LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(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-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	3.530	168	170	177	rBV	11339	26782	1.19%	0.136%
2	4.410	243	247	256	rVB	705350	1370061	60.76%	6.937%
3	4.913	288	291	293	rBV	1849611	2087462	92.57%	10.569%
4	5.336	326	328	332	rBV	26601	25932	1.15%	0.131%
5	6.033	386	389	391	rBV	1956497	2238208	99.26%	11.332%
6	6.125	395	397	400	rVV	1935553	1847174	81.92%	9.352%
7	6.353	415	417	420	rVB	375559	350112	15.53%	1.773%
8	6.513	428	431	433	rBV	1798425	1554357	68.93%	7.870%
9	6.936	465	468	470	rBV	1337118	1326885	58.84%	6.718%
10	7.645	528	530	532	rBV	531604	452351	20.06%	2.290%
11	8.730	622	625	627	rBV	2403543	2254912	100.00%	11.417%
12	9.131	658	660	662	rBV	440235	390679	17.33%	1.978%
13	9.382	680	682	685	rVB	484492	455837	20.22%	2.308%
14	10.171	748	751	753	rBV	1359207	1362938	60.44%	6.901%
15	10.319	762	764	770	rVB	39586	45342	2.01%	0.230%
16	10.765	801	803	804	rBV	32937	29345	1.30%	0.149%
17	10.845	808	810	813	rBV	455877	473925	21.02%	2.400%
18	11.428	859	861	865	rBV	107186	114912	5.10%	0.582%
19	12.045	913	915	917	rBV	58631	49573	2.20%	0.251%
20	12.262	932	934	935	rBV	56765	54346	2.41%	0.275%
21	12.297	935	937	938	rVB	18399	24063	1.07%	0.122%
22	12.434	946	949	952	rBV	1685536	1884985	83.59%	9.544%
23	13.360	1028	1030	1036	rBV	76339	151924	6.74%	0.769%
24	13.451	1036	1038	1043	rVB	368944	457277	20.28%	2.315%
25	13.977	1082	1084	1091	rBV	37227	64143	2.84%	0.325%
26	14.388	1119	1120	1122	rBV2	21375	26026	1.15%	0.132%
27	14.434	1122	1124	1130	rVB	49457	78407	3.48%	0.397%
28	14.548	1133	1134	1136	rBV	42361	47110	2.09%	0.239%
29	14.674	1143	1145	1147	rBV	21316	31008	1.38%	0.157%
30	14.720	1147	1149	1151	rBV	24216	29666	1.32%	0.150%
31	14.765	1151	1153	1155	rBV	221968	269968	11.97%	1.367%
32	15.154	1184	1187	1190	rBV	28078	38134	1.69%	0.193%
33	15.714	1233	1236	1241	rBV2	10751	25455	1.13%	0.129%
34	15.828	1244	1246	1250	rBV2	16139	29094	1.29%	0.147%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.148	1271	1274	1278	rVB	13435	24235	1.07%	0.123%
36	16.251	1280	1283	1291	rBV4	16148	58061	2.57%	0.294%

