LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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	2.913	80	81	102	rBV4	74213	382786	5.72%	0.613%
2	4.822	245	248	270	rVB	1980872	3578281	53.46%	5.729%
3	5.267	284	287	289	rBV	4869316	6315510	94.36%	10.111%
4	6.319	376	379	381	rBV	6010942	6693345	100.00%	10.716%
5	6.422	386	388	391	rBV	4750042	6033147	90.14%	9.659%
6	6.650	406	408	411	rBV	1378945	1236066	18.47%	1.979%
7	6.810	419	422	424	rBV	3993108	4296493	64.19%	6.878%
8	7.222	455	458	460	rBV	3701969	3816699	57.02%	6.110%
9	7.942	518	521	523	rBV	1314410	1584160	23.67%	2.536%
10	9.016	612	615	618	rBV	5276620	5491614	82.05%	8.792%
11	9.108	620	623	625	rBV	127914	134361	2.01%	0.215%
12	9.416	648	650	652	rBV	923314	918670	13.73%	1.471%
13	9.633	667	669	671	rBV	219301	207903	3.11%	0.333%
14	9.679	671	673	676	rBV	1232585	1796642	26.84%	2.876%
15	9.873	686	690	693	rBV2	33467	89308	1.33%	0.143%
16	10.136	709	713	715	rBV	286014	279418	4.17%	0.447%
17	10.353	729	732	735	rBV	95321	150904	2.25%	0.242%
18	10.468	740	742	745	rBV2	3224796	4266159	63.74%	6.830%
19	10.605	752	754	760	rVB	274236	322133	4.81%	0.516%
20	11.051	791	793	794	rBV	123752	93687	1.40%	0.150%
21	11.165	800	803	805	rBV	1425083	1793592	26.80%	2.871%
22	11.222	805	808	813	rVB3	39552	95621	1.43%	0.153%
