LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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	2.235	11	13	29	rVB	50306	113238	3.86%	0.423%
2	5.116	262	265	269	rBV	488154	619712	21.11%	2.317%
3	5.527	298	301	304	rBV	2234151	2640574	89.96%	9.872%
4	6.544	387	390	393	rBV	2246002	2429178	82.76%	9.082%
5	6.693	400	403	405	rBV	2056260	2935307	100.00%	10.974%
6	6.921	420	423	425	rBV	664352	624071	21.26%	2.333%
7	7.082	434	437	439	rBV	2053697	2383476	81.20%	8.911%
8	7.482	469	472	474	rBV	1690002	1958392	66.72%	7.322%
9	8.202	532	535	537	rBV	881236	766678	26.12%	2.866%
10	9.276	626	629	632	rBV	2678389	2514253	85.66%	9.400%
11	9.665	661	663	666	rBV	396000	393542	13.41%	1.471%
12	9.893	681	683	686	rBV	42357	33811	1.15%	0.126%
13	9.950	686	688	691	rBV	697968	730732	24.89%	2.732%
14	10.396	723	727	728	rBV	49211	58953	2.01%	0.220%
15	10.739	754	757	759	rBV	1613833	1569939	53.48%	5.870%
16	10.865	766	768	772	rVB	63462	68279	2.33%	0.255%
17	11.436	815	818	819	rBV	698038	715560	24.38%	2.675%
18	11.962	863	864	866	rVV	42060	32671	1.11%	0.122%
19	12.042	869	871	875	rVB2	22619	36383	1.24%	0.136%
20	12.248	885	889	891	rVB	23024	29391	1.00%	0.110%
21	12.636	921	923	926	rVB	228392	262973	8.96%	0.983%
22	12.865	939	943	945	rBV3	241388	422626	14.40%	1.580%
23	12.922	945	948	950	rVB2	87890	94428	3.22%	0.353%
24	13.014	954	956	959	rVB	2029062	2035742	69.35%	7.611%
25	13.196	967	972	974	rBV2	22131	39197	1.34%	0.147%
26	13.551	1000	1003	1005	rBV	149641	133764	4.56%	0.500%
27	13.596	1005	1007	1011	rVB2	44311	70419	2.40%	0.263%
28	13.699	1011	1016	1019	rVB2	25926	34643	1.18%	0.130%
29	13.814	1019	1026	1027	rBV2	27316	62543	2.13%	0.234%
30	13.916	1032	1035	1038	rVB2	141274	226593	7.72%	0.847%
31	14.065	1045	1048	1049	rBV2	714173	867346	29.55%	3.243%
32	14.088	1049	1050	1055	rVB	123240	105393	3.59%	0.394%
33	14.236	1061	1063	1065	rBV2	73306	76793	2.62%	0.287%
34	14.545	1087	1090	1091	rBV	89130	93298	3.18%	0.349%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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

35	14.842	1114	1116	1120	rBV	58591	70093	2.39%	0.262%
36	14.922	1120	1123	1125	rVV2	23040	35577	1.21%	0.133%
37	15.082	1135	1137	1142	rBV	90322	196306	6.69%	0.734%
38	15.174	1143	1145	1148	rVV2	50573	82677	2.82%	0.309%
39	15.379	1161	1163	1166	rBV	52559	66354	2.26%	0.248%
40	15.437	1166	1168	1171	rVV	60436	75548	2.57%	0.282%
41	15.505	1171	1174	1177	rVV	421751	615395	20.97%	2.301%
42	15.551	1177	1178	1186	rVB	45036	60031	2.05%	0.224%
43	15.985	1213	1216	1218	rBV	31699	51862	1.77%	0.194%
44	16.477	1254	1259	1264	rBV5	21755	65260	2.22%	0.244%
45	16.922	1295	1298	1304	rVB2	24541	53858	1.83%	0.201%
46	17.345	1333	1335	1341	rVB	18052	45114	1.54%	0.169%
47	17.528	1348	1351	1354	rBV5	17735	36690	1.25%	0.137%
48	17.757	1368	1371	1376	rVB4	16072	41596	1.42%	0.156%
49	18.580	1436	1443	1449	rBV9	15291	70835	2.41%	0.265%