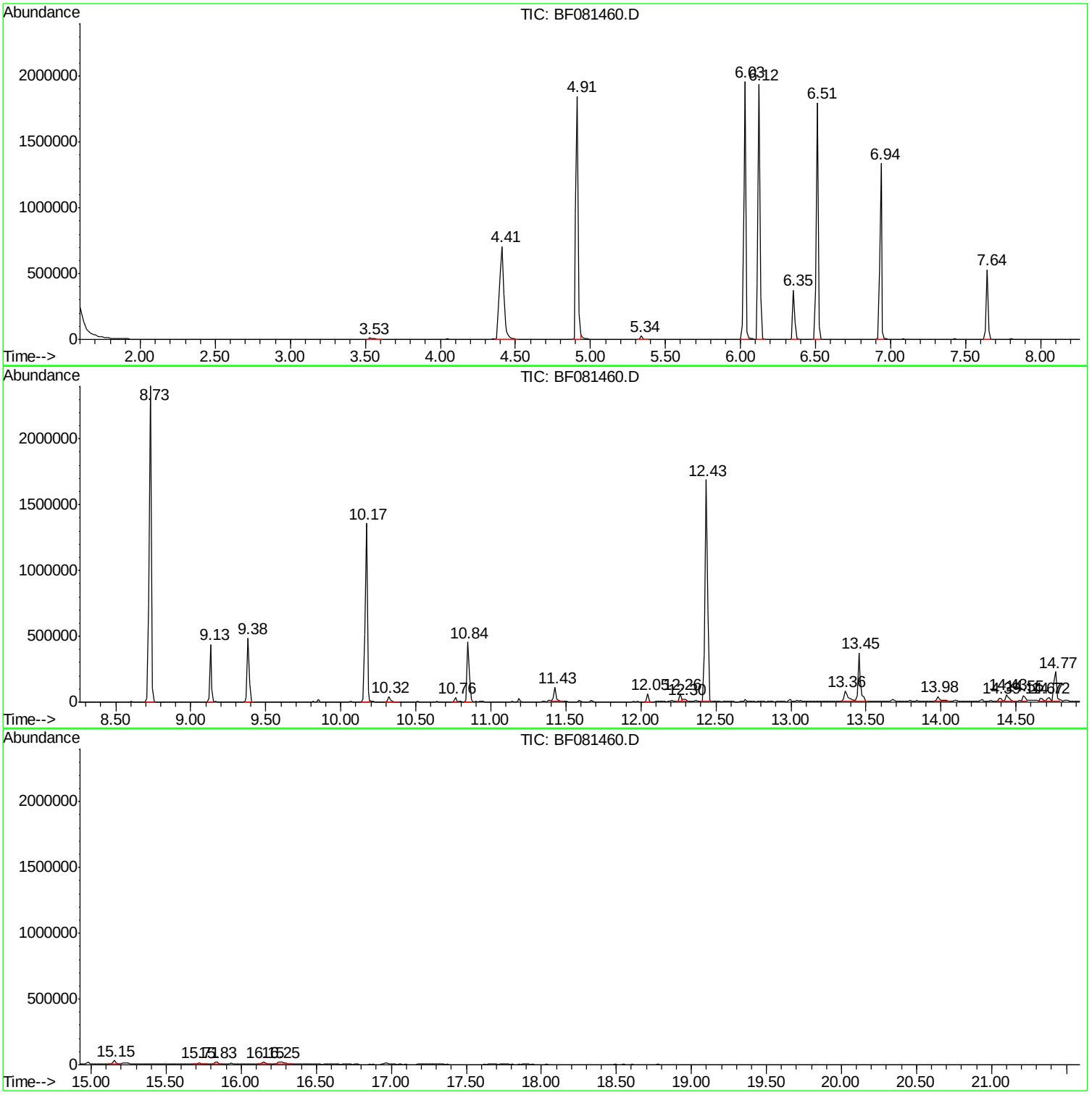
Sum of corrected areas: 19750689

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07(0-0.16)

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

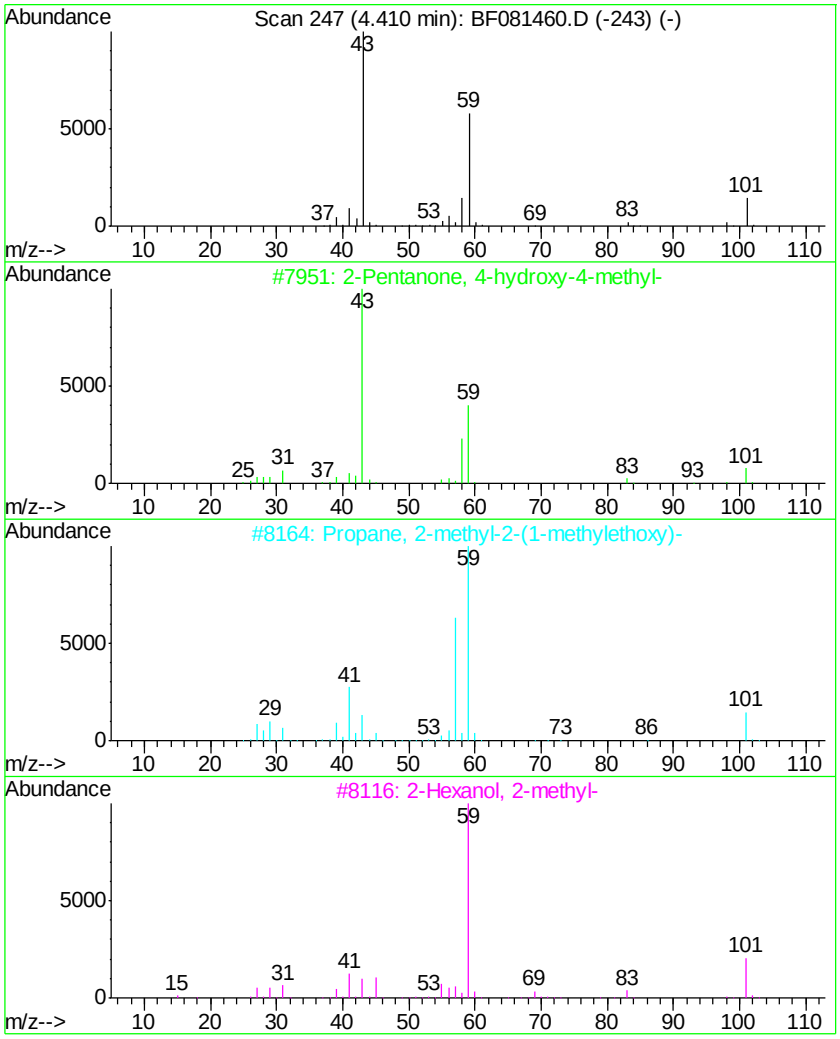
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

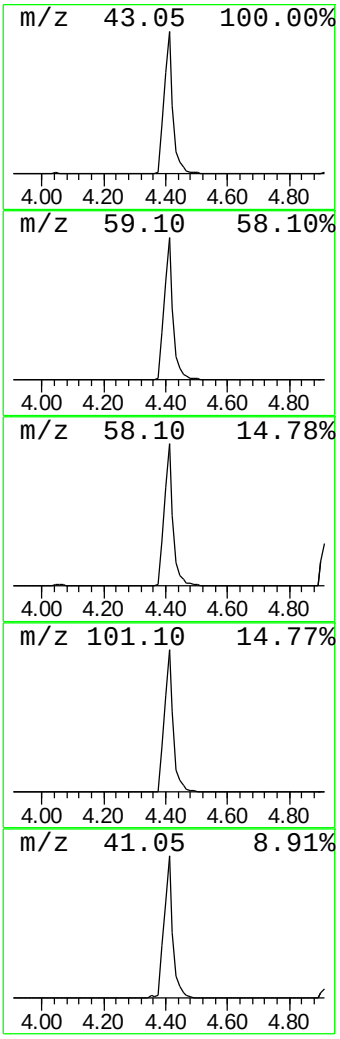
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	78.26 ng	1370060	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





