LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

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-BF112115.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	4.787	243	245	256	rVB	934177	1471626	20.81%	2.971%
2	5.256	284	286	296	rBV	3012761	3617993	51.16%	7.304%
3	6.307	376	378	386	rBV	1717700	2285501	32.32%	4.614%
4	6.422	386	388	391	rBV	4979584	5555289	78.55%	11.216%
5	6.650	406	408	410	rBV	1286901	1258940	17.80%	2.542%
6	6.810	419	422	424	rBV	5290539	5547254	78.43%	11.199%
7	7.222	455	458	461	rVV	4114632	4439610	62.77%	8.963%
8	7.302	463	465	467	rVV2	65652	83033	1.17%	0.168%
9	7.347	467	469	473	rVB2	59515	76678	1.08%	0.155%
10	7.679	494	498	500	rBV3	24497	70967	1.00%	0.143%
11	7.942	518	521	523	rBV	1117110	1531230	21.65%	3.091%
12	8.090	532	534	539	rBV5	35720	98265	1.39%	0.198%
13	8.890	600	604	608	rBV5	28027	72723	1.03%	0.147%
14	9.016	612	615	618	rBV	5764231	7072504	100.00%	14.279%
15	9.679	671	673	676	rBV	1158438	1486292	21.02%	3.001%
16	10.033	700	704	706	rBV2	50416	78107	1.10%	0.158%
17	10.468	740	742	745	rBV2	2736556	3776523	53.40%	7.624%
18	11.154	800	802	805	rBV	922666	1268109	17.93%	2.560%
19	11.714	848	851	853	rBV	222267	251820	3.56%	0.508%
20	12.411	908	912	915	rBV3	35027	94973	1.34%	0.192%
21	12.491	917	919	923	rVV	366176	427239	6.04%	0.863%
22	12.582	925	927	930	rVV	117245	114292	1.62%	0.231%
23	12.754	939	942	944	rBV	4128661	5768585	81.56%	11.646%
24	13.291	986	989	990	rBV	62088	82598	1.17%	0.167%
25	13.782	1030	1032	1035	rBV	1275962	1222766	17.29%	2.469%
26	15.154	1149	1152	1154	rBV	578835	885438	12.52%	1.788%
27	15.200	1154	1156	1159	rVB	59340	79389	1.12%	0.160%
28	15.565	1186	1188	1192	rBV	70242	123166	1.74%	0.249%
29	16.000	1223	1226	1230	rVB	104772	192502	2.72%	0.389%
30	16.503	1266	1270	1273	rBV	79977	171235	2.42%	0.346%
31	17.086	1318	1321	1325	rVB	62725	133228	1.88%	0.269%
32	17.783	1378	1382	1385	rVB2	34257	93102	1.32%	0.188%
33	18.606	1451	1454	1459	rVB4	31264	100617	1.42%	0.203%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

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-BF112115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

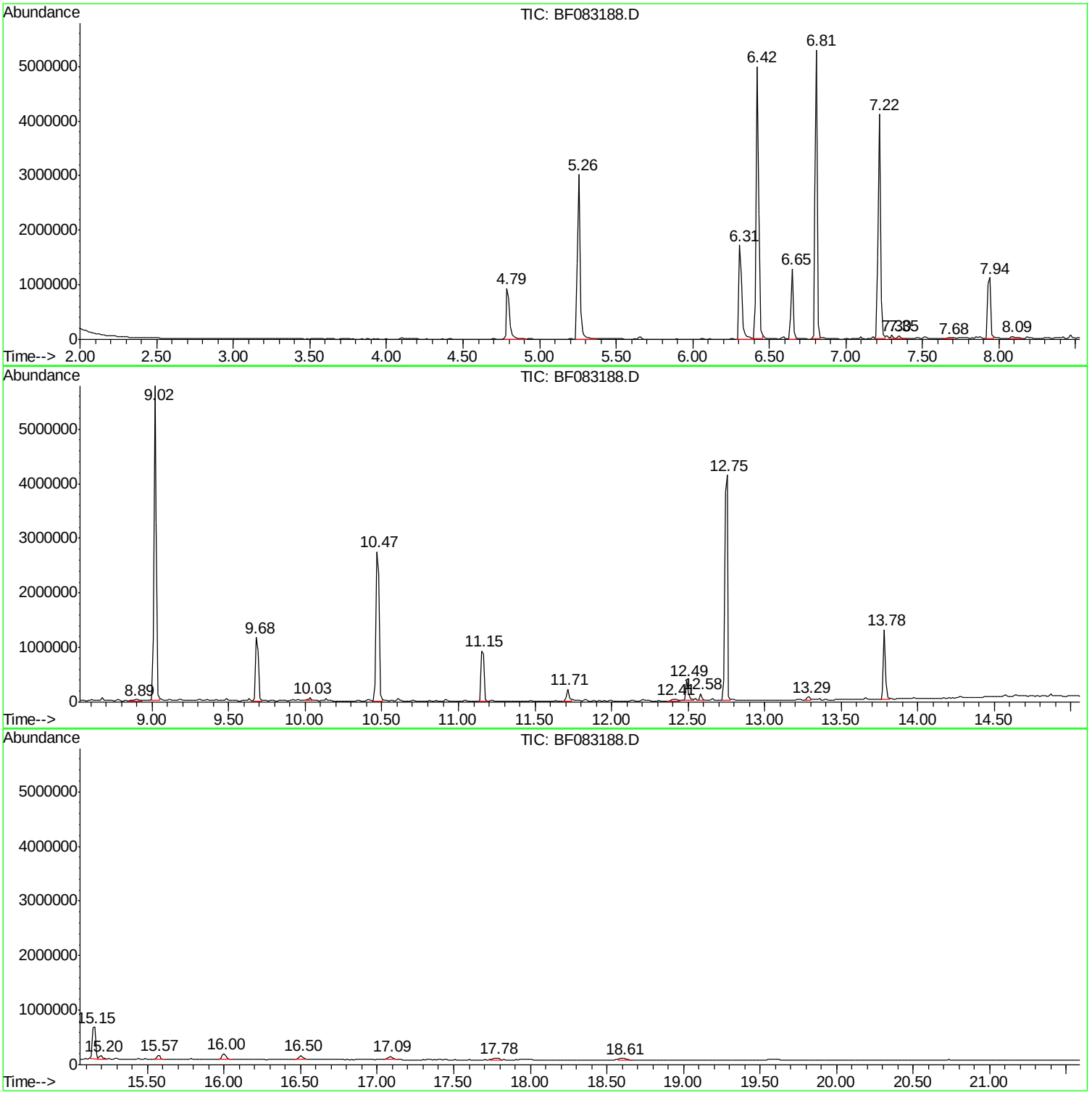
Sum of corrected areas: 49531594

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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\BF112215\
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Acq On : 23 Nov 2015 5:30
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Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

