LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

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-BF121315.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	5.104	261	264	271	rBV	406357	628725	18.75%	2.109%
2	5.527	298	301	303	rBV	2728963	3037138	90.59%	10.188%
3	6.544	386	390	392	rBV	2710854	2989330	89.17%	10.027%
4	6.682	399	402	405	rBV	2622880	2842449	84.79%	9.535%
5	6.922	420	423	425	rBV	570995	722743	21.56%	2.424%
6	7.070	434	436	439	rVB	2051985	2296452	68.50%	7.703%
7	7.470	468	471	474	rBV	1447289	1936704	57.77%	6.497%
8	8.202	532	535	537	rBV	1101867	1013357	30.23%	3.399%
9	9.276	626	629	631	rBV	3622113	3352507	100.00%	11.246%
10	9.665	661	663	665	rBV	713648	590168	17.60%	1.980%
11	9.893	681	683	686	rBV	61357	49598	1.48%	0.166%
12	9.950	686	688	691	rVB	1216446	1090217	32.52%	3.657%
13	10.396	723	727	728	rBV	73957	96709	2.88%	0.324%
14	10.613	743	746	749	rBV	35049	55555	1.66%	0.186%
15	10.739	754	757	759	rBV	2086528	2225835	66.39%	7.466%
16	10.865	765	768	772	rBV	120797	148088	4.42%	0.497%
17	11.311	805	807	808	rBV	85717	69648	2.08%	0.234%
18	11.436	815	818	820	rVB	791508	1066355	31.81%	3.577%
19	11.962	862	864	866	rBV	59900	61385	1.83%	0.206%
20	13.014	953	956	958	rBV	3158866	2959061	88.26%	9.926%
21	13.494	996	998	1000	rVB	43708	54314	1.62%	0.182%
22	13.551	1000	1003	1006	rVV	64120	83221	2.48%	0.279%
23	13.642	1008	1011	1012	rVV	44834	61256	1.83%	0.205%
24	13.677	1012	1014	1015	rVV2	75966	85756	2.56%	0.288%
25	13.711	1015	1017	1020	rVB2	37664	53856	1.61%	0.181%
26	13.871	1028	1031	1033	rBV	30715	36897	1.10%	0.124%
27	13.905	1033	1034	1038	rVV	304218	332533	9.92%	1.115%
28	13.985	1038	1041	1043	rVV	86837	99457	2.97%	0.334%
29	14.054	1045	1047	1050	rVB	851136	850977	25.38%	2.855%
30	14.739	1101	1107	1108	rVB3	31615	65071	1.94%	0.218%
31	14.922	1120	1123	1125	rBV	99233	139634	4.17%	0.468%
32	15.174	1142	1145	1148	rBV	41119	49679	1.48%	0.167%
33	15.494	1170	1173	1176	rBV	551928	666678	19.89%	2.236%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

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-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