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

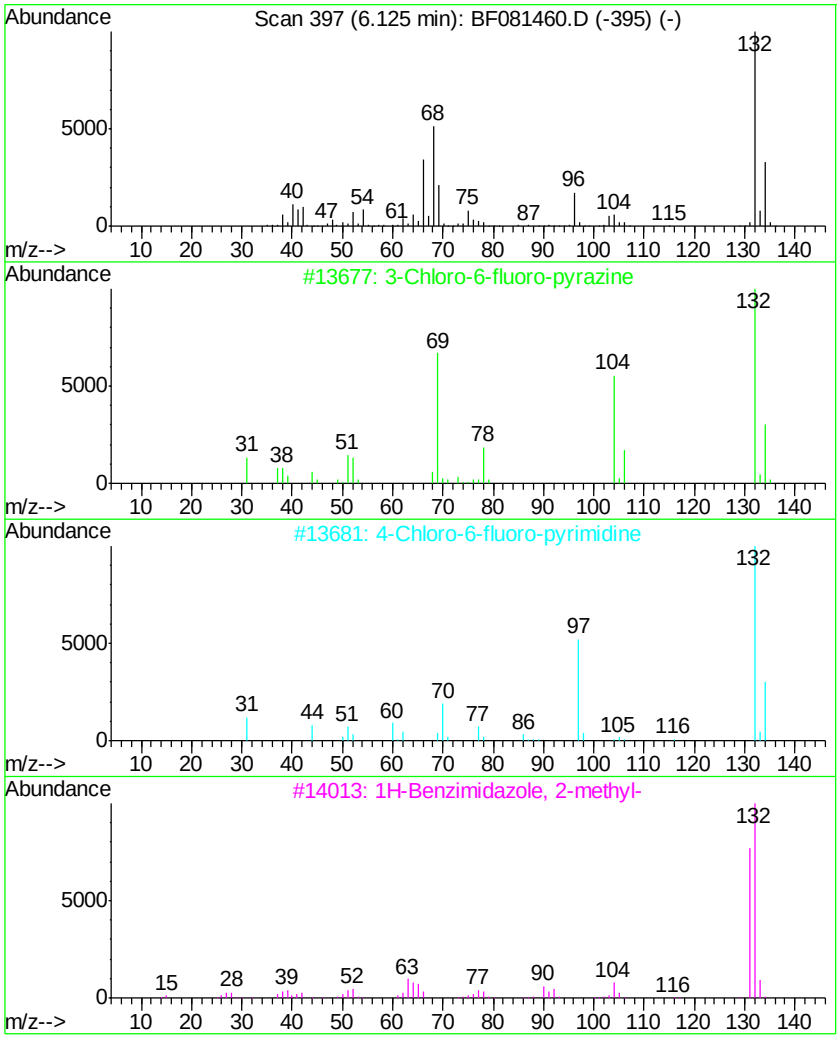
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

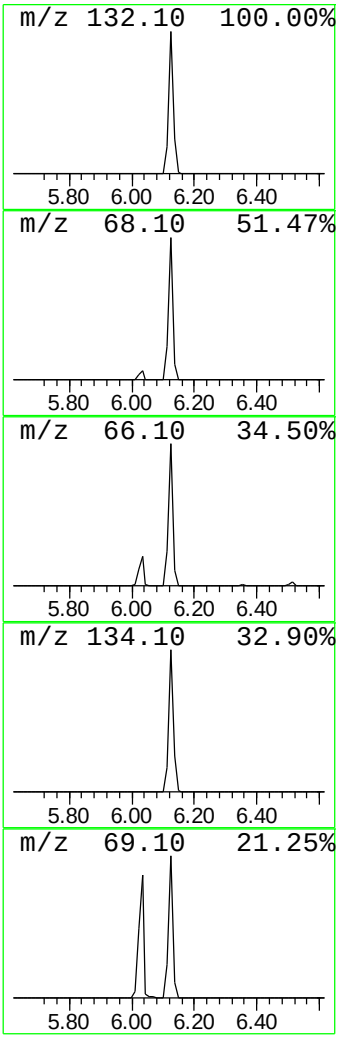
****

Peak Number 2 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	105.52 ng	1847170	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	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