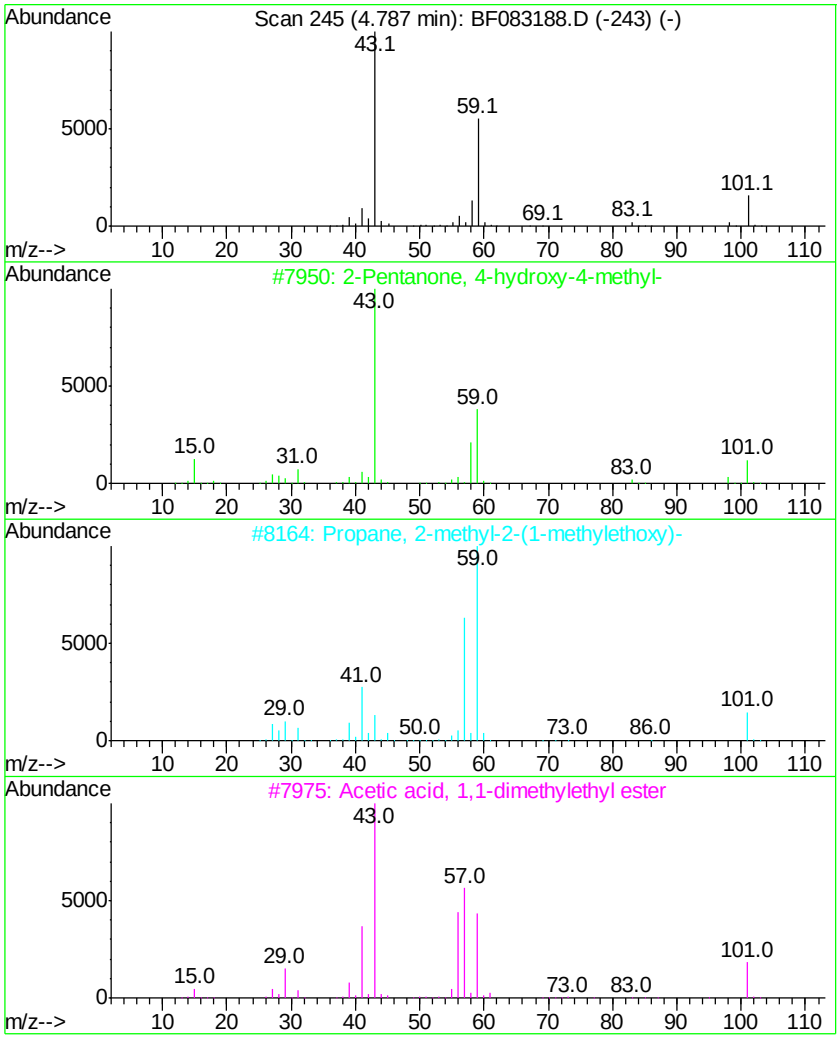
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

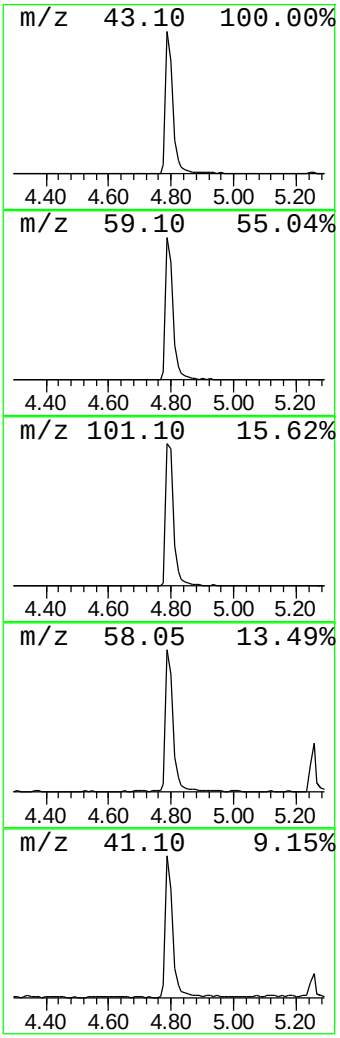
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	23.38 ng	1471630	1,4-Dichlorobenzene-d4	6.65

