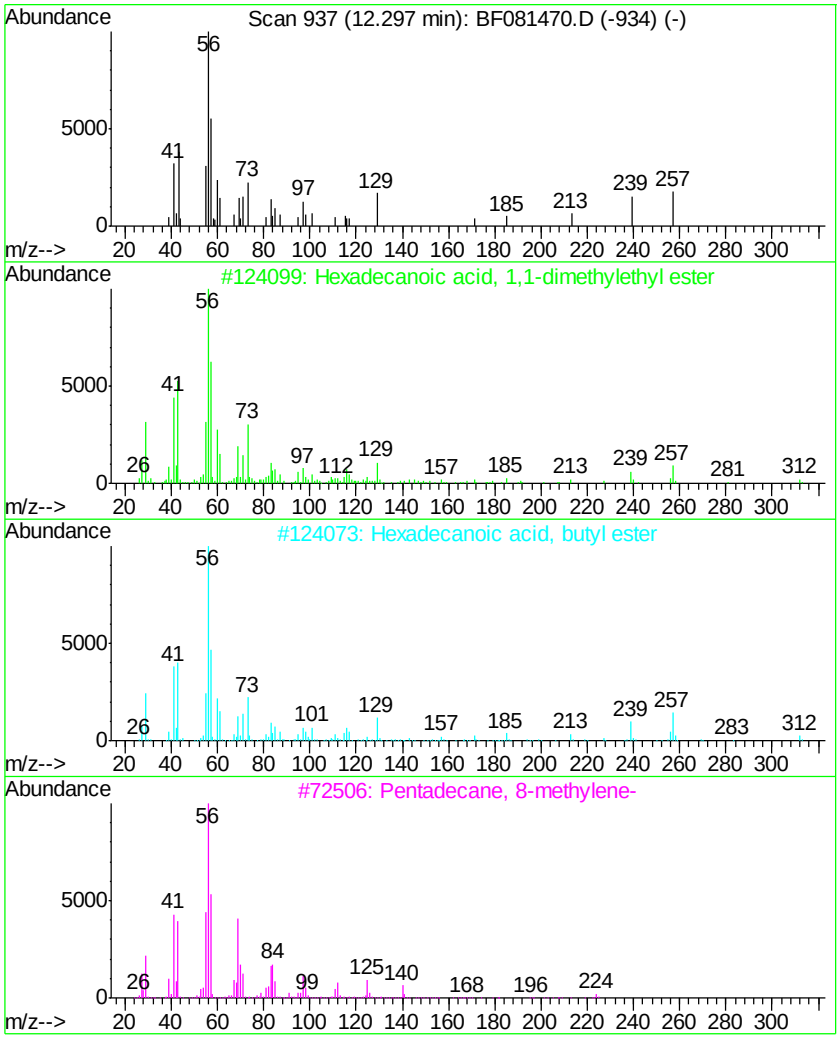
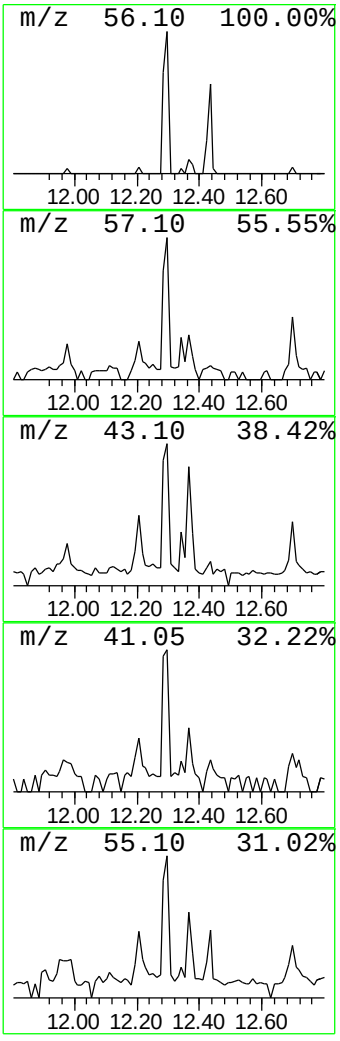
Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	3.15 ng	56616	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	43
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
4	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27
5	2-Chloro-2-methylnonane	176	C10H21Cl	004325-50-2	25





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Acq On : 5 Sep 2015 17:52
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Sample : G3559-04
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Instrument : BNA_F