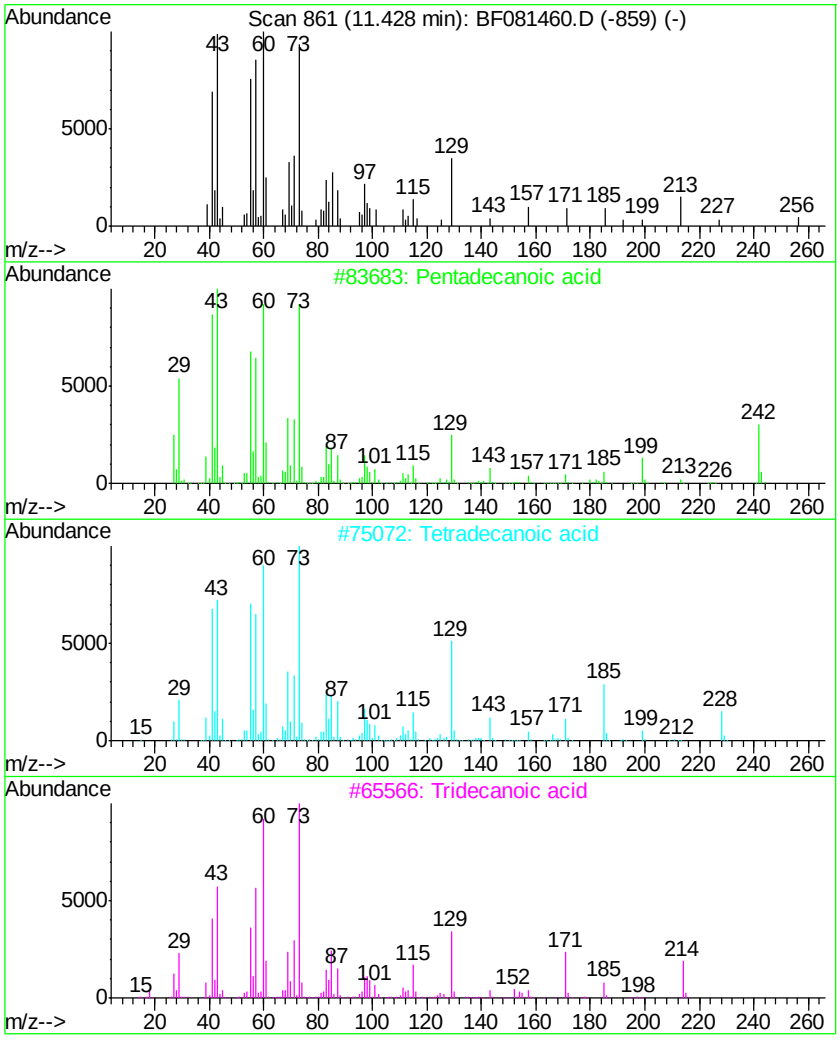
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

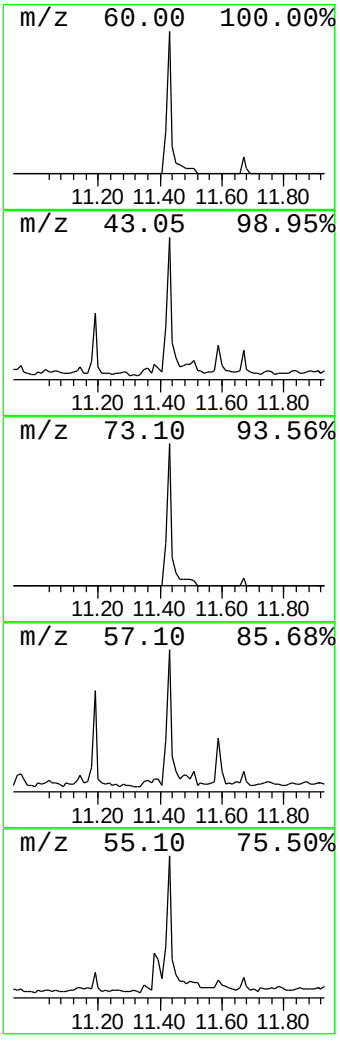
****

Peak Number 4 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	4.85 ng	114912	Phenanthrene-d10	10.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

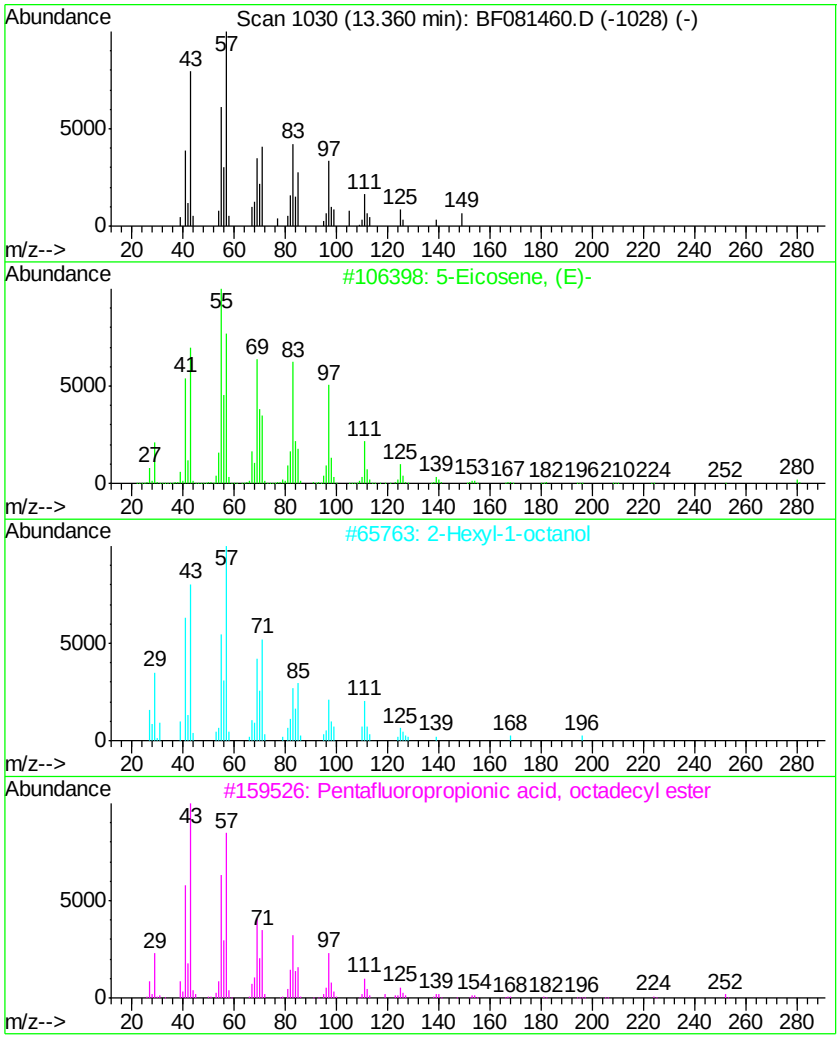
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