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	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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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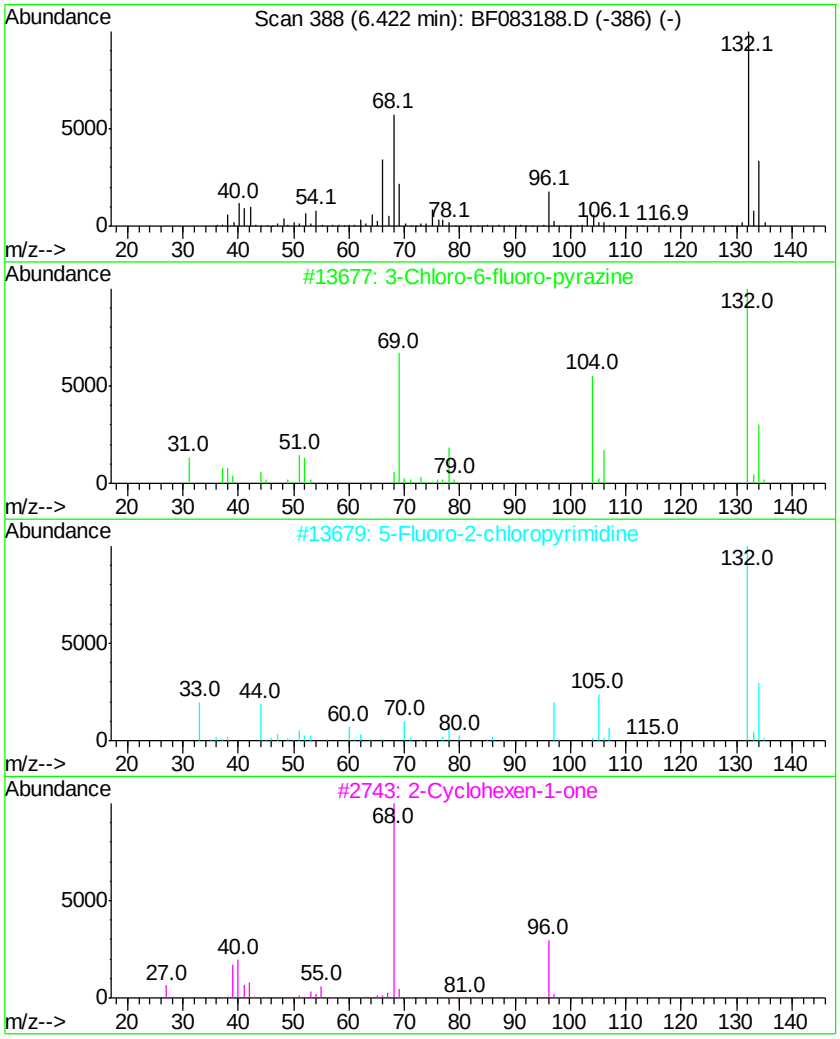
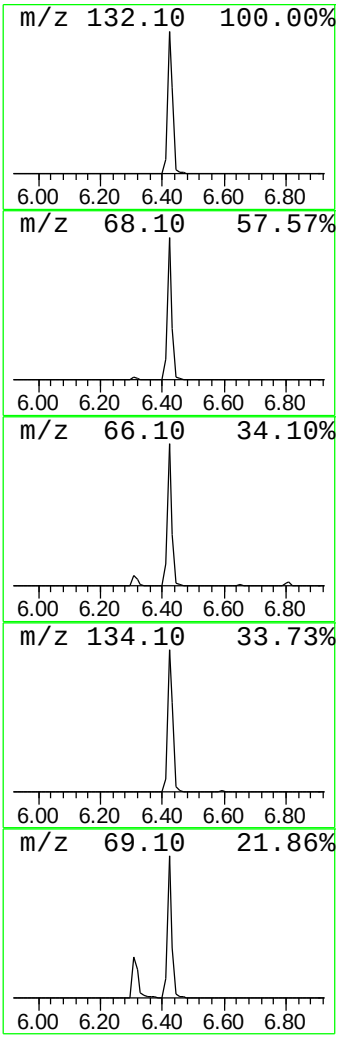
Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	88.25 ng	5555290	1,4-Dichlorobenzene-d4	6.65