ClientSampleId : MGP224BR-23-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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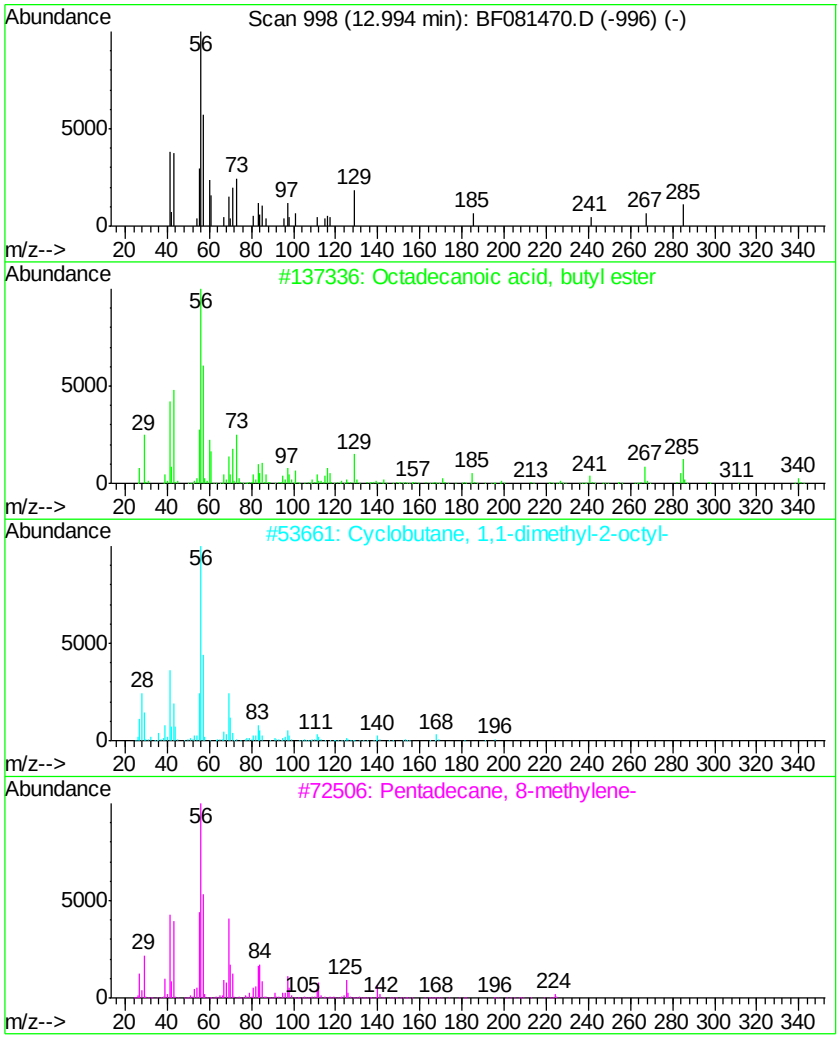
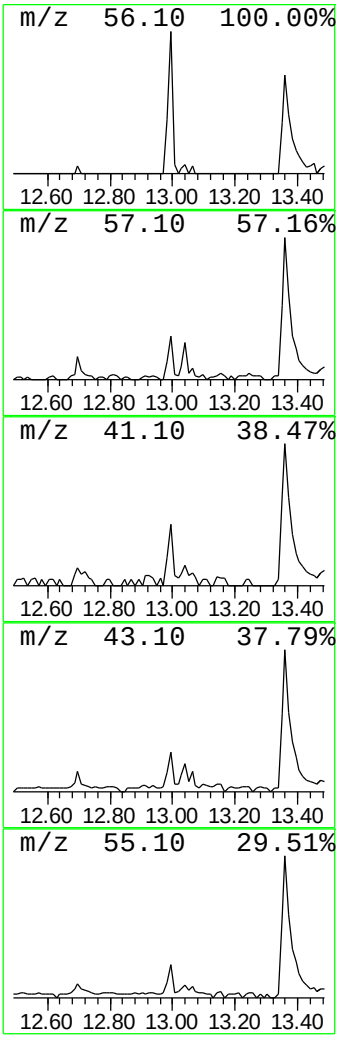
Peak Number 6 unknown12.99 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	2.23 ng	40068	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	43
2	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





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Misc :
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Instrument : BNA_F
ClientSampleId : MGP224BR-23-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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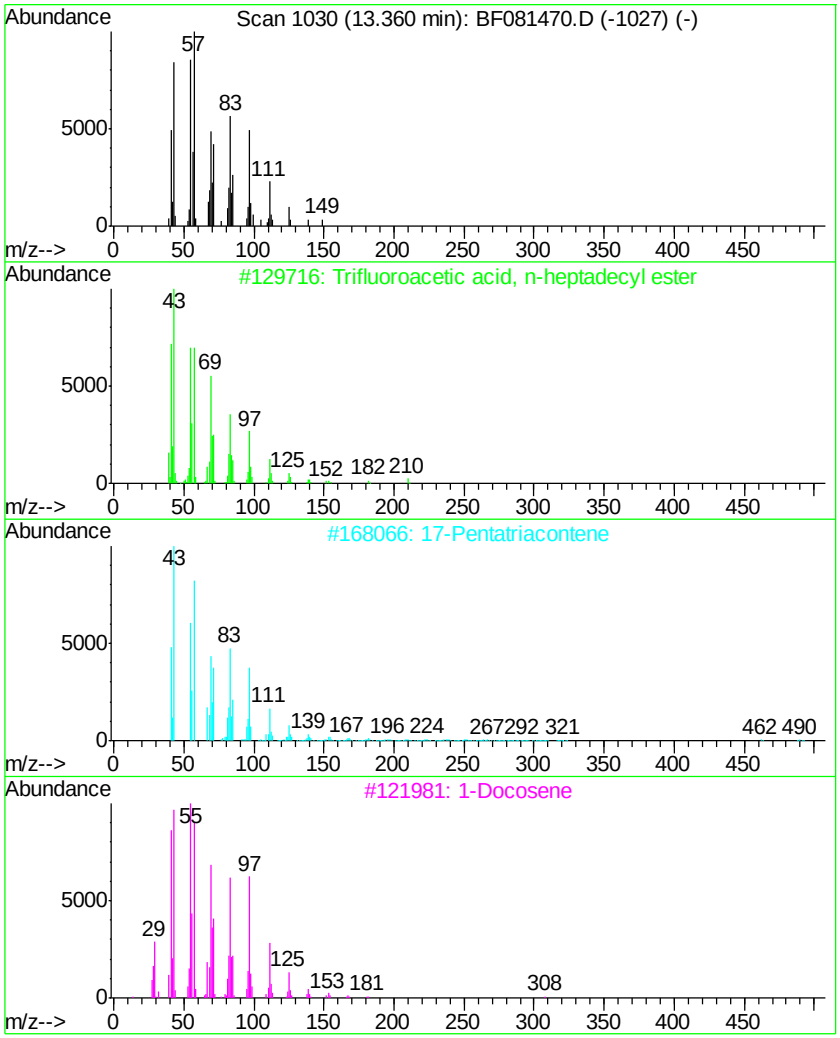