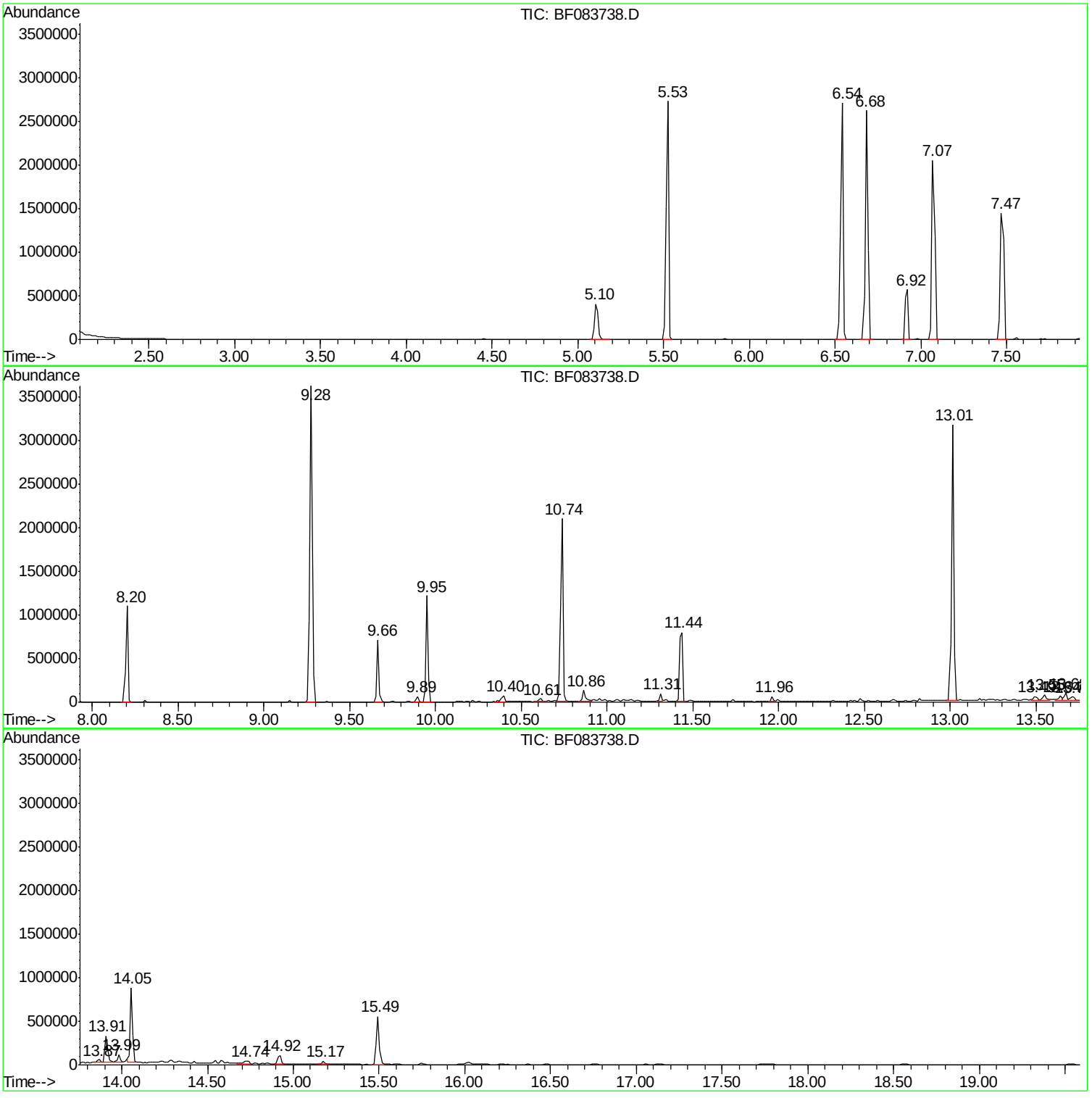
Sum of corrected areas: 29811353

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

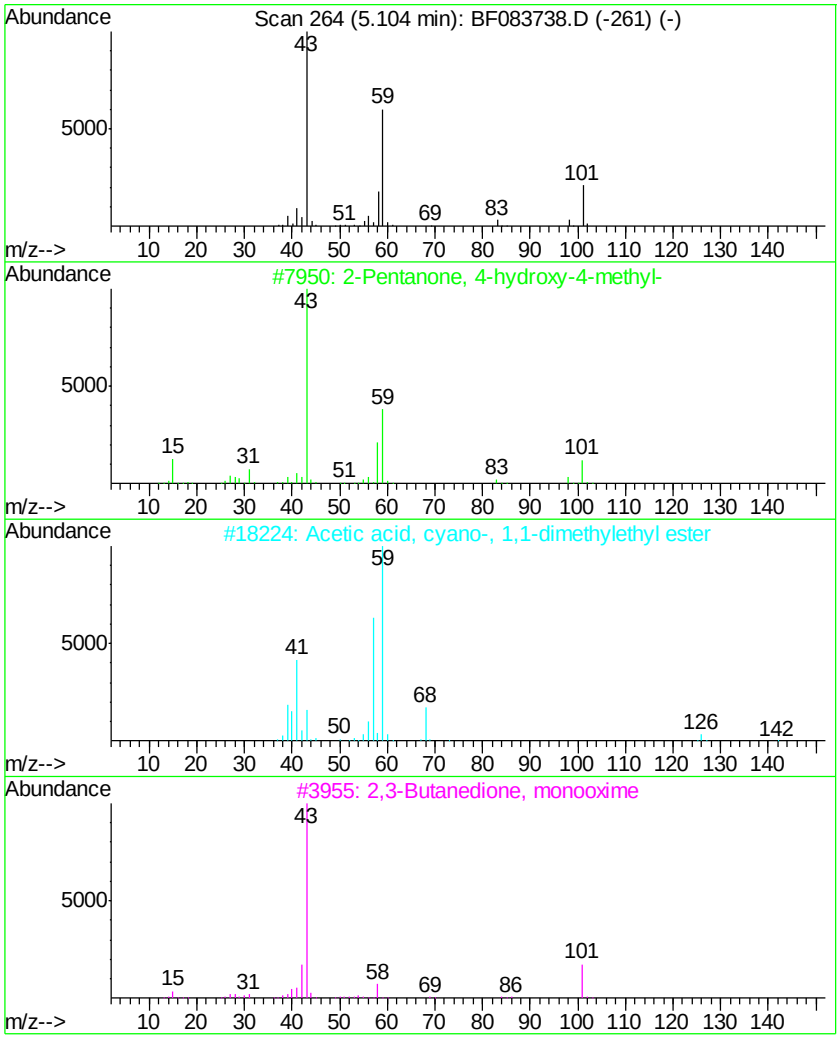
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