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	12
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.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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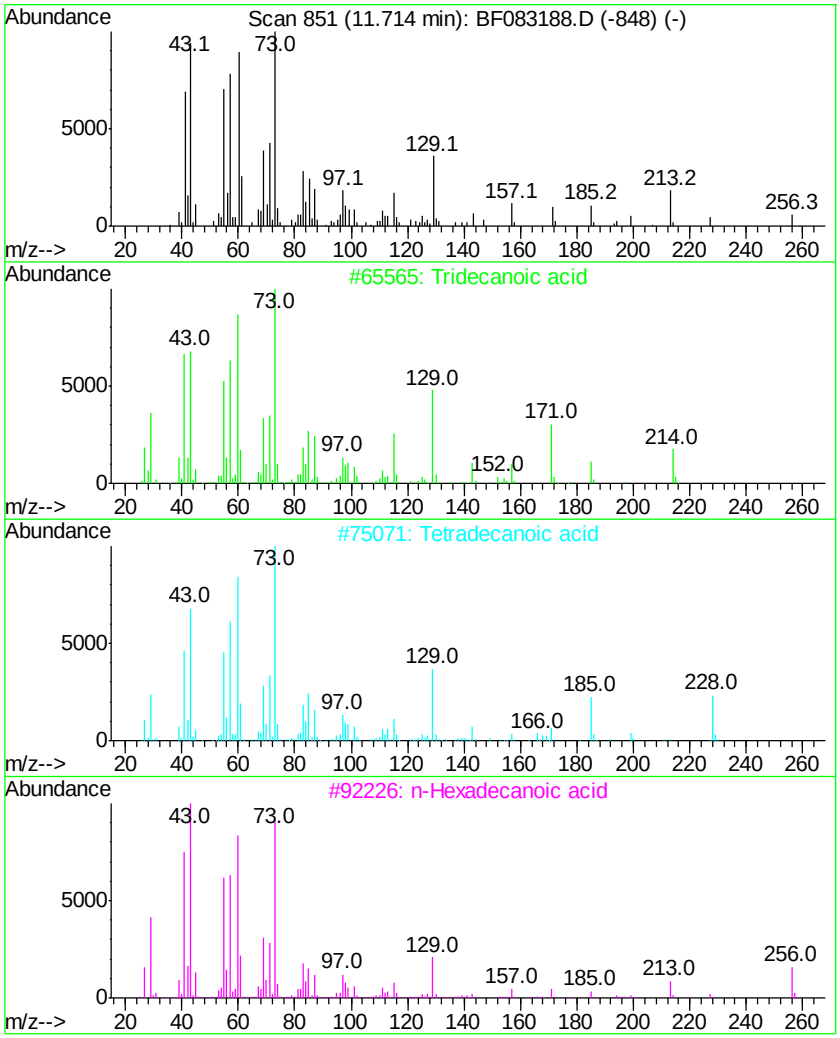
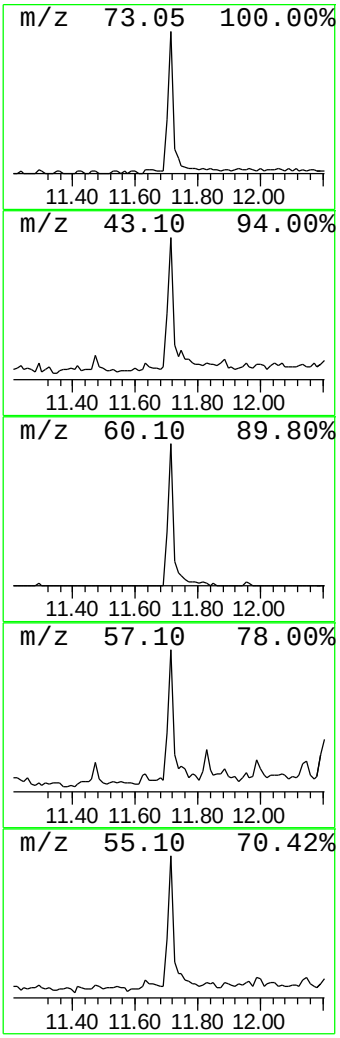
Peak Number 4 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	3.97 ng	251820	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.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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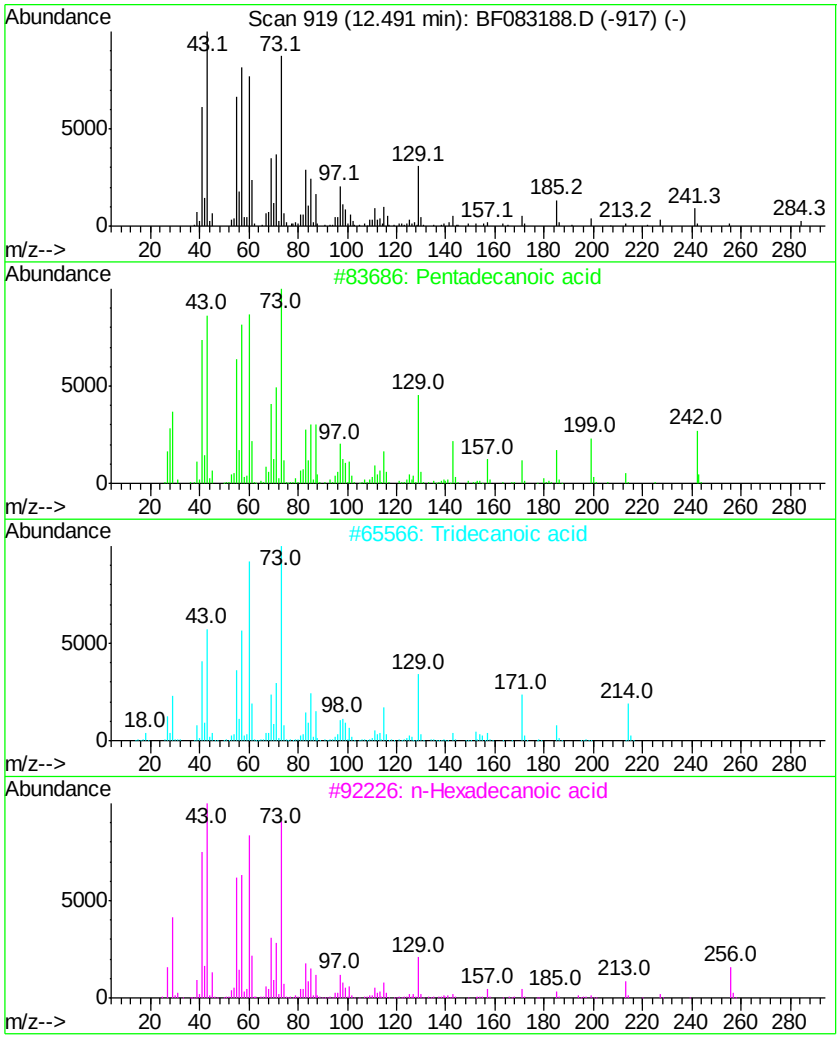
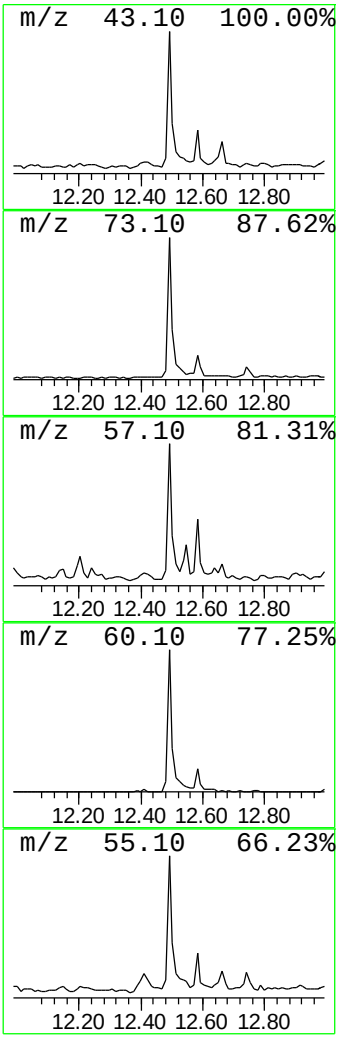
Peak Number 5 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	6.99 ng	427239	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Heptanoic acid	130	C7H14O2	000111-14-8	35





Library Search Compound Report

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Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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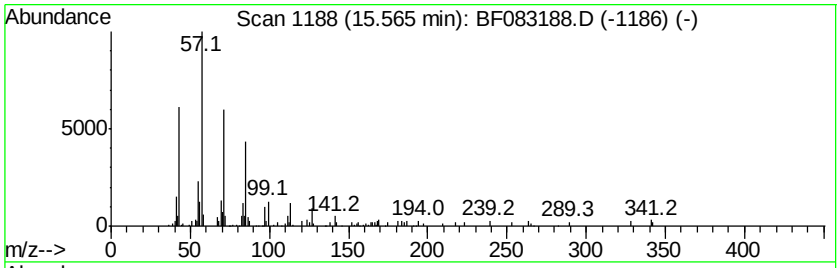
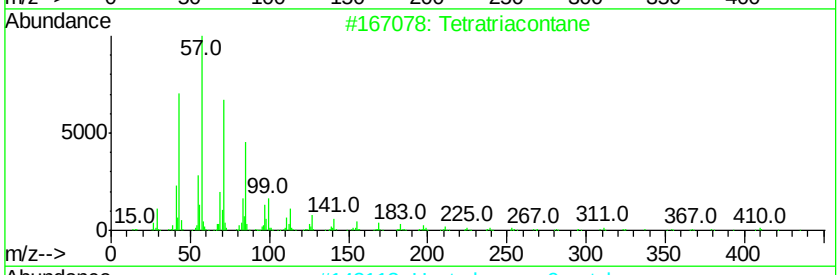
****