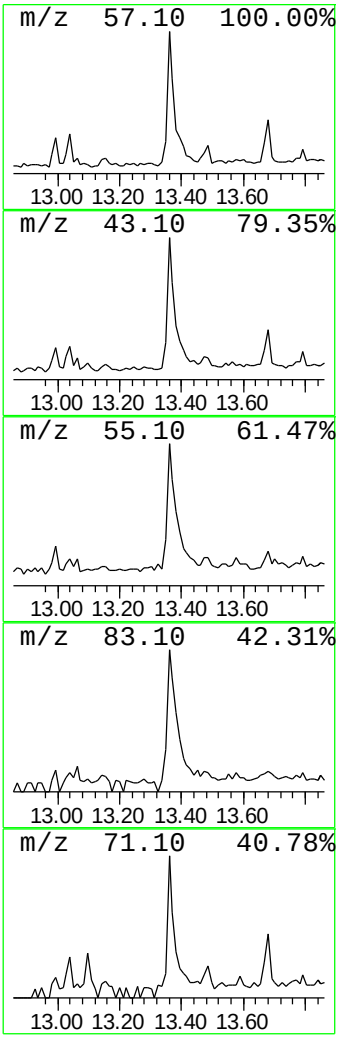
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	6.64 ng	151924	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	81
2	2-Hexyl-1-octanol	214	C14H30O	019780-79-1	80
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	80
4	1-Docosene	308	C22H44	001599-67-3	74
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

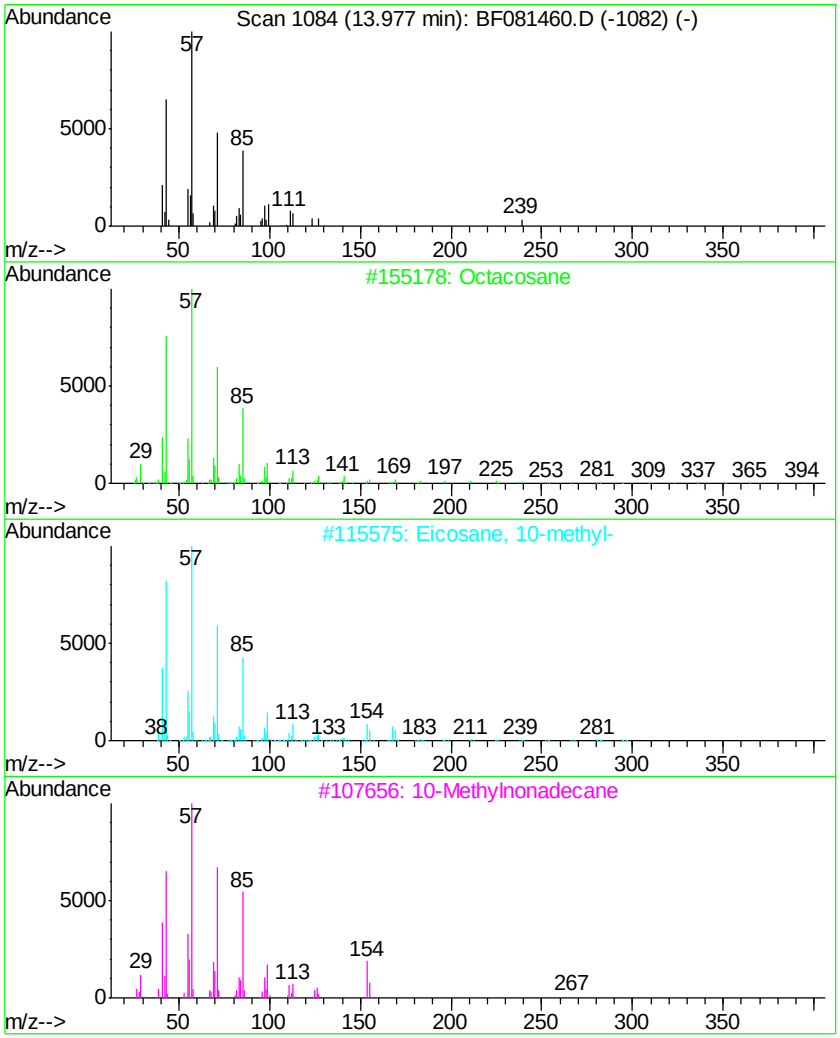
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