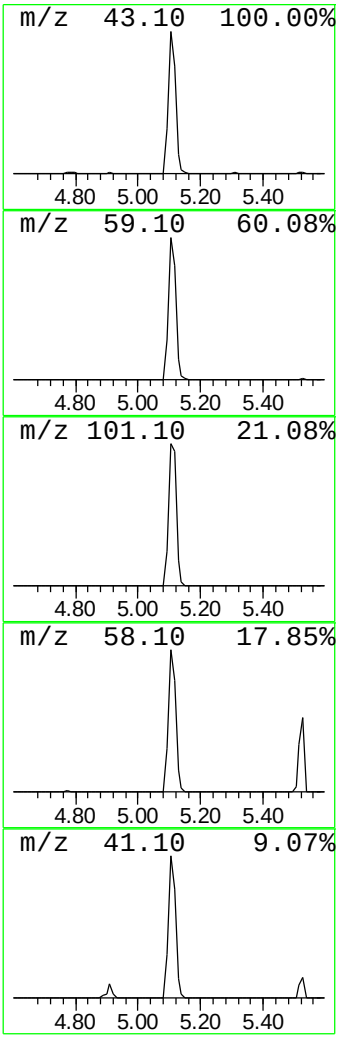
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	17.40 ng	628725	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

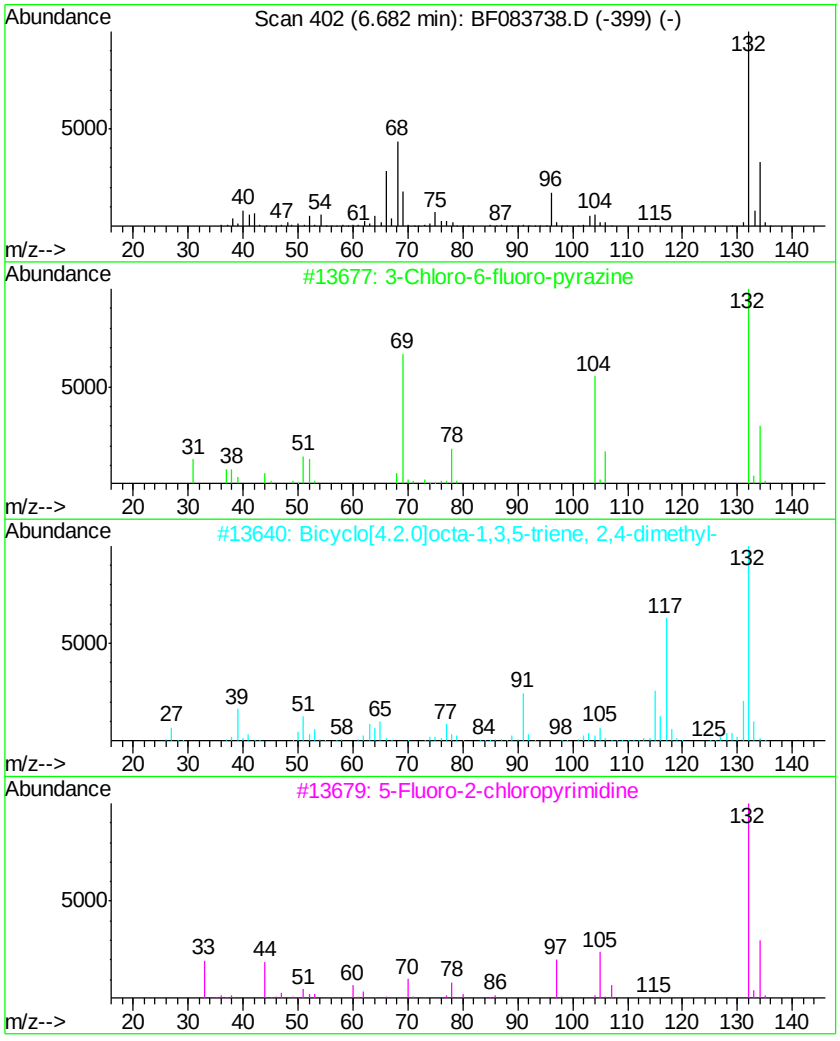
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