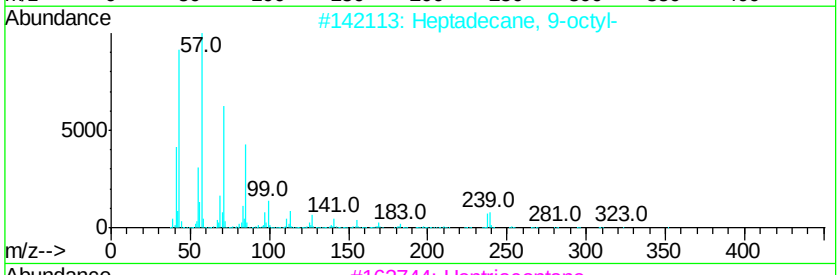
Peak Number 6 Tetratriacontane Concentration Rank 9

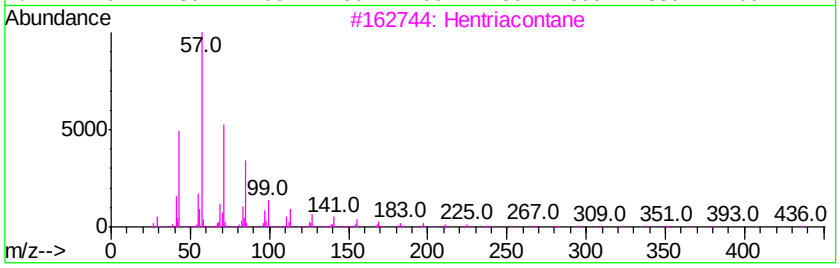
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.78 ng	123166	Perylene-d12	15.15

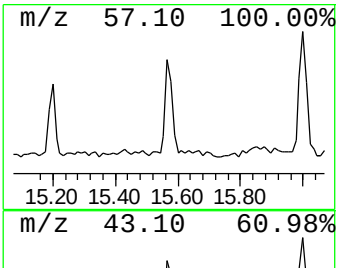
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90

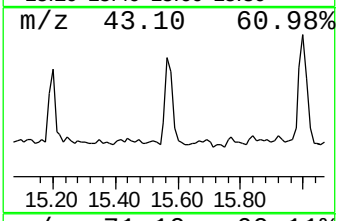


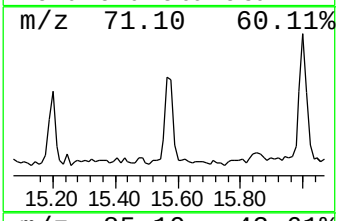


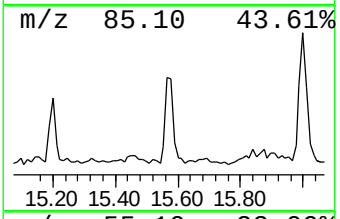


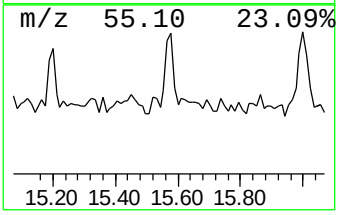












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Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

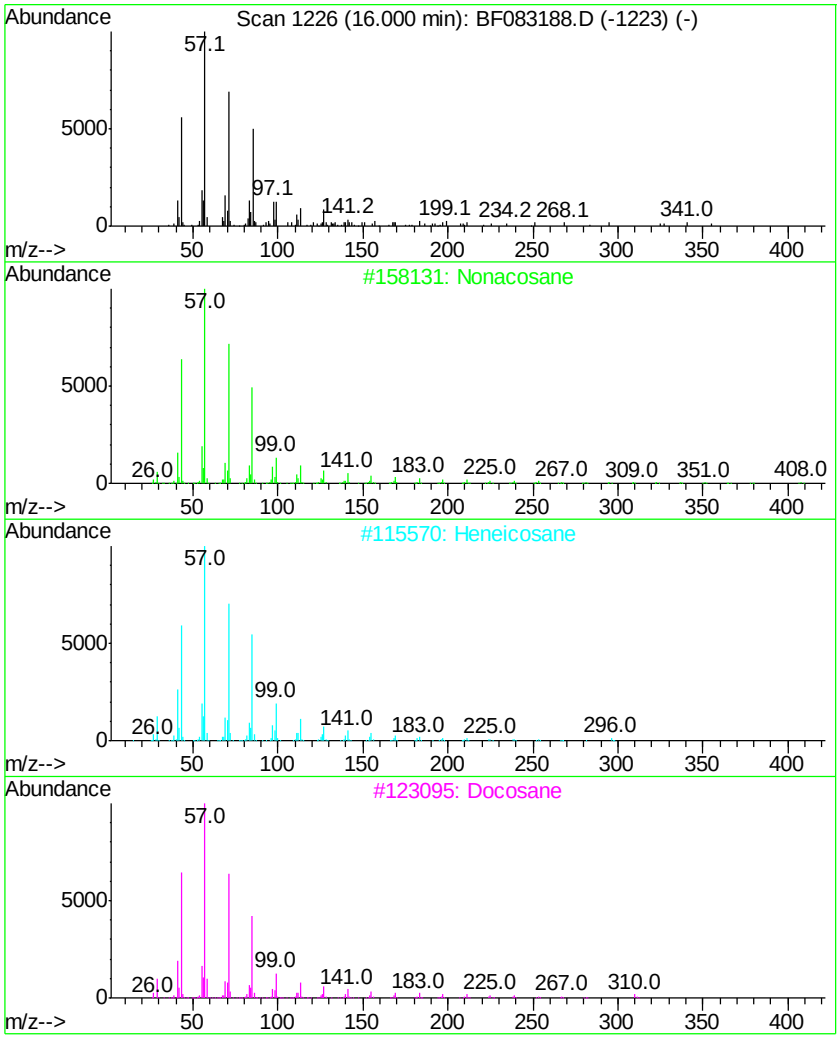
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

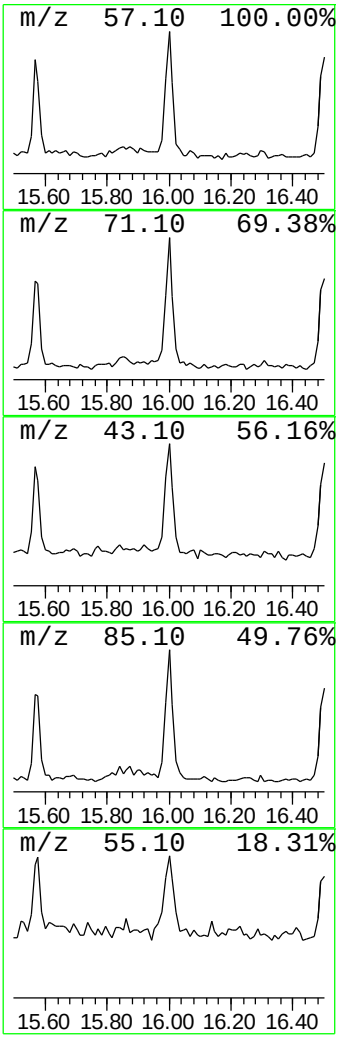
****

Peak Number 7 Nonacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	4.35 ng	192502	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane	408	C29H60	000630-03-5	87
2	Heneicosane	296	C21H44	000629-94-7	86
3	Docosane	310	C22H46	000629-97-0	86
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
5	Eicosane	282	C20H42	000112-95-8	86