Sum of corrected areas: 26747094

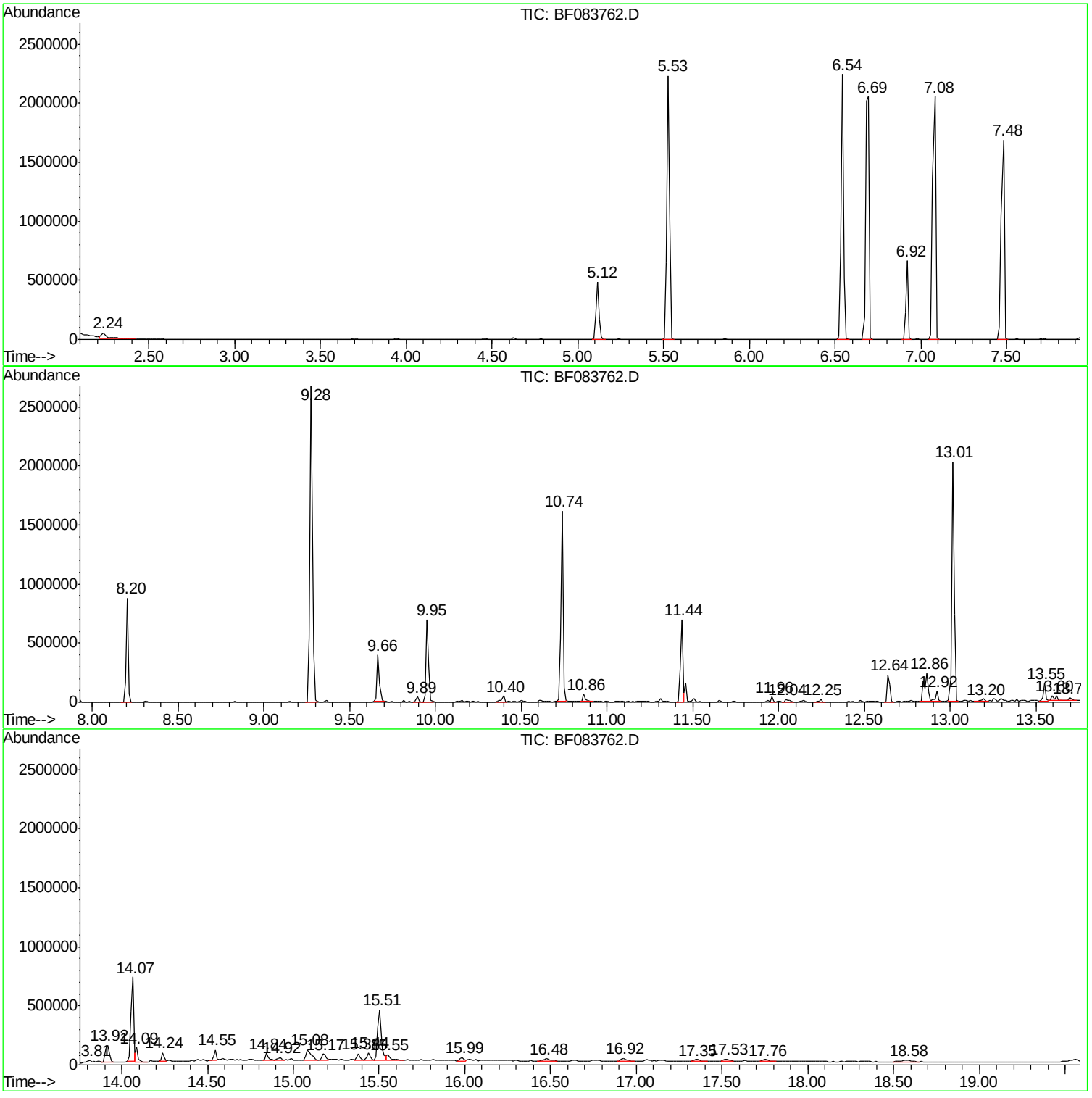
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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 : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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

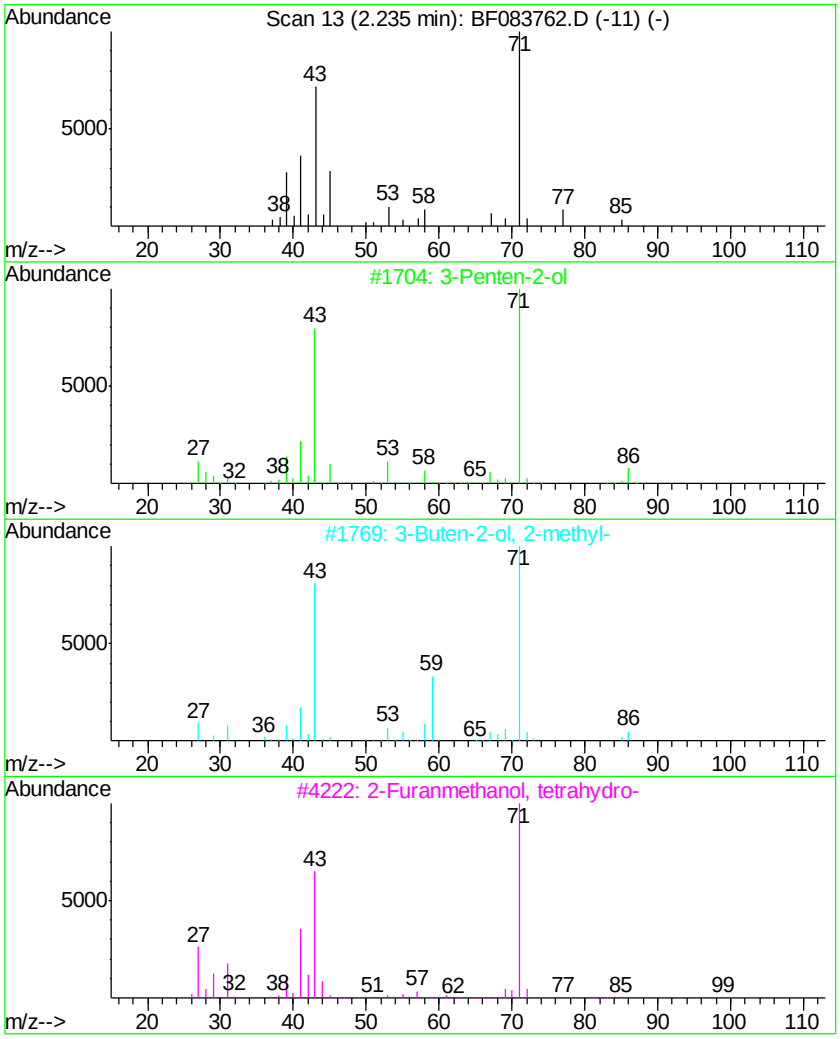
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