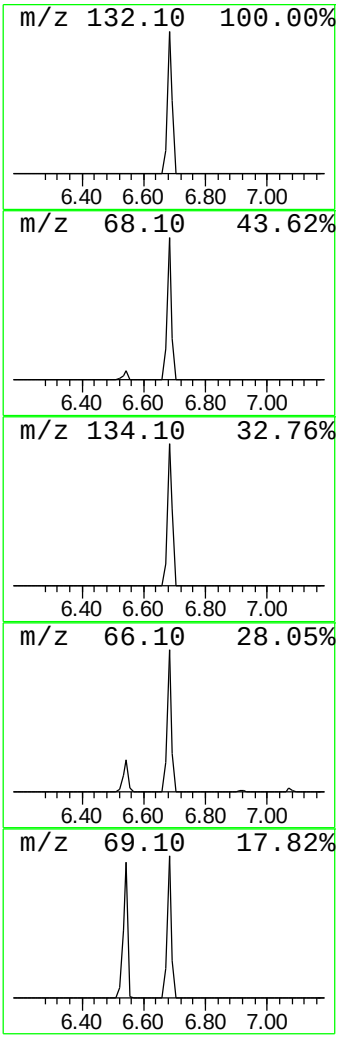
****

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	78.66 ng	2842450	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

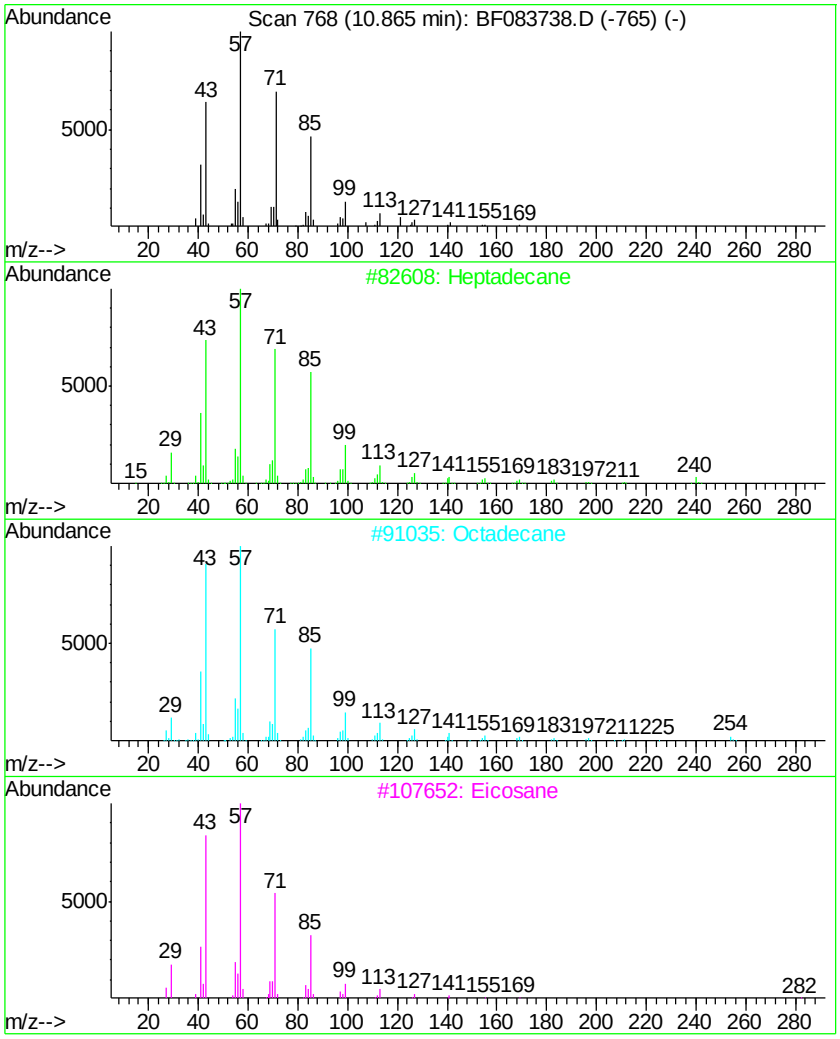
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

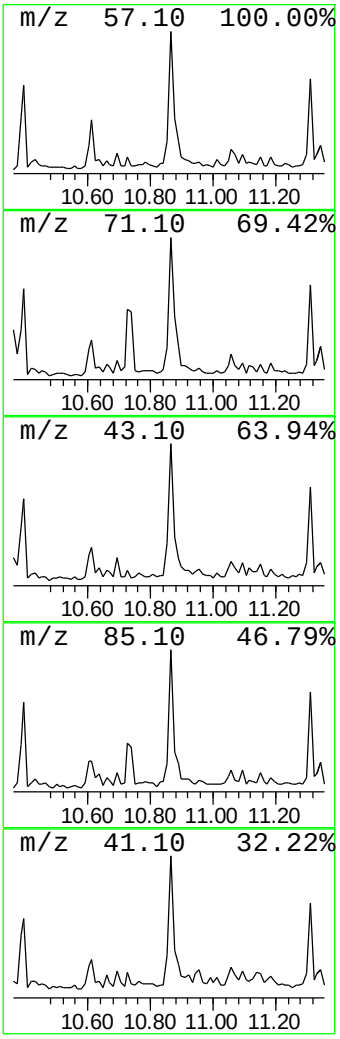
****

Peak Number 4 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.78 ng	148088	Phenanthrene-d10	11.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexadecane	226	C16H34	000544-76-3	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