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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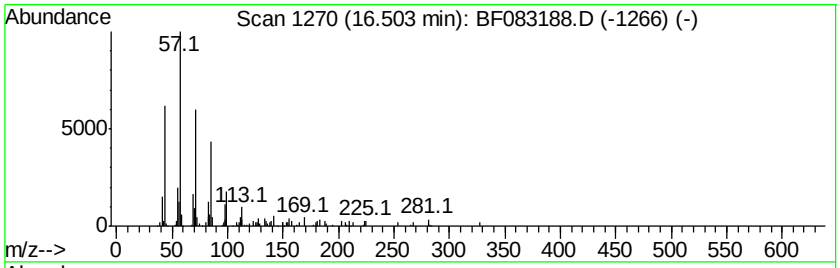
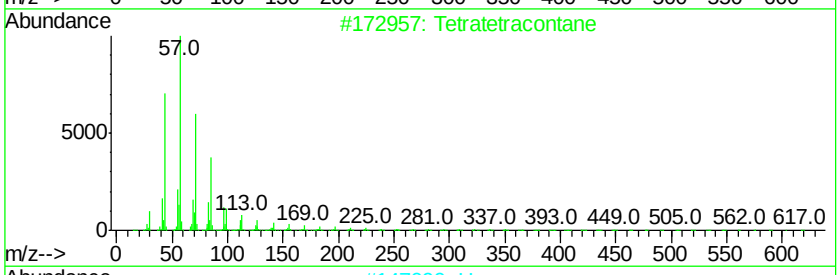
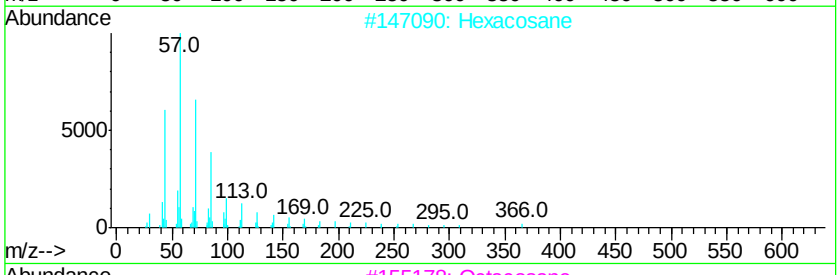
Peak Number 8 Tetratetracontane Concentration Rank 7

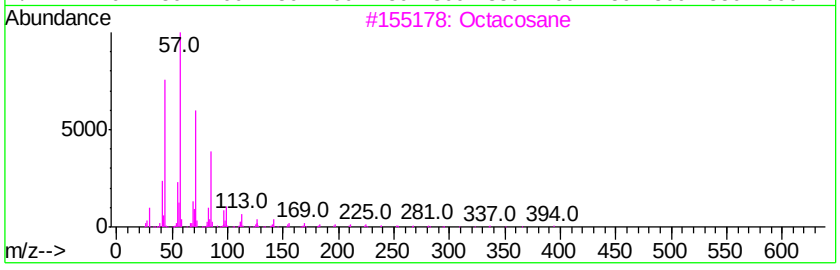
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	3.87 ng	171235	Perylene-d12	15.15

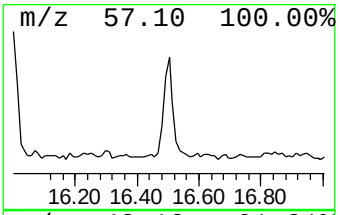
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Triacontane	422	C30H62	000638-68-6	87
5	Hentriacontane	437	C31H64	000630-04-6	87