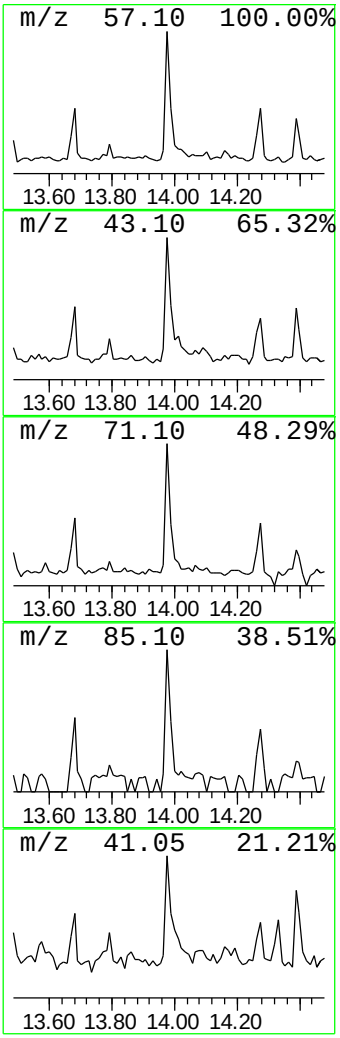
****

Peak Number 6 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	2.81 ng	64143	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
3	10-Methylnonadecane	282	C20H42	056862-62-5	80
4	Tetracosane	338	C24H50	000646-31-1	80
5	Hentriacontane	437	C31H64	000630-04-6	78





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

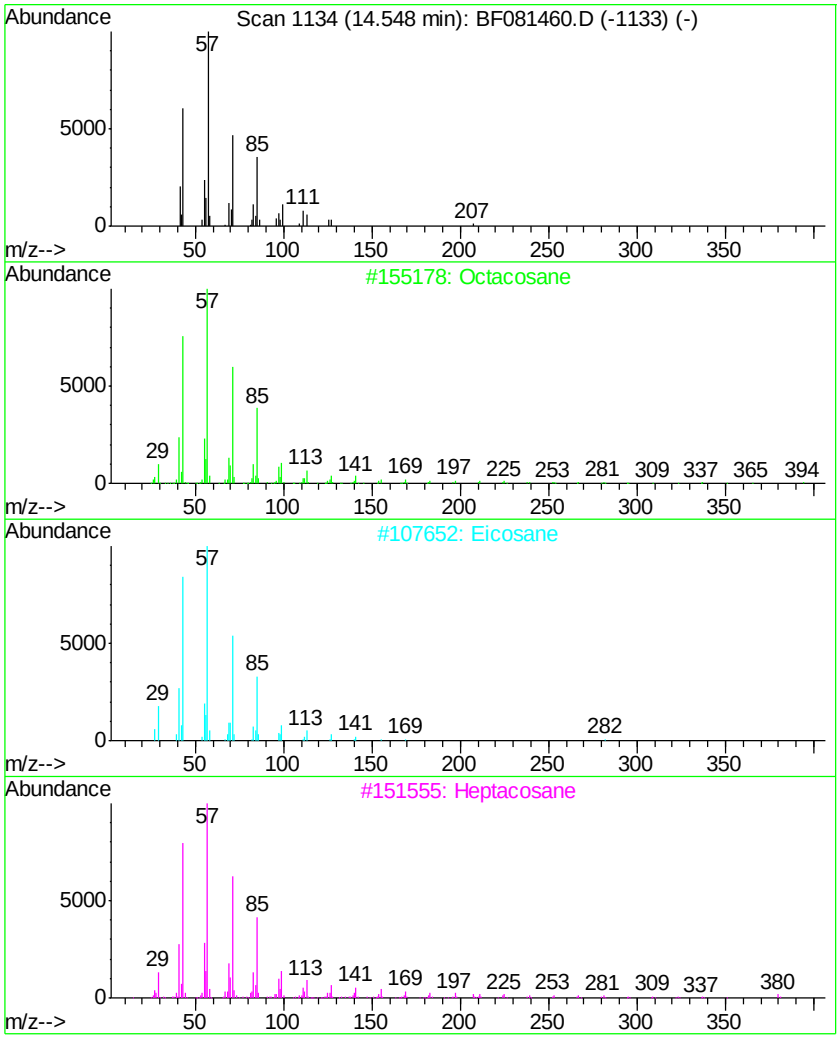
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