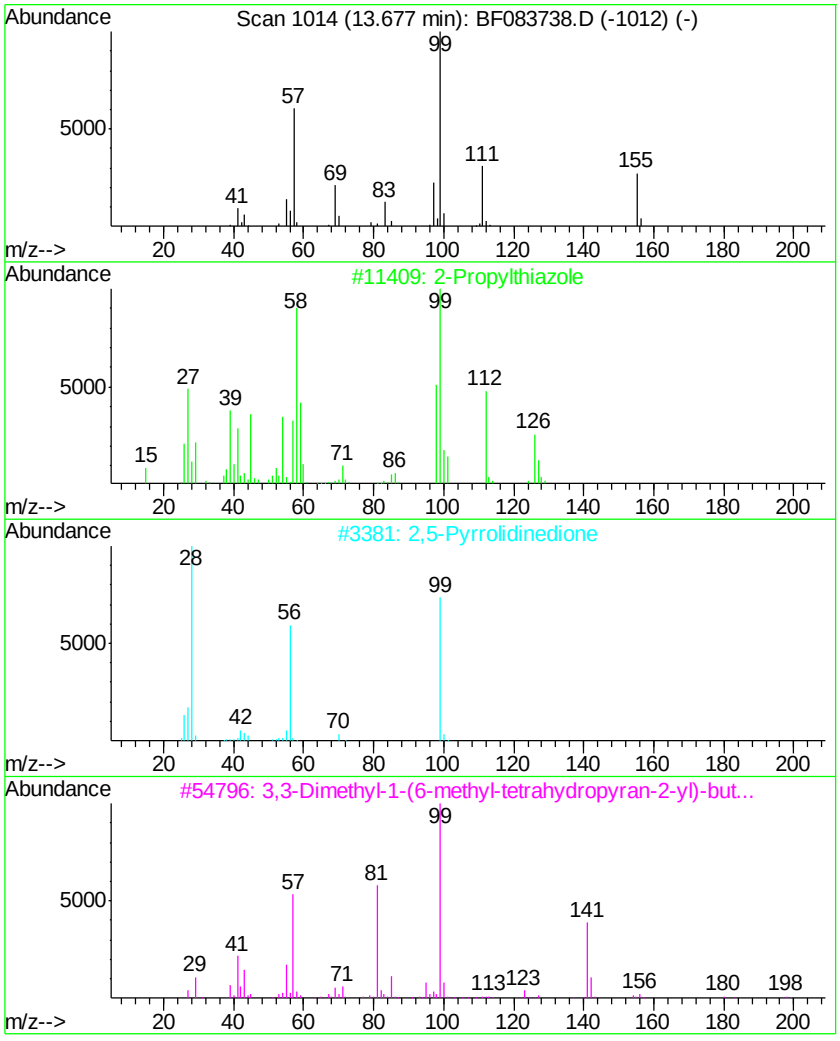
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

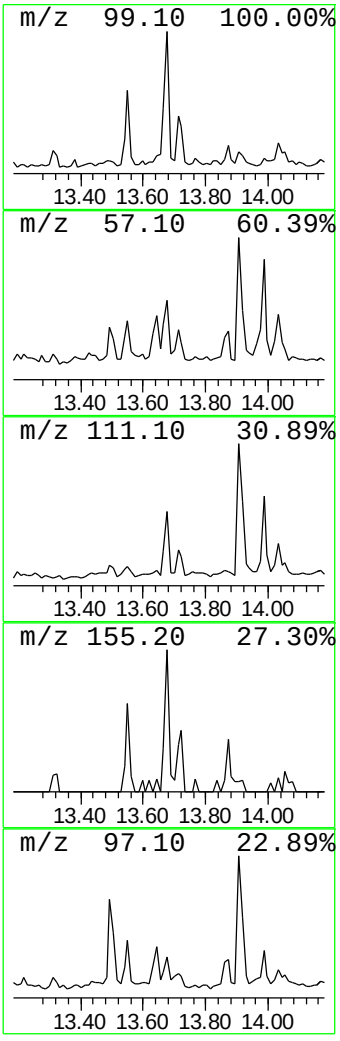
****

Peak Number 5 unknown13.68 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	2.02 ng	85756	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propylthiazole	127	C6H9NS	017626-75-4	35
2	2,5-Pyrrolidinedione	99	C4H5NO2	000123-56-8	32
3	3,3-Dimethyl-1-(6-methyl-tetrahy...	198	C12H22O2	343947-11-5	28
4	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	28
5	(.+/-.)-Dethiobiotin	214	C10H18N2O3	000636-20-4	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