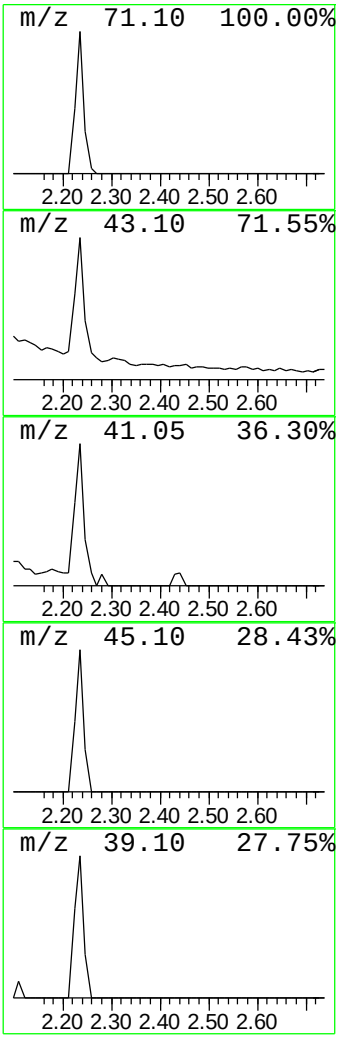
****

Peak Number 1 3-Penten-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	3.63 ng	113238	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	72
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	59
3	2-Furanmethanol, tetrahydro-	102	C5H10O2	000097-99-4	50
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	40
5	Z-1-Methoxy-2-hexene	114	C7H14O	1000279-60-9	39





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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

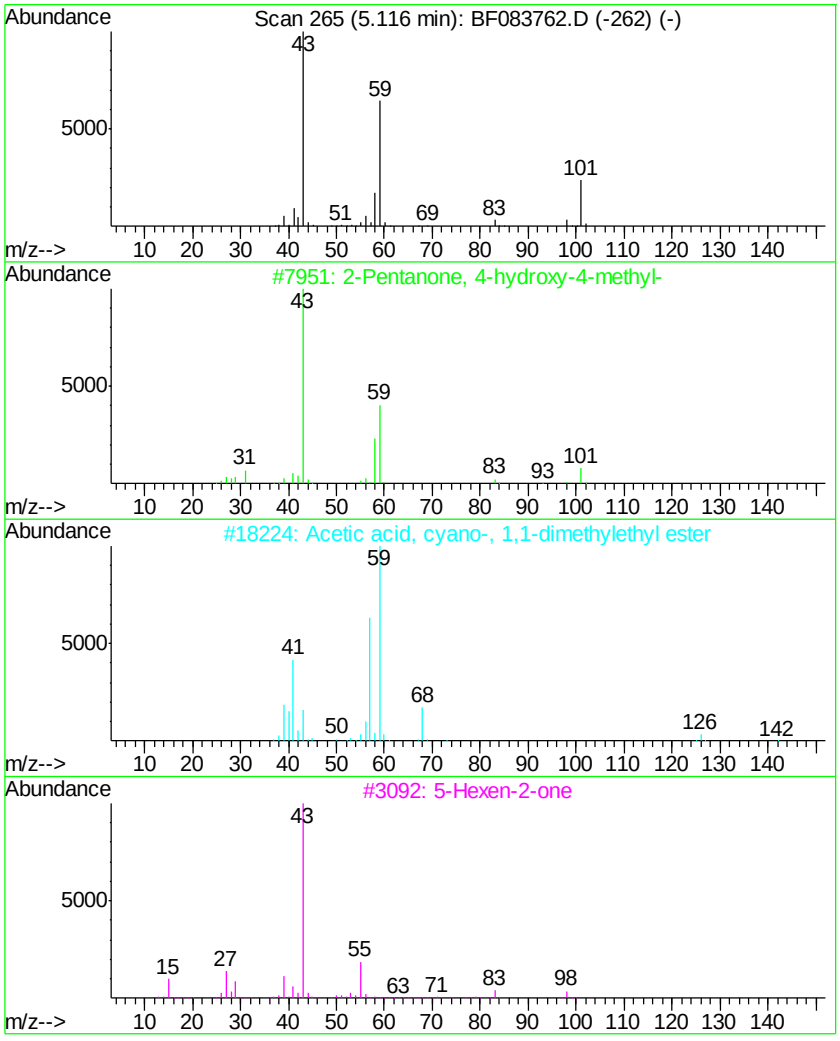
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

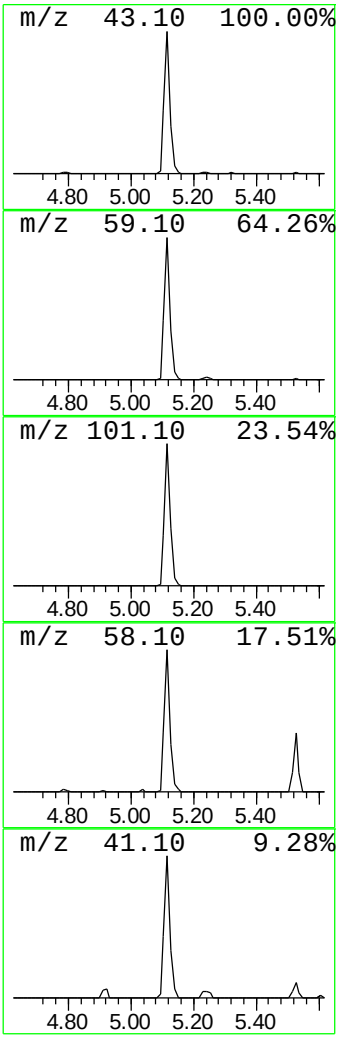
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	19.86 ng	619712	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	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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