23	11.714	849	851	856	rBV	485279	464861	6.95%	0.744%
24	12.411	907	912	917	rBV7	22081	68387	1.02%	0.109%
25	12.502	917	920	922	rBV	736368	1068832	15.97%	1.711%
26	12.582	925	927	931	rVB	188864	211246	3.16%	0.338%
27	12.708	936	938	939	rBV	179445	177001	2.64%	0.283%
28	12.754	939	942	944	rVB	4192142	6063233	90.59%	9.707%
29	13.039	965	967	969	rVB	95327	112212	1.68%	0.180%
30	13.234	981	984	986	rBV2	44329	111565	1.67%	0.179%
31	13.291	986	989	990	rVV2	126240	148805	2.22%	0.238%
32	13.668	1019	1022	1026	rBV	306991	532355	7.95%	0.852%
33	13.782	1030	1032	1035	rBV	1793750	1733100	25.89%	2.775%
34	13.977	1047	1049	1054	rBV	67646	105471	1.58%	0.169%

LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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

35	14.171	1064	1066	1068	rBV	125887	129698	1.94%	0.208%
36	14.285	1074	1076	1077	rBV	41622	74079	1.11%	0.119%
37	14.548	1097	1099	1105	rBV3	130284	324037	4.84%	0.519%
38	15.154	1149	1152	1154	rBV	977932	1372379	20.50%	2.197%
39	15.577	1186	1189	1192	rBV	49856	80869	1.21%	0.129%
40	16.000	1224	1226	1231	rVB5	50963	108133	1.62%	0.173%

Sum of corrected areas: 62462762

Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
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Acq On : 22 Nov 2015 8:27