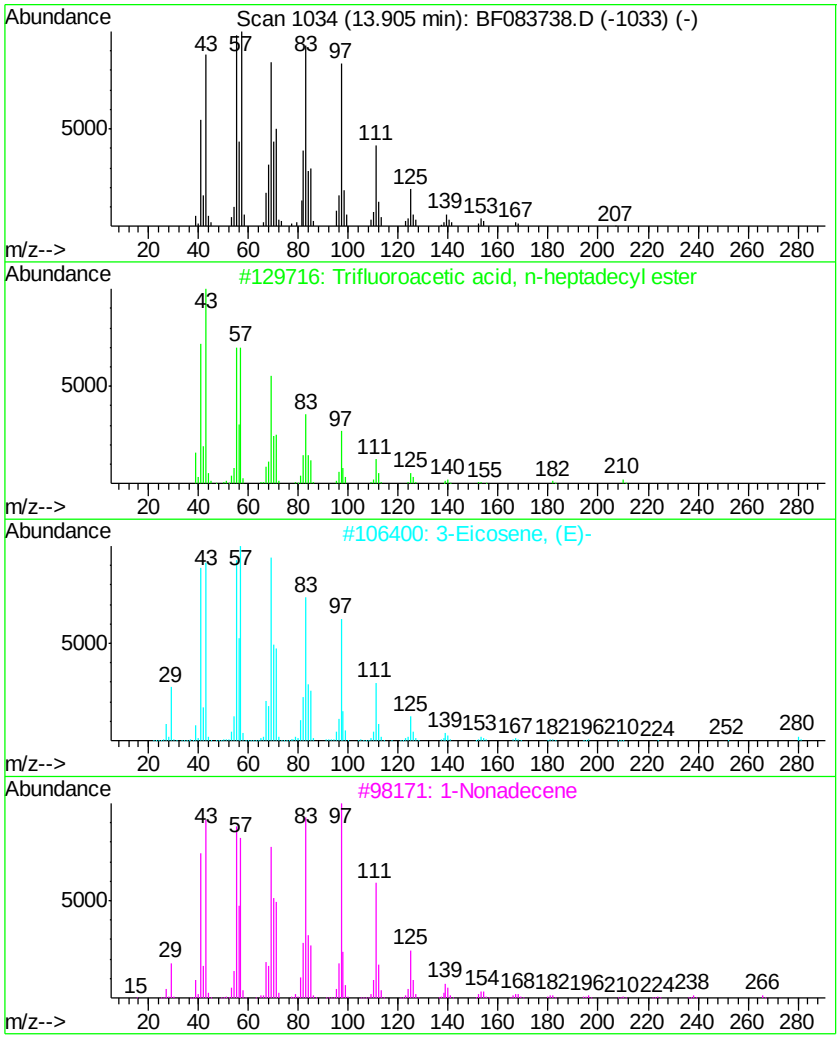
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

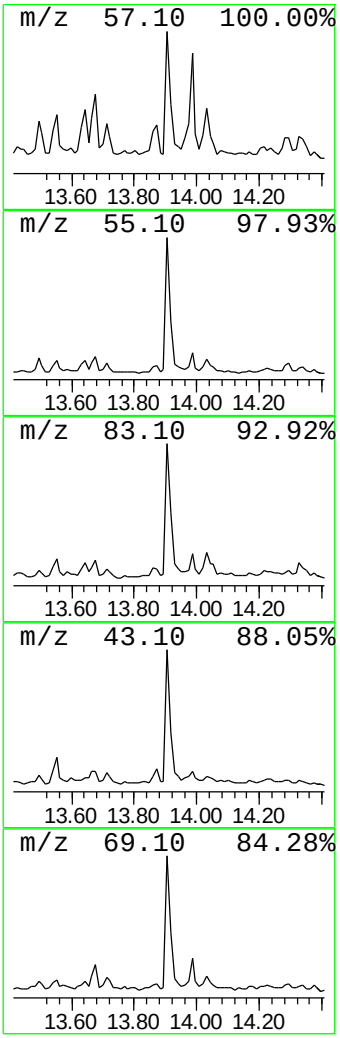
****

Peak Number 6 Trifluoroacetic acid, n-hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	7.82 ng	332533	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