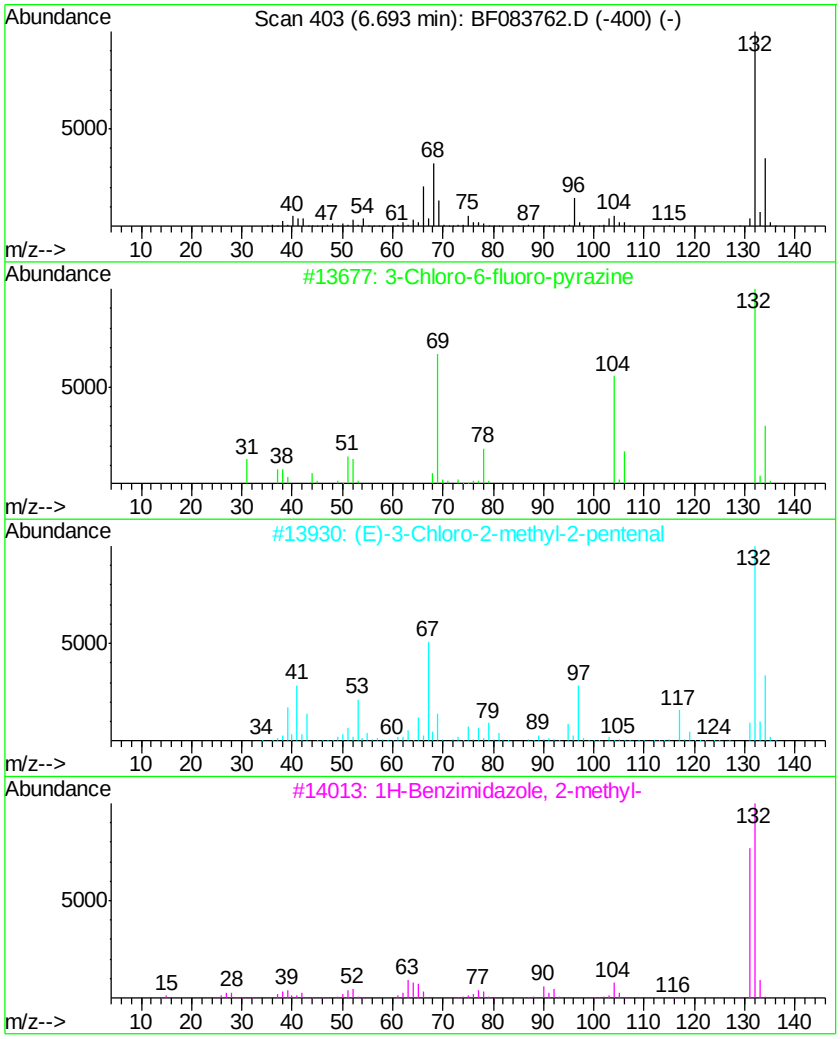
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

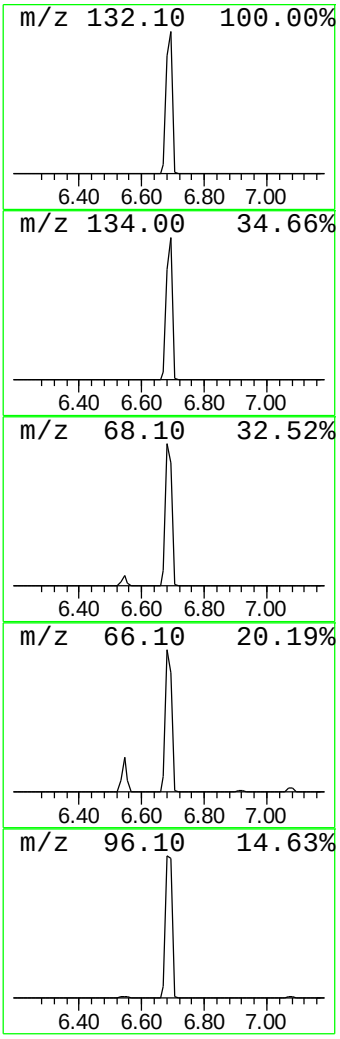
****

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	94.07 ng	2935310	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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