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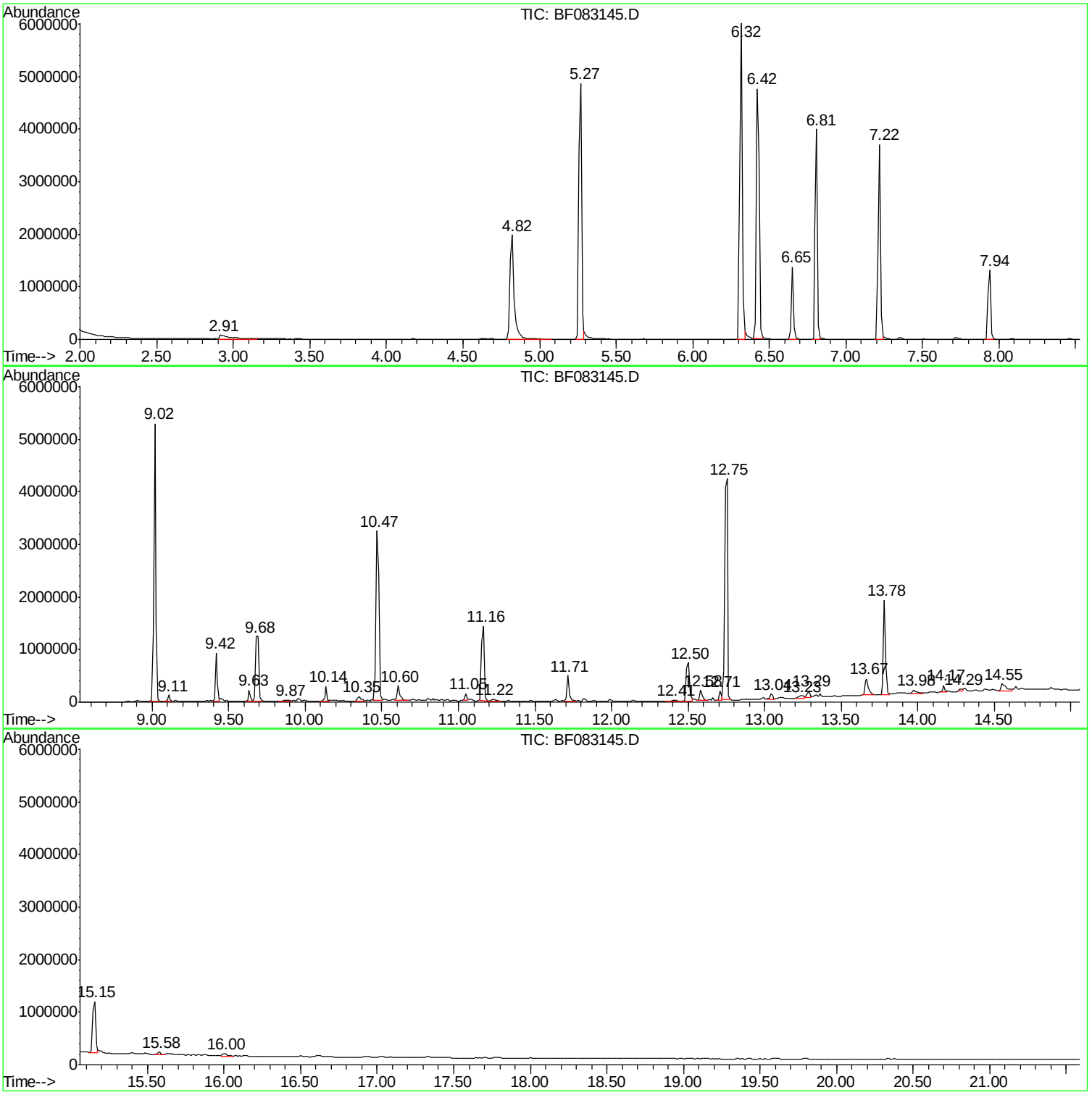
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-22(1-2.2)

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



Library Search Compound Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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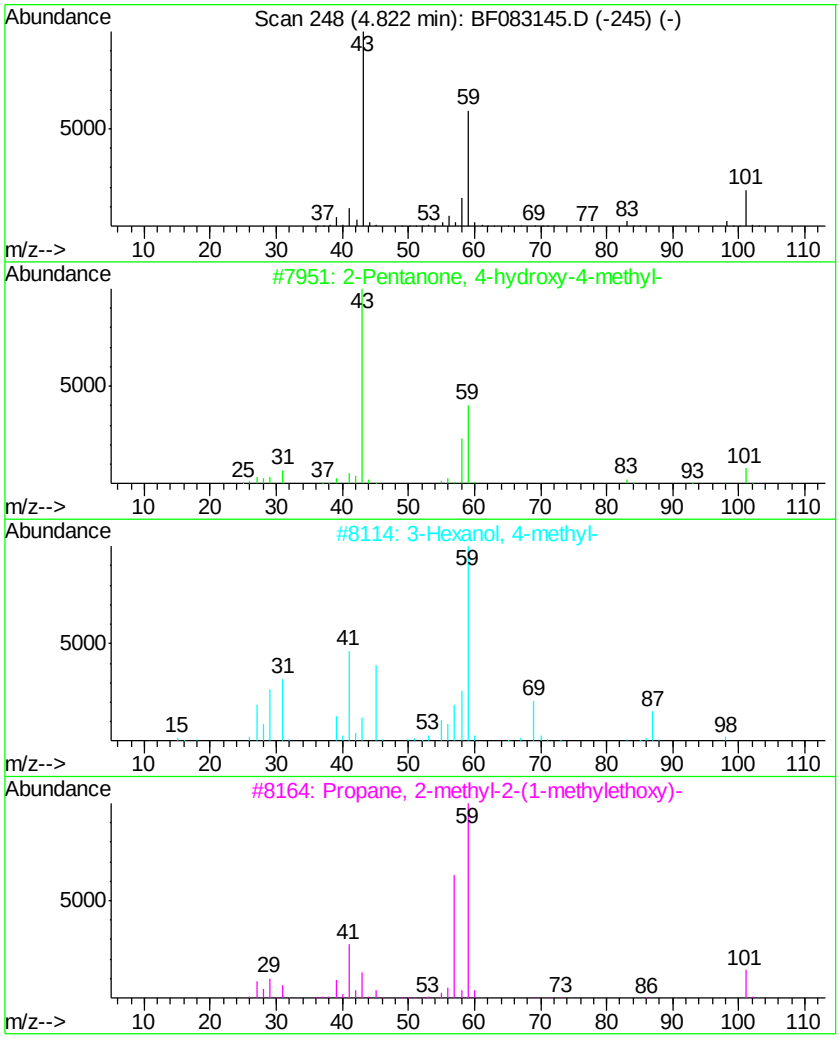
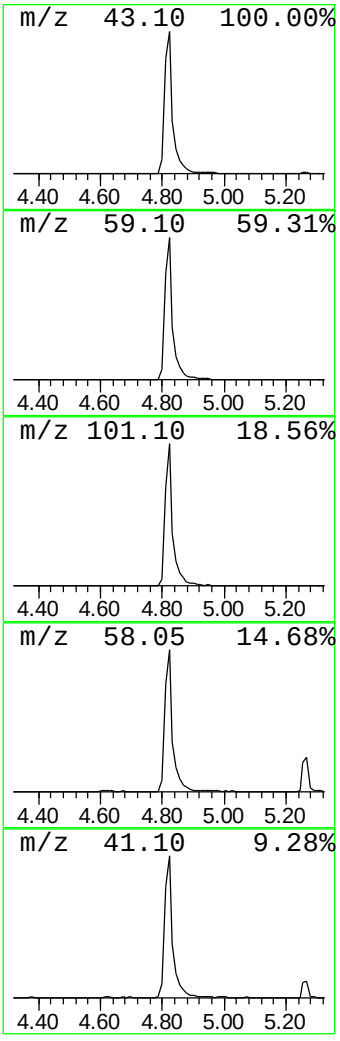
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	57.90 ng	3578280	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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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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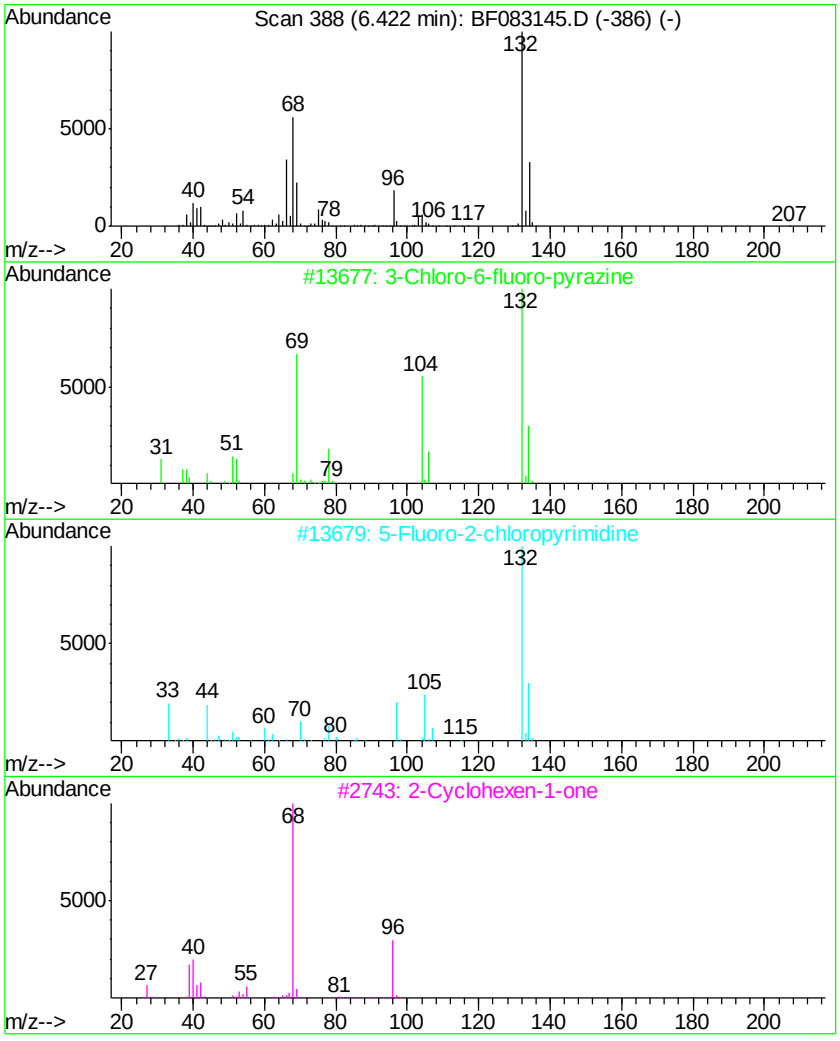