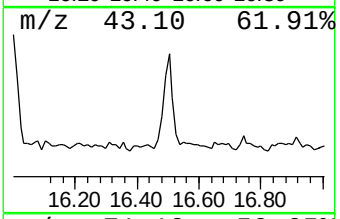


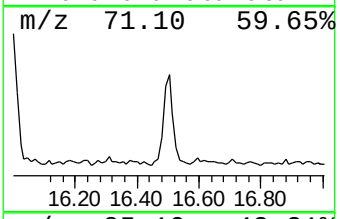


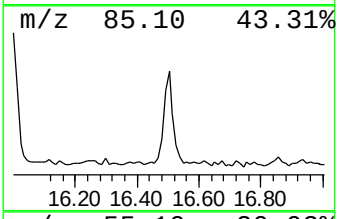


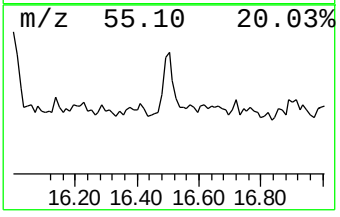












Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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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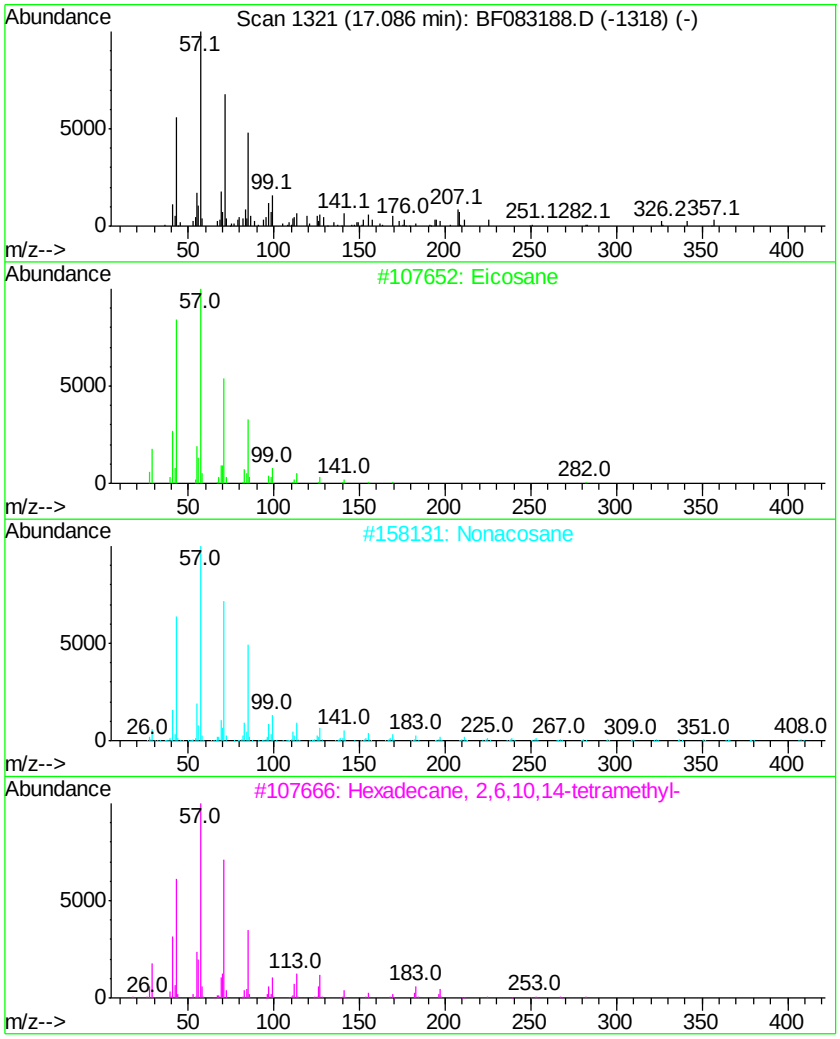
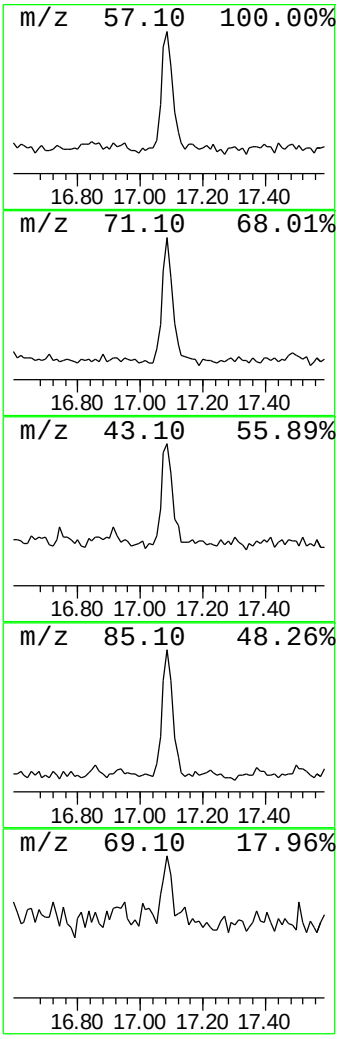
Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.09	3.01 ng	133228	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Nonacosane	408	C29H60	000630-03-5	83
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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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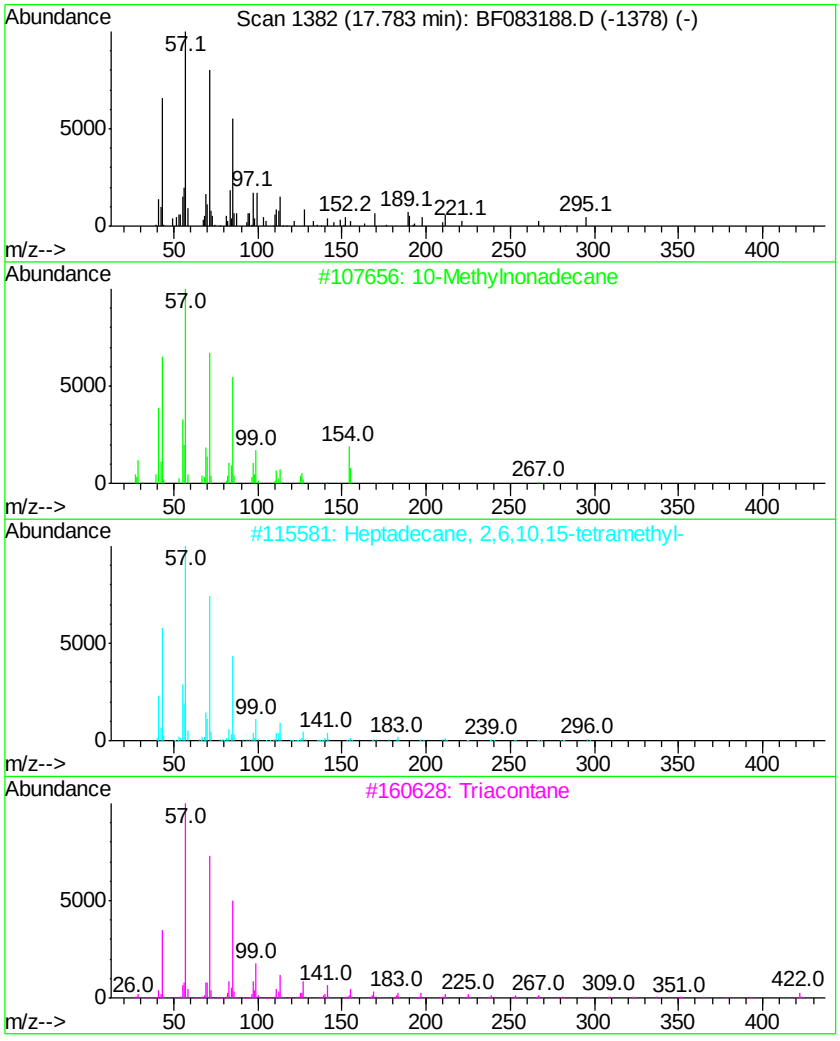
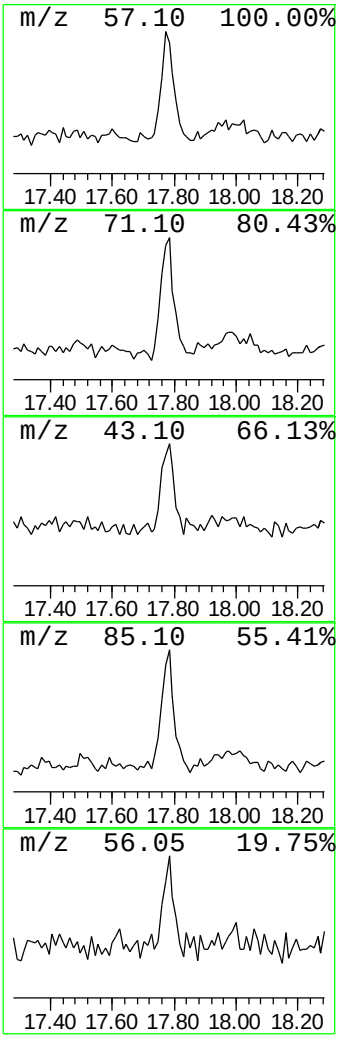
Peak Number 10 10-Methylnonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.78	2.10 ng	93102	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	86
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3	Triacontane	422	C30H62	000638-68-6	80
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.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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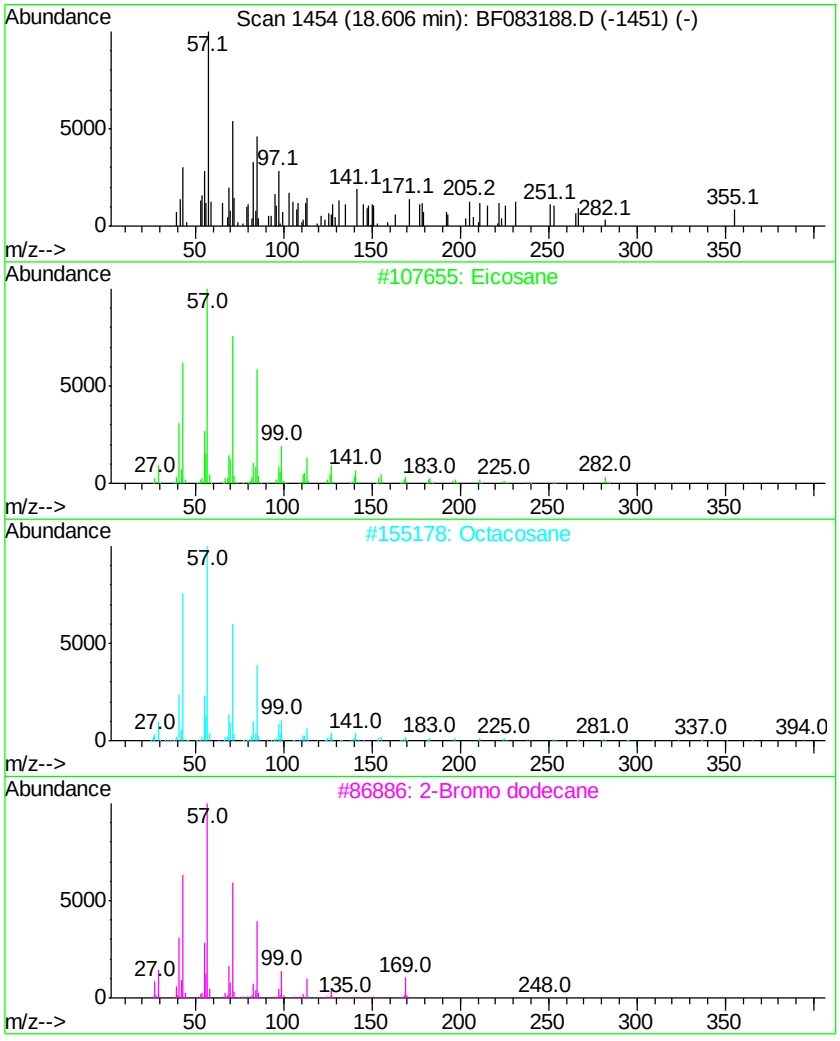