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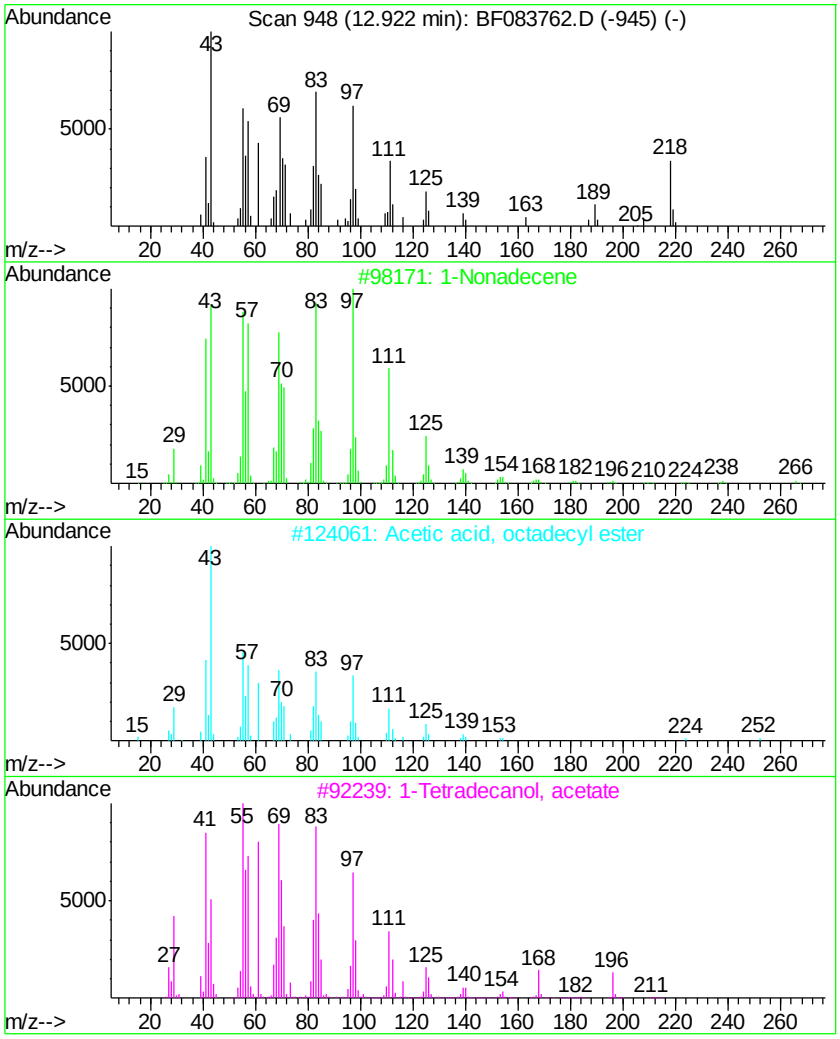
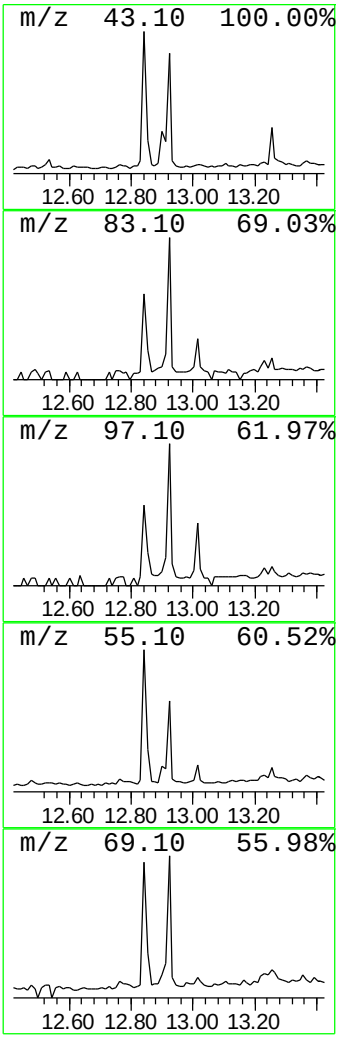
Peak Number 5 1-Nonadecene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	2.18 ng	94428	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	81
3	1-Tetradecanol, acetate	256	C16H32O2	000638-59-5	64
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	64
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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

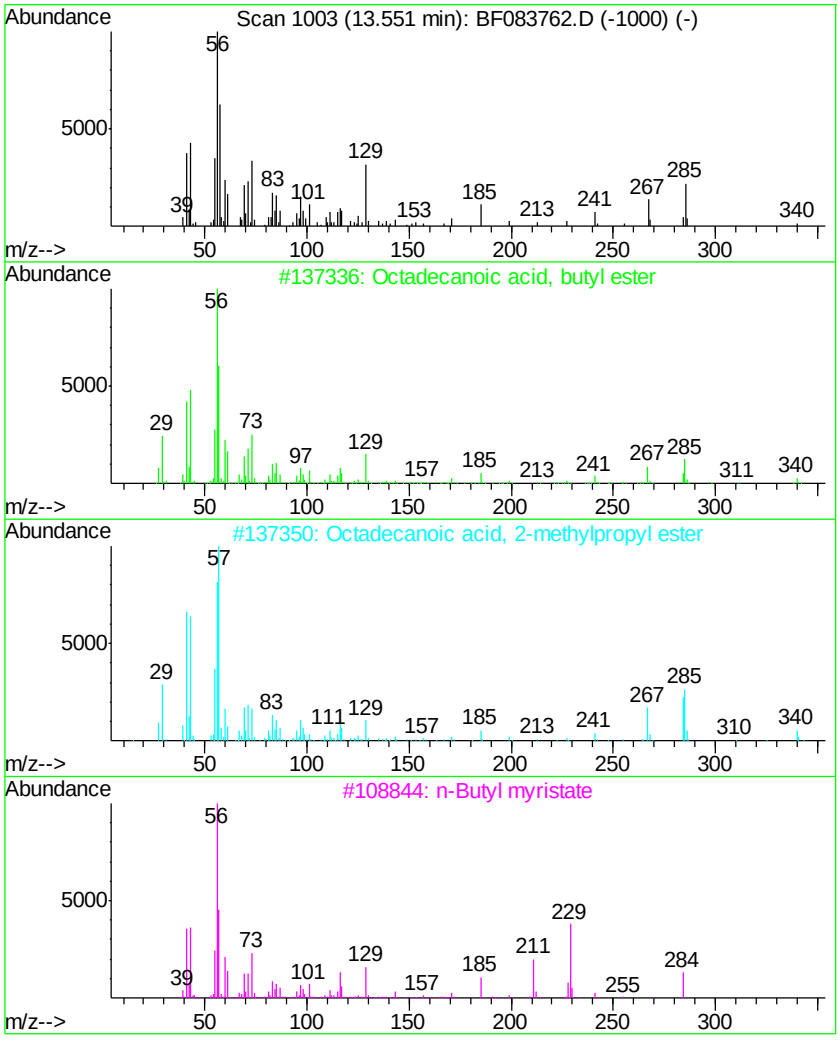
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