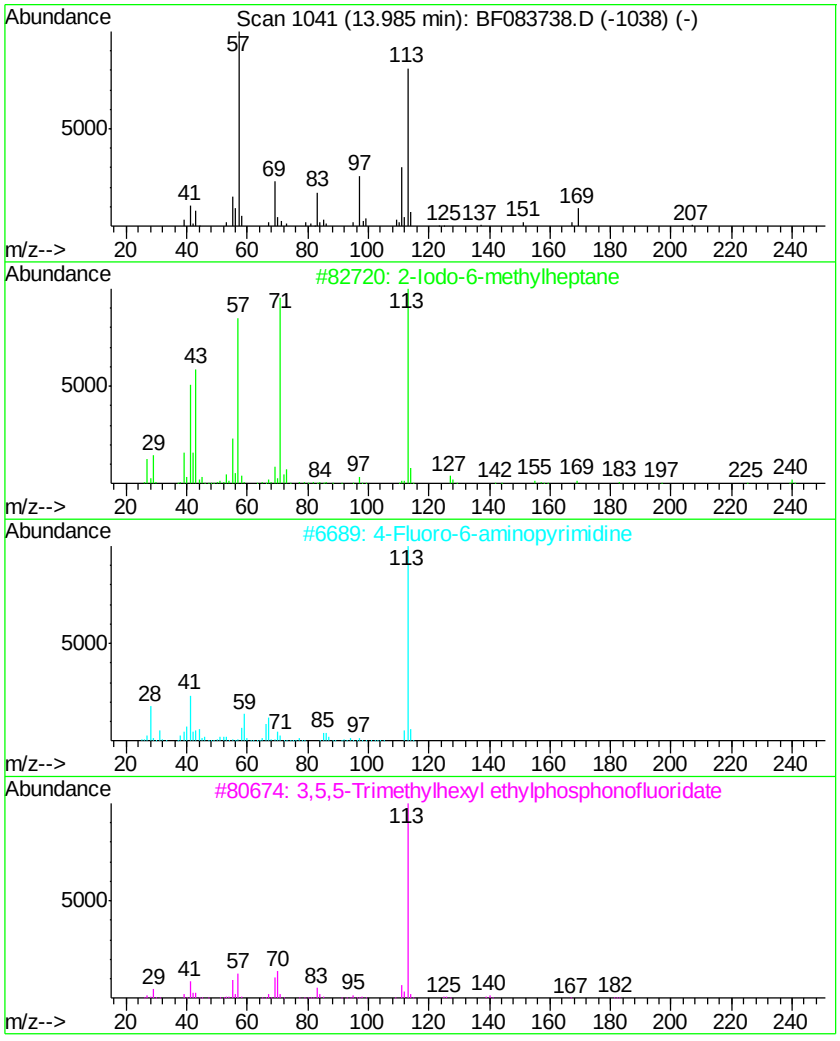
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

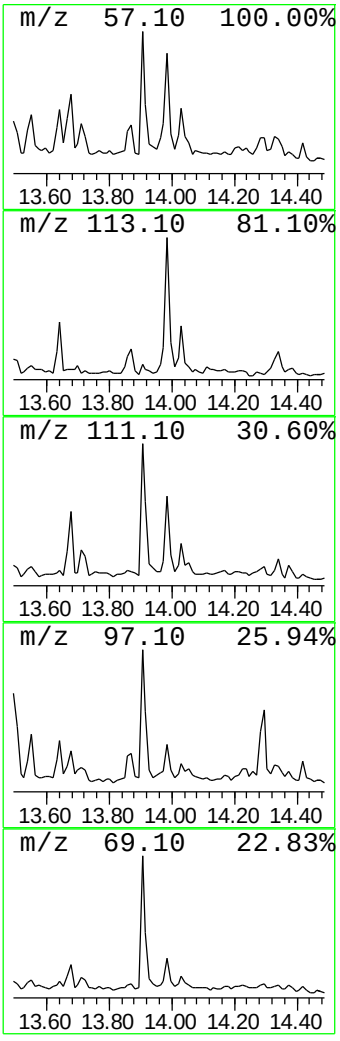
****

Peak Number 7 unknown13.99 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	2.34 ng	99457	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Iodo-6-methylheptane	240	C8H17I	088373-60-8	40
2	4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	38
3	3,5,5-Trimethylhexyl ethylphosph...	238	C11H24FO2P	1000298-45-0	38
4	1H-Pyrazole, 4-nitro-	113	C3H3N3O2	002075-46-9	37
5	Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	36