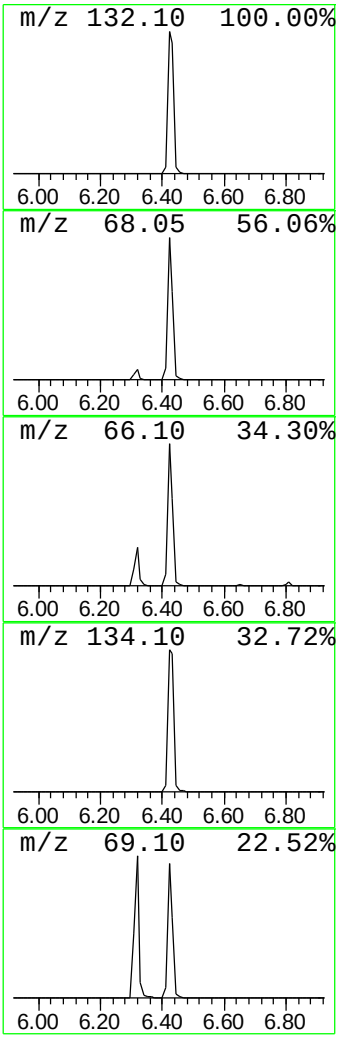
Peak Number 3 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	97.62 ng	6033150	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	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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

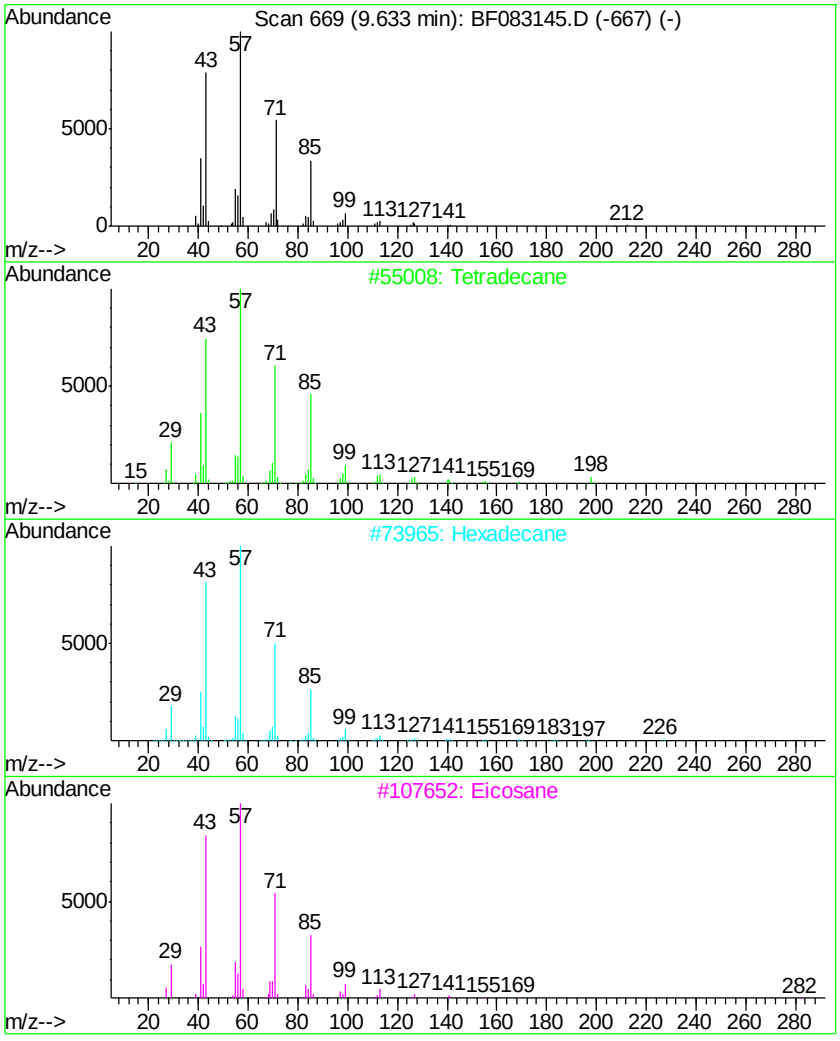
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

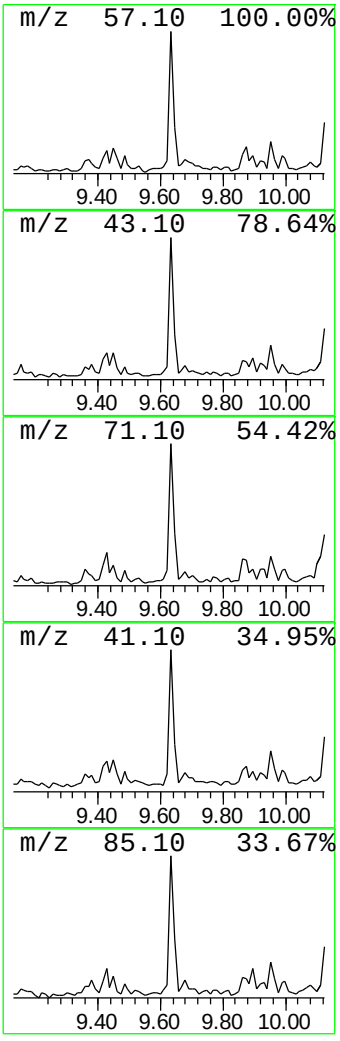
****

Peak Number 5 Tetradecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	2.31 ng	207903	Acenaphthene-d10	9.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Eicosane	282	C20H42	000112-95-8	83