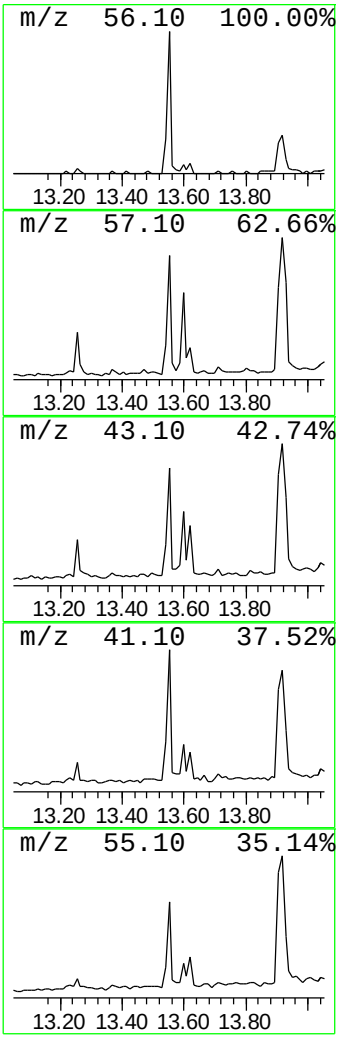
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	3.08 ng	133764	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	53
3	n-Butyl myristate	284	C18H36O2	000110-36-1	53
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	Cyclohexanamine	99	C6H13N	000108-91-8	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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

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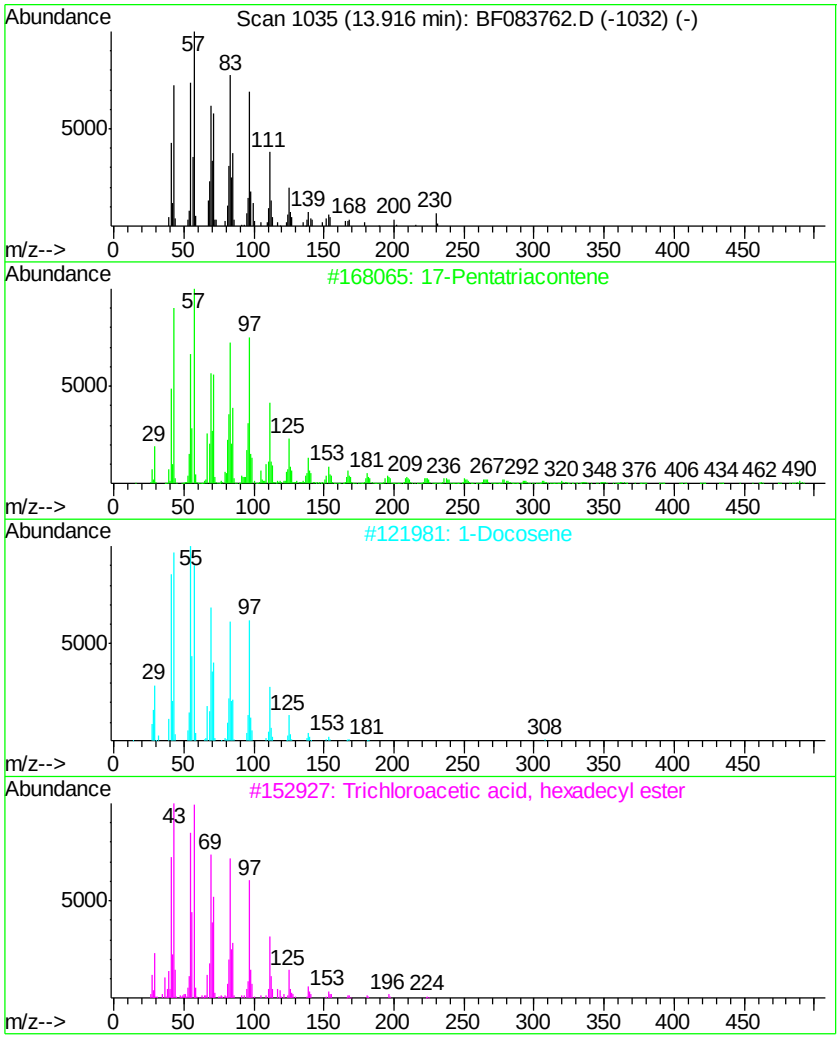
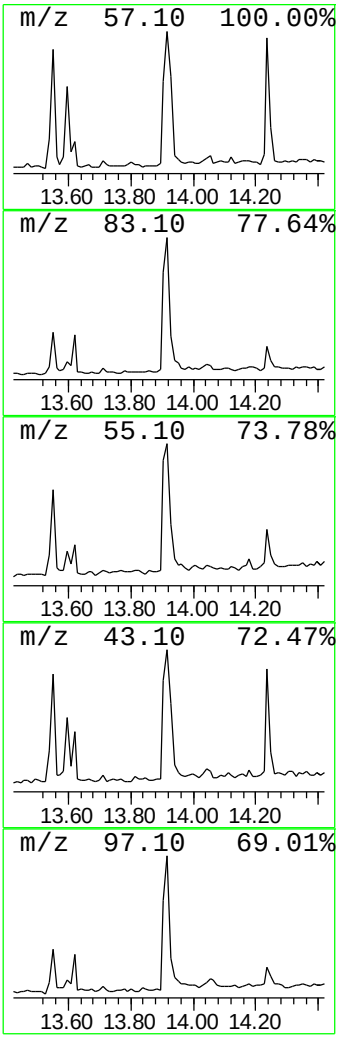
Peak Number 7 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	5.22 ng	226593	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	1-Docosene	308	C22H44	001599-67-3	90
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	87
5	1-Nonadecene	266	C19H38	018435-45-5	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05(0-0.16)