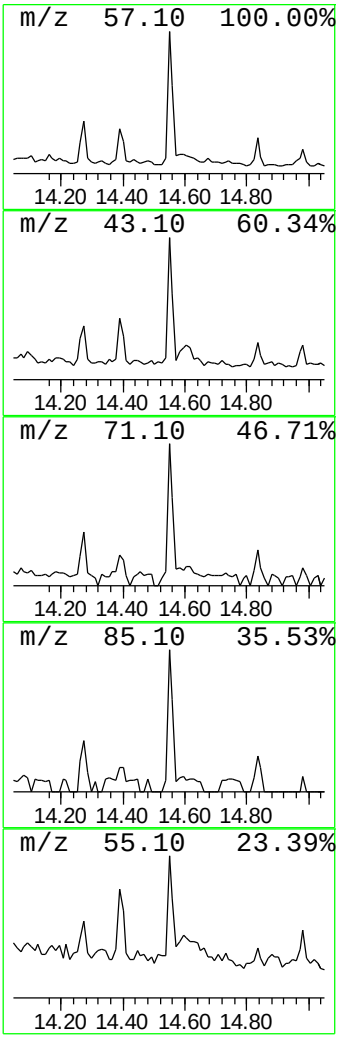
****

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	3.49 ng	47110	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Eicosane	282	C20H42	000112-95-8	86
3	Heptacosane	380	C27H56	000593-49-7	80
4	Hexatriacontane	507	C36H74	000630-06-8	80
5	Hentriacontane	437	C31H64	000630-04-6	78





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

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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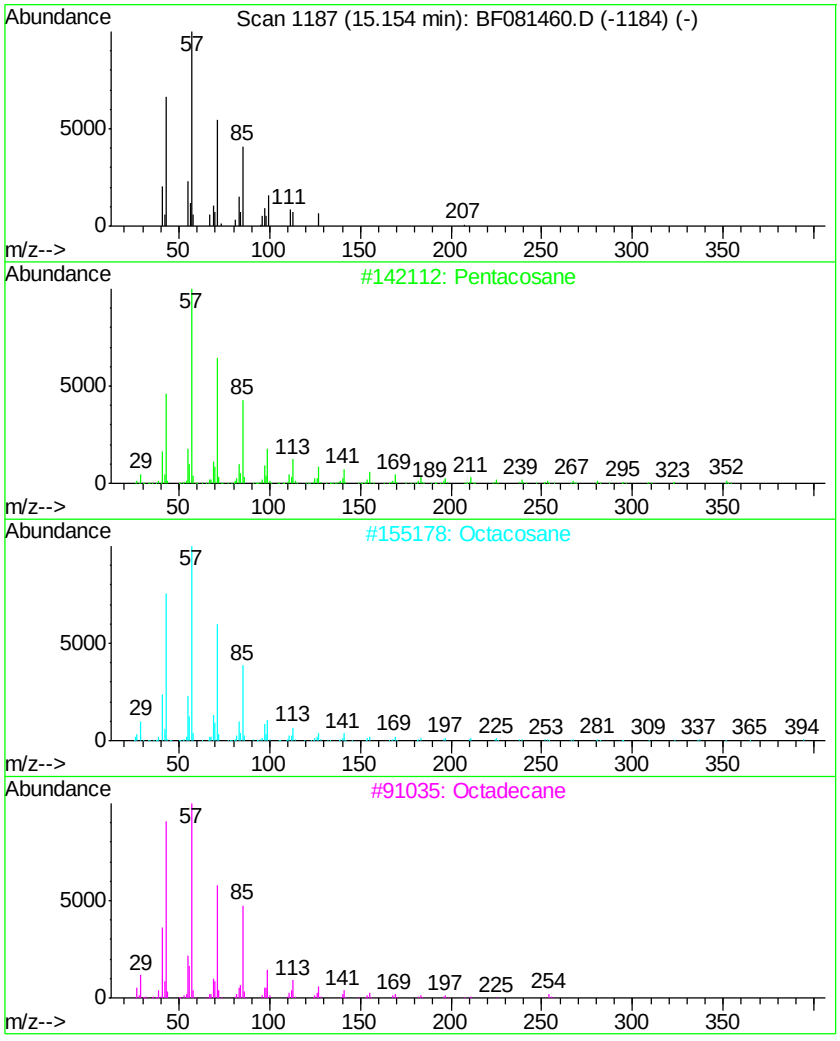
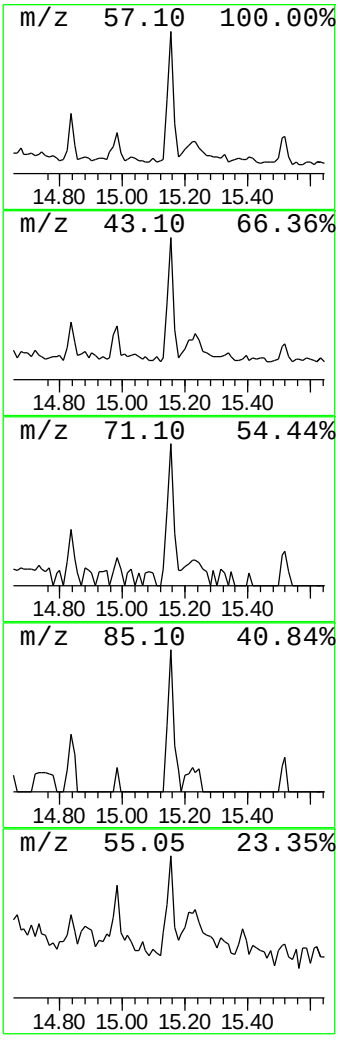
Peak Number 8 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	2.83 ng	38134	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Octadecane	254	C18H38	000593-45-3	86
4	Tetratriacontane	479	C34H70	014167-59-0	86
5	Tetracosane	338	C24H50	000646-31-1	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