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	59
5	Pentadecane	212	C15H32	000629-62-9	53





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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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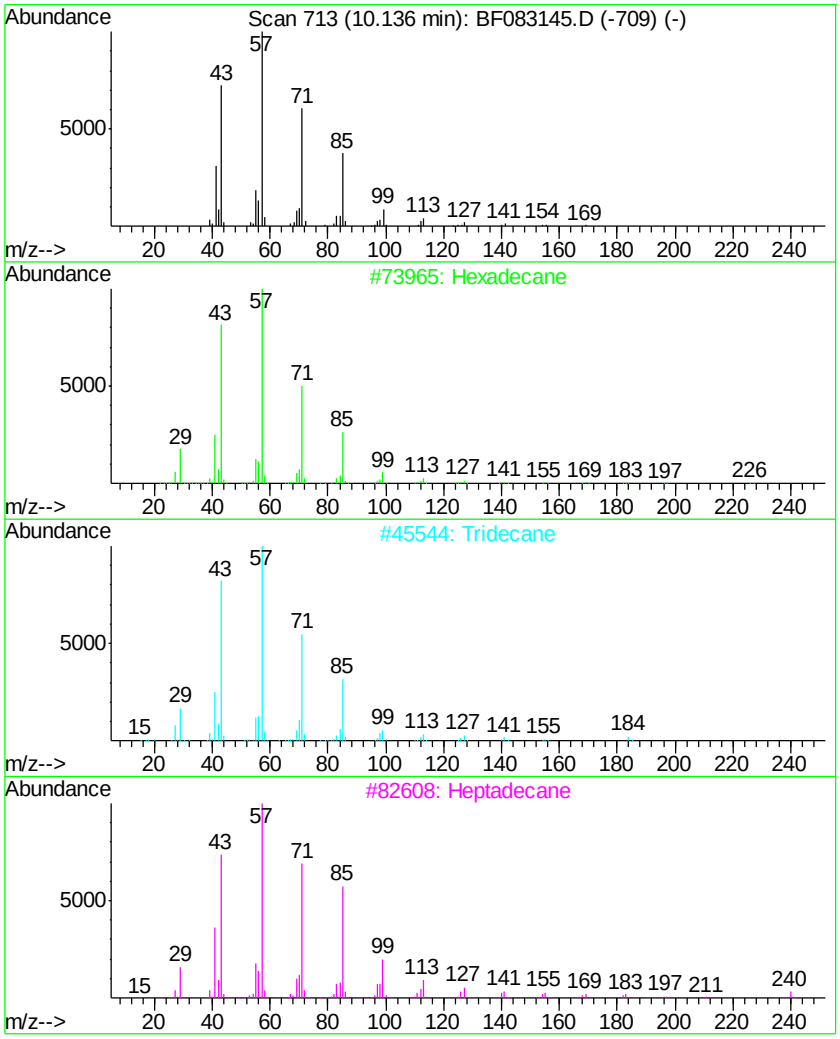
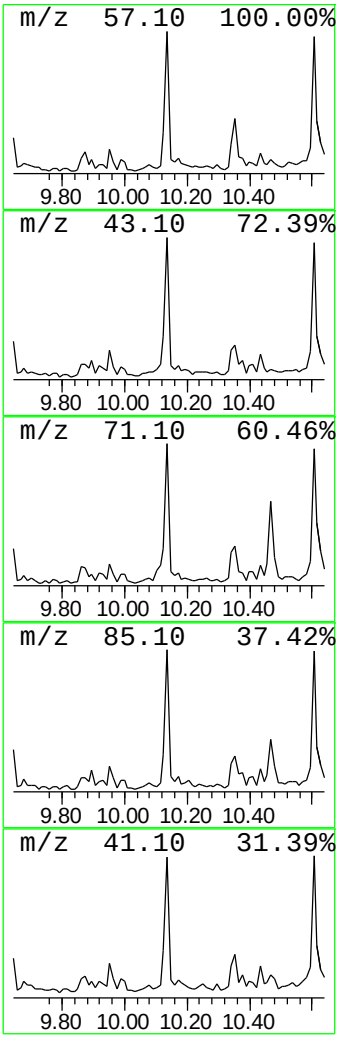
Peak Number 6 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	3.11 ng	279418	Acenaphthene-d10	9.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tridecane	184	C13H28	000629-50-5	