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

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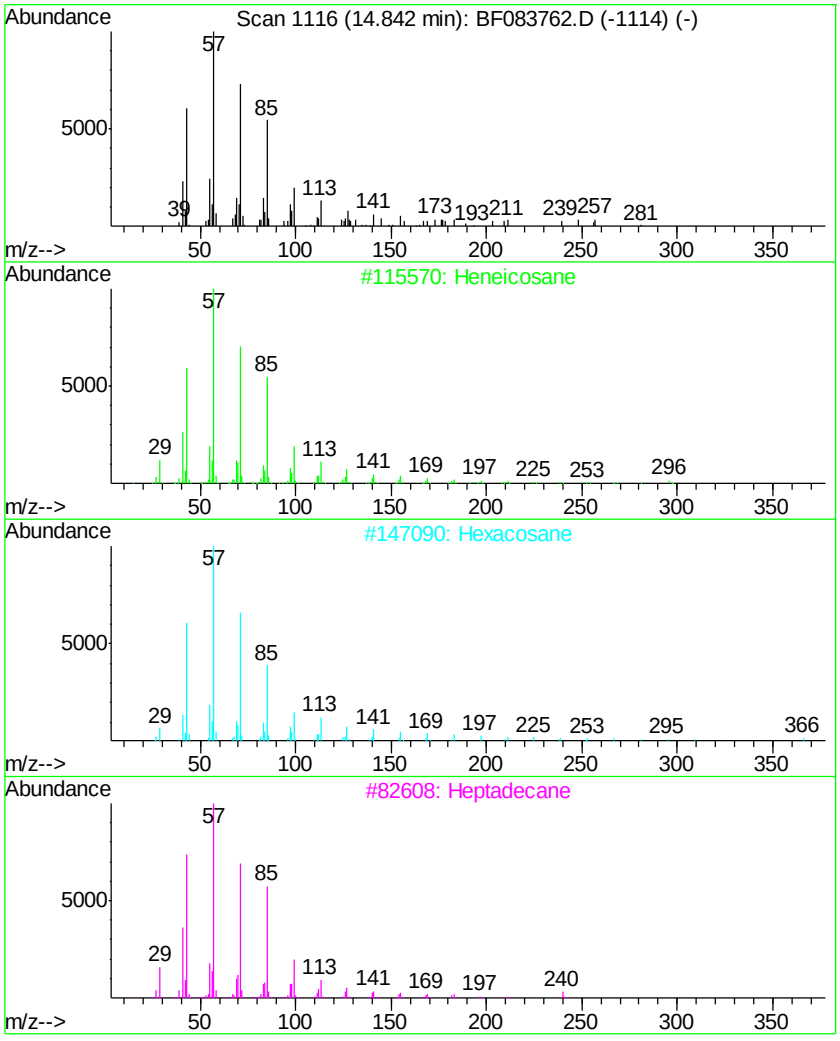
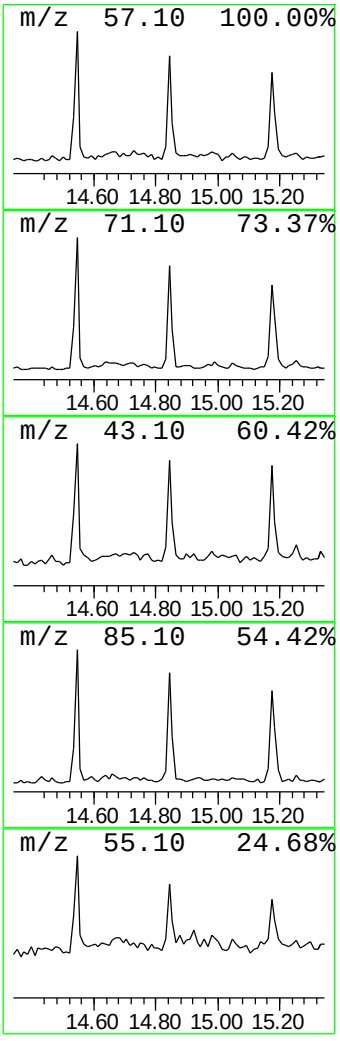
Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.28 ng	70093	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Pentacosane	352	C25H52	000629-99-2	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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