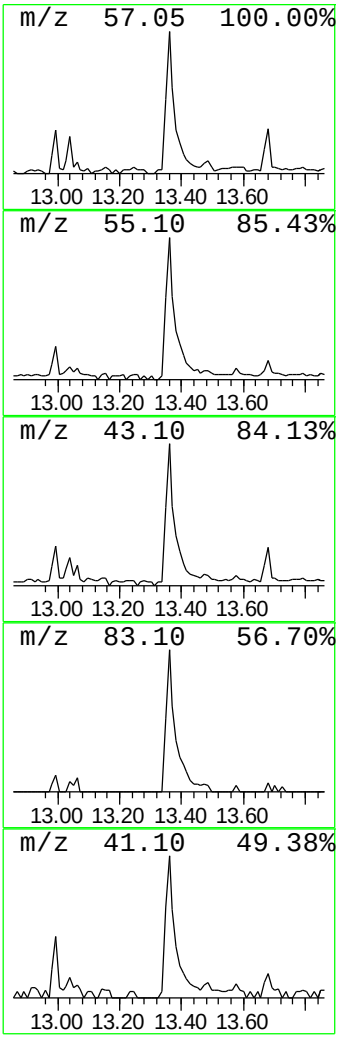
Peak Number 7 Trifluoroacetic acid, n-hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	13.39 ng	240523	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	86
2	17-Pentatriacontene	491	C35H70	006971-40-0	83
3	1-Docosene	308	C22H44	001599-67-3	81
4	1-Tetracosanol	354	C24H50O	000506-51-4	81
5	1-Hexacosanol	382	C26H54O	000506-52-5	70





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

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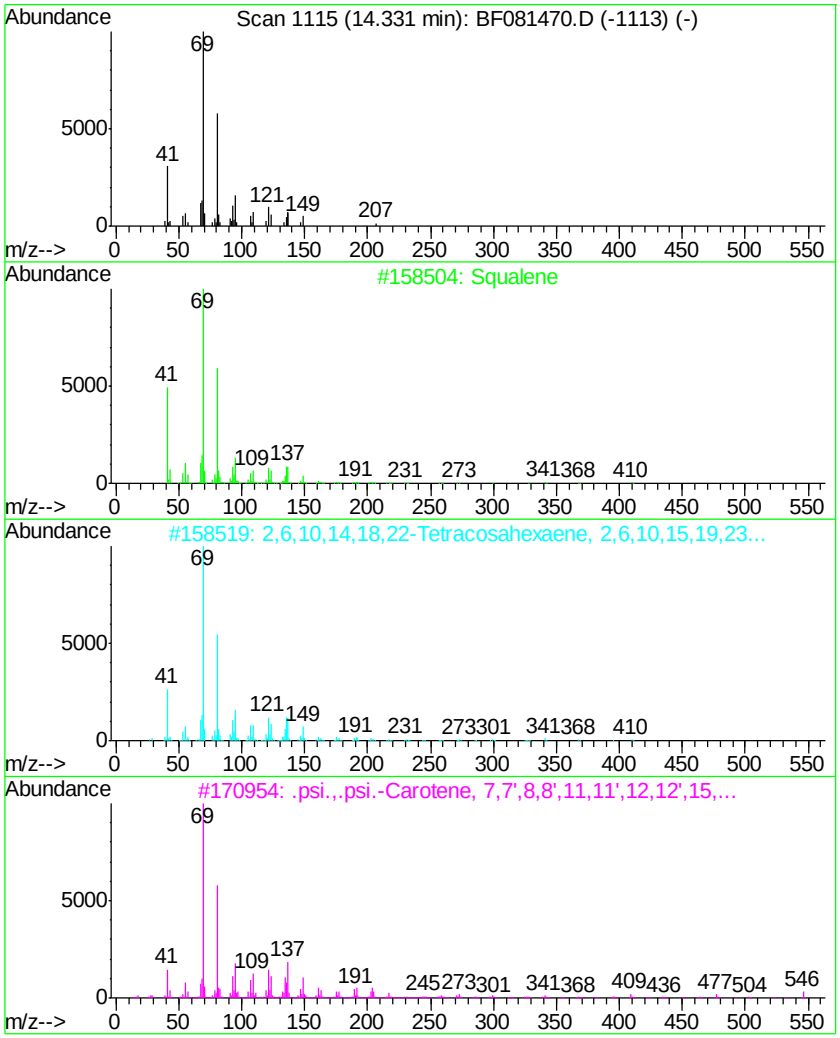
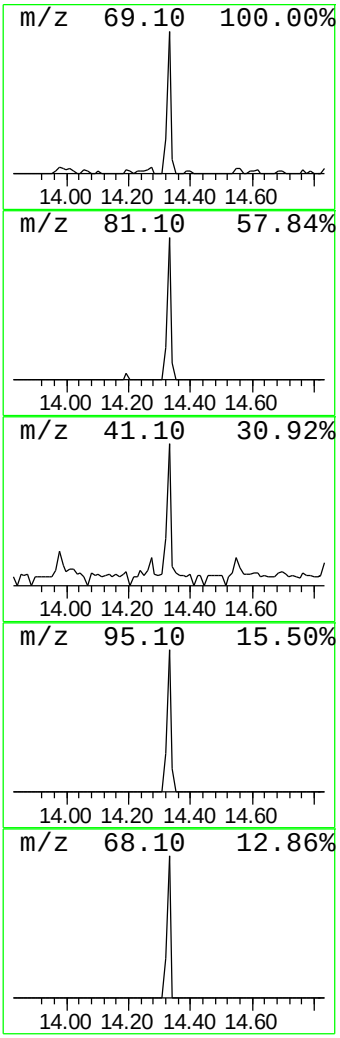
Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	3.51 ng	46704	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





Tentatively Identified Compound (LSC) summary

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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...	4.40	61.3	ng	1075000	1	6.35	350658	20.0
unknown6.12	6.12	103.1	ng	1808380	1	6.35	350658	20.0
n-Hexadecanoic acid	11.43	6.5	ng	146533	4	10.85	454114	20.0
Hexadecanoic acid...	12.30	3.1	ng	56616	5	13.45	359161	20.0
unknown12.99	12.99	2.2	ng	40068	5	13.45	359161	20.0
Trifluoroacetic a...	13.36	13.4	ng	240523	5	13.45	359161	20.0
Squalene	14.33	3.5	ng	46704	6	14.77	265850	20.0