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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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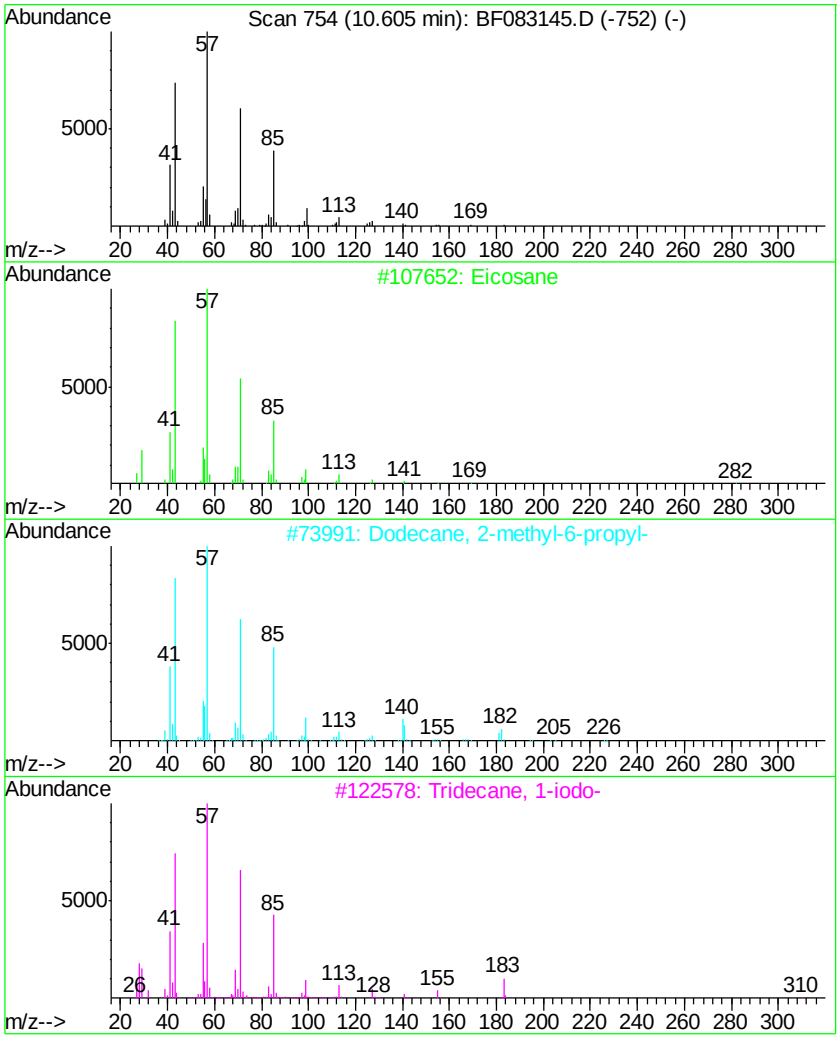
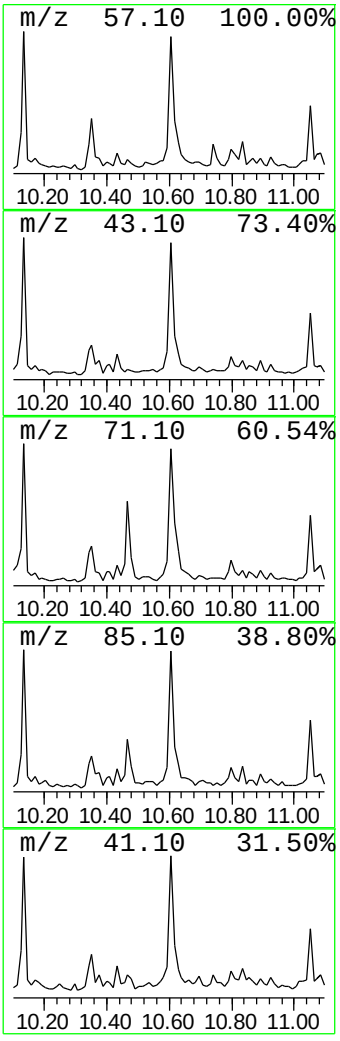
Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	3.59 ng	322133	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
4	Tetradecane	198	C14H30	000629-59-4	83
5	Tetracosane	338	C24H50	000646-31-1	83





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Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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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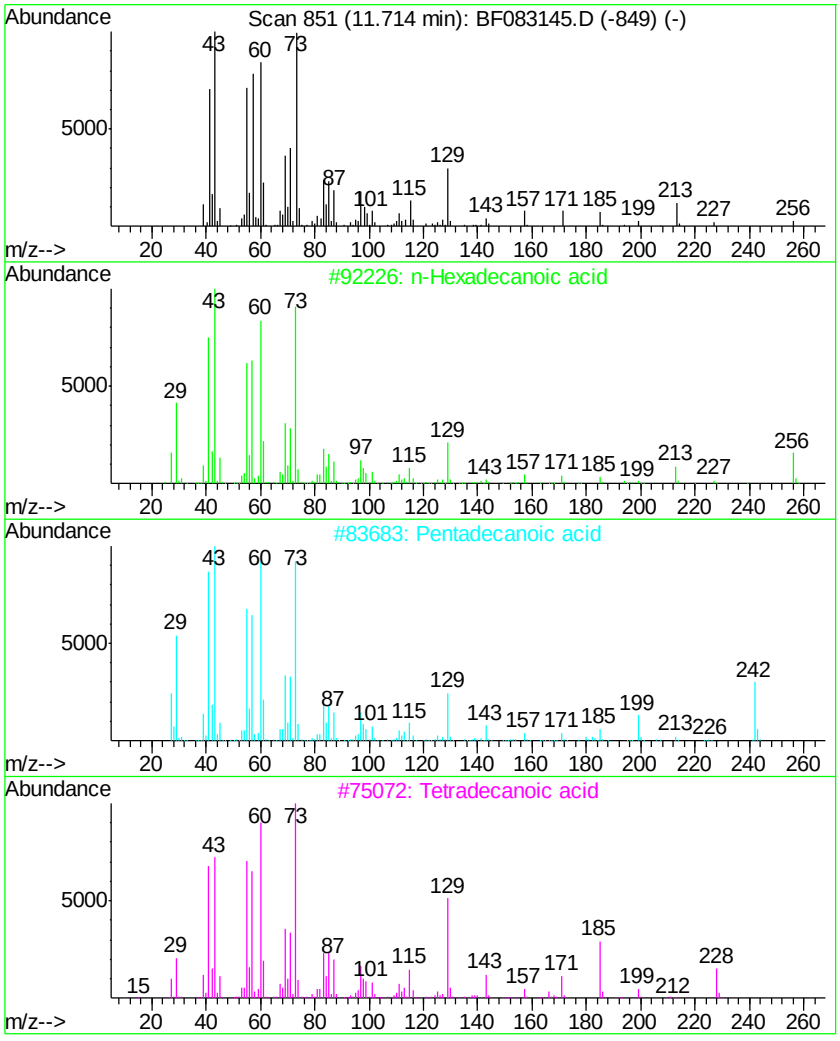