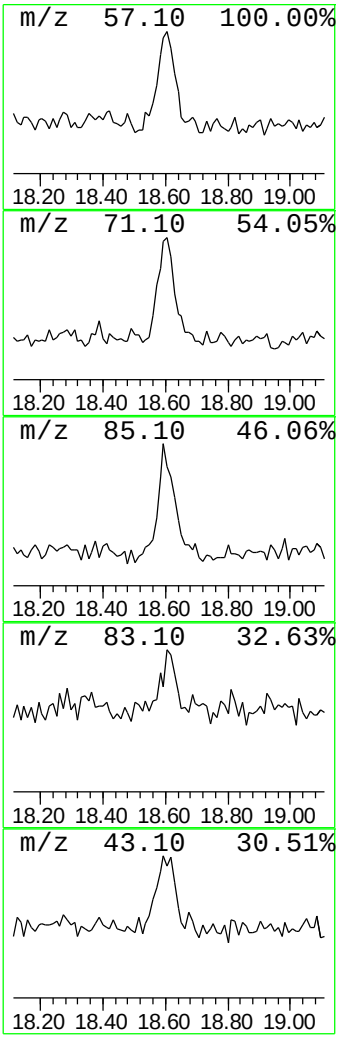
Peak Number 11 unknown18.61 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.61	2.27 ng	100617	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	43
2	Octacosane	394	C28H58	000630-02-4	43
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	38
4	Tetradecane	198	C14H30	000629-59-4	38
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112215\
Data File : BF083188.D
Acq On : 23 Nov 2015 5:30
Operator : UM/IZ
Sample : G4437-01
Misc :
ALS Vial : 74 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-35

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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...	4.79	23.4	ng	1471630	1	6.65	1258940	20.0
unknown6.42	6.42	88.3	ng	5555290	1	6.65	1258940	20.0
Tridecanoic acid	11.71	4.0	ng	251820	4	11.16	1268110	20.0
Pentadecanoic acid	12.49	7.0	ng	427239	5	13.78	1222770	20.0
Tetratriacontane	15.57	2.8	ng	123166	6	15.15	885438	20.0
Nonacosane	16.00	4.3	ng	192502	6	15.15	885438	20.0
Tetratetracontane	16.50	3.9	ng	171235	6	15.15	885438	20.0
Eicosane	17.09	3.0	ng	133228	6	15.15	885438	20.0
10-Methylnonadecane	17.78	2.1	ng	93102	6	15.15	885438	20.0
unknown18.61	18.61	2.3	ng	100617	6	15.15	885438	20.0