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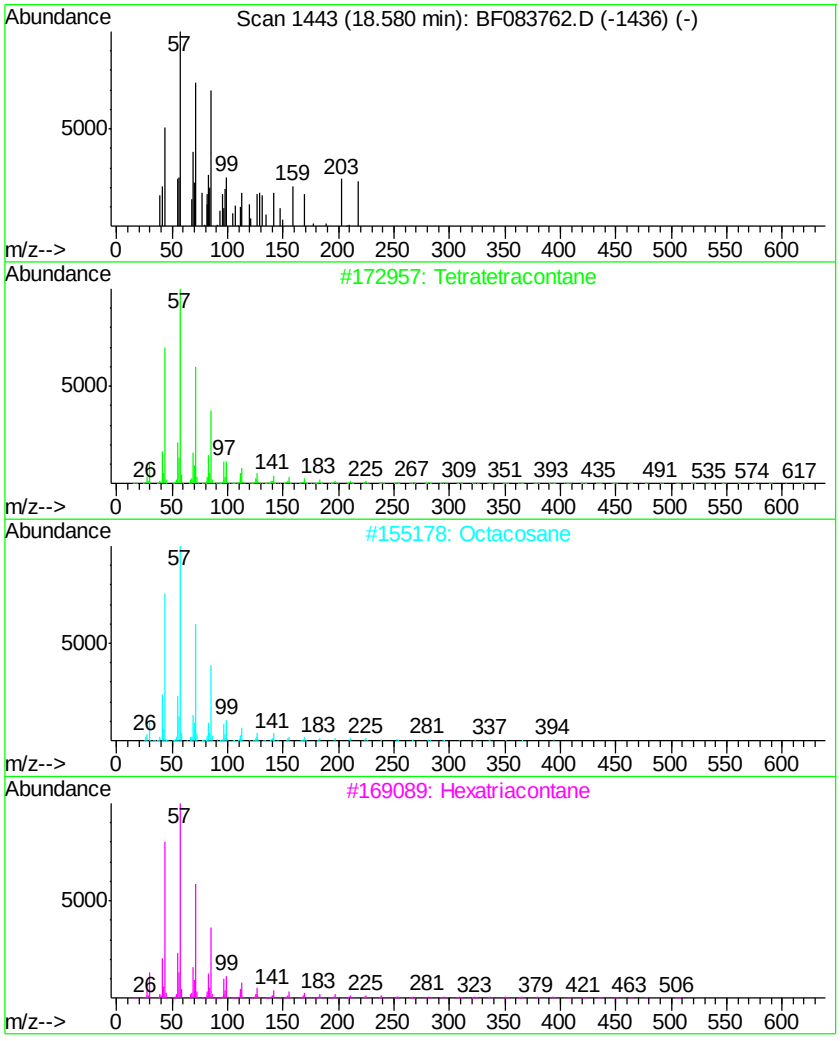
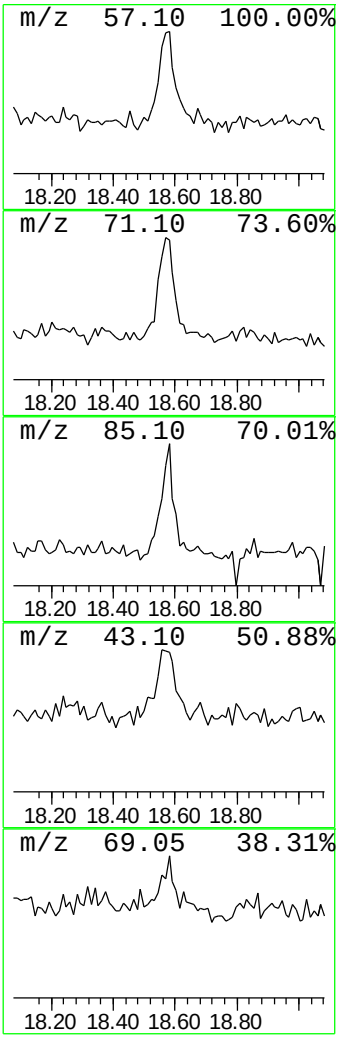
Peak Number 10 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	2.30 ng	70835	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	50
2	Octacosane	394	C28H58	000630-02-4	50
3	Hexatriacontane	507	C36H74	000630-06-8	47
4	Eicosane	282	C20H42	000112-95-8	47
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083762.D
Acq On : 14 Dec 2015 6:57
Operator : UM/IZ
Sample : G4648-07
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05(0-0.16)

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
3-Penten-2-ol	2.24	3.6	ng	113238	1	6.92	624071	20.0
2-Pentanone, 4-hy...	5.12	19.9	ng	619712	1	6.92	624071	20.0
unknown6.69	6.69	94.1	ng	2935310	1	6.92	624071	20.0
1-Nonadecene	12.92	2.2	ng	94428	5	14.07	867346	20.0
Octadecanoic acid...	13.55	3.1	ng	133764	5	14.07	867346	20.0
17-Pentatriacontene	13.92	5.2	ng	226593	5	14.07	867346	20.0
Heneicosane	14.84	2.3	ng	70093	6	15.51	615395	20.0
Tetratetracontane	18.58	2.3	ng	70835	6	15.51	615395	20.0