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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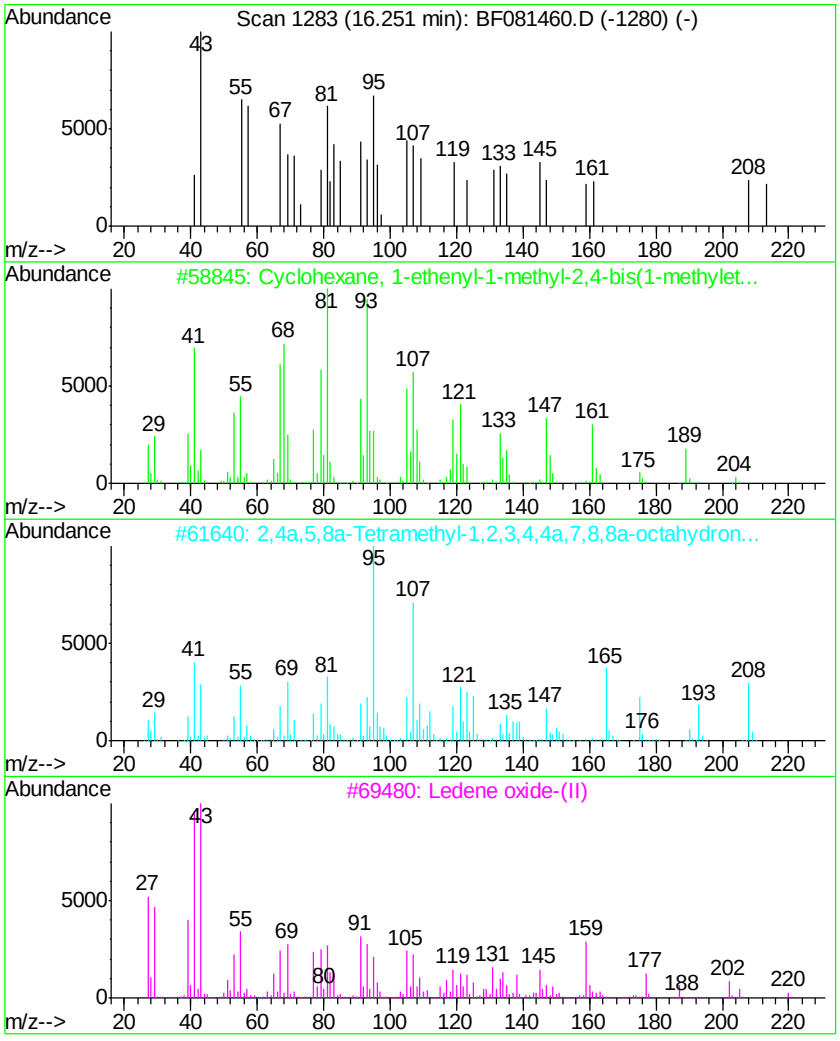
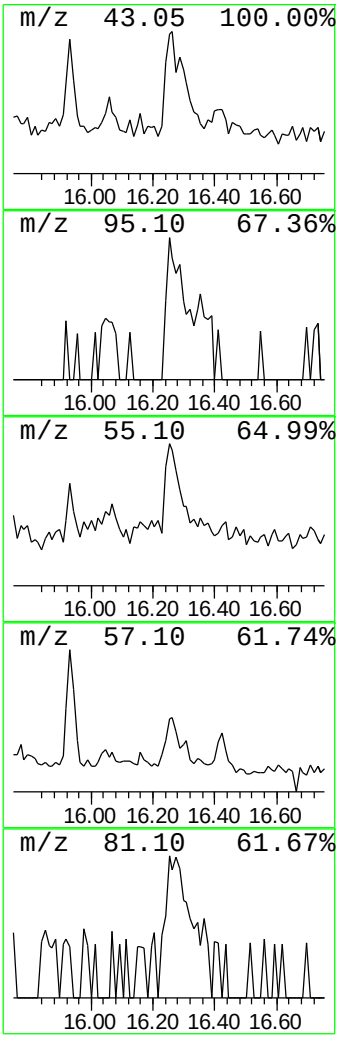
Peak Number 10 unknown16.25 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	4.30 ng	58061	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	25
2	2,4a,5,8a-Tetramethyl-1,2,3,4,4a...	208	C14H24O	020558-22-9	25
3	Ledene oxide-(II)	220	C15H24O	1000159-36-7	25
4	cis-Z-.alpha.-Bisabolene epoxide	220	C15H24O	1000131-71-2	23
5	1,5,9,13-Tetradecatetraene	190	C14H22	051487-38-8	17





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090415\
Data File : BF081460.D
Acq On : 5 Sep 2015 12:44
Operator : UM/IZ
Sample : G3511-09
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07(0-0.16)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.41	78.3	ng	1370060	1	6.35	350112	20.0
unknown6.12	6.12	105.5	ng	1847170	1	6.35	350112	20.0
Pentadecanoic acid	11.43	4.8	ng	114912	4	10.85	473925	20.0
5-Eicosene, (E)-	13.36	6.6	ng	151924	5	13.45	457277	20.0
Octacosane	13.98	2.8	ng	64143	5	13.45	457277	20.0
Eicosane	14.55	3.5	ng	47110	6	14.77	269968	20.0
Pentacosane	15.15	2.8	ng	38134	6	14.77	269968	20.0
unknown16.25	16.25	4.3	ng	58061	6	14.77	269968	20.0