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

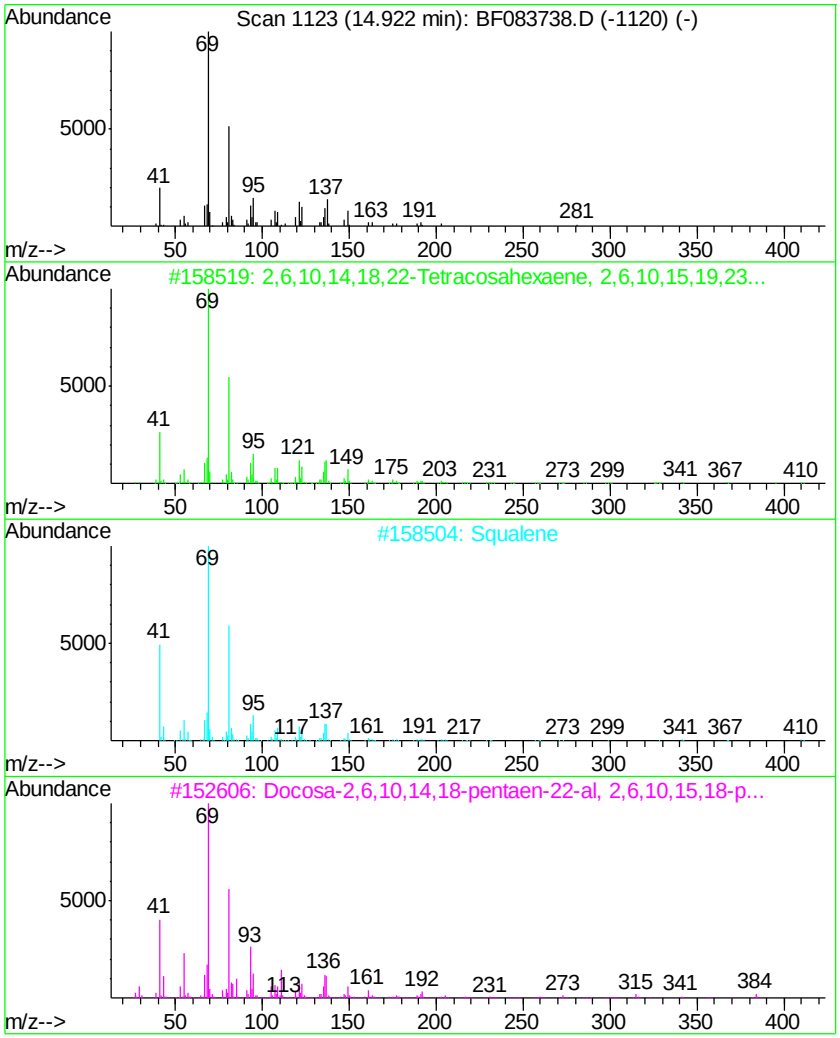
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

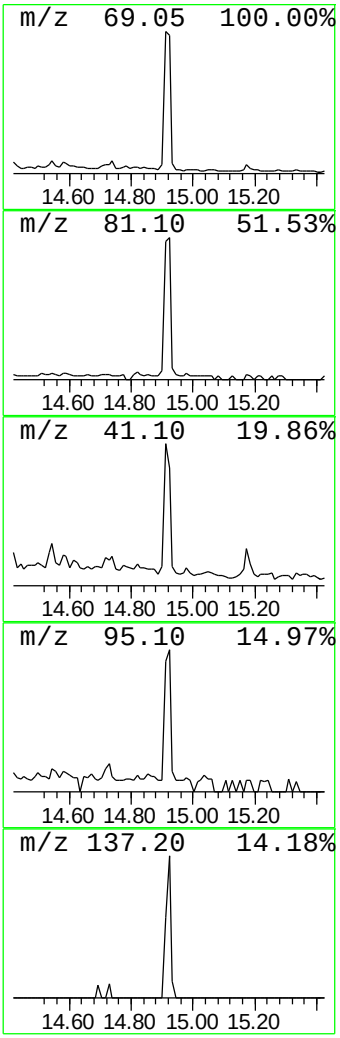
****

Peak Number 8 2,6,10,14,18,22-Tetracosahe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.19 ng	139634	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
2	Squalene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
4	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	53
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083738.D
Acq On : 13 Dec 2015 19:24
Operator : UM/IZ
Sample : G4648-18
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(27-29.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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...	5.10	17.4	ng	628725	1	6.92	722743	20.0
unknown6.68	6.68	78.7	ng	2842450	1	6.92	722743	20.0
Heptadecane	10.86	2.8	ng	148088	4	11.44	1066360	20.0
unknown13.68	13.68	2.0	ng	85756	5	14.05	850977	20.0
Trifluoroacetic a...	13.91	7.8	ng	332533	5	14.05	850977	20.0
unknown13.99	13.99	2.3	ng	99457	5	14.05	850977	20.0
2,6,10,14,18,22-T...	14.92	4.2	ng	139634	6	15.49	666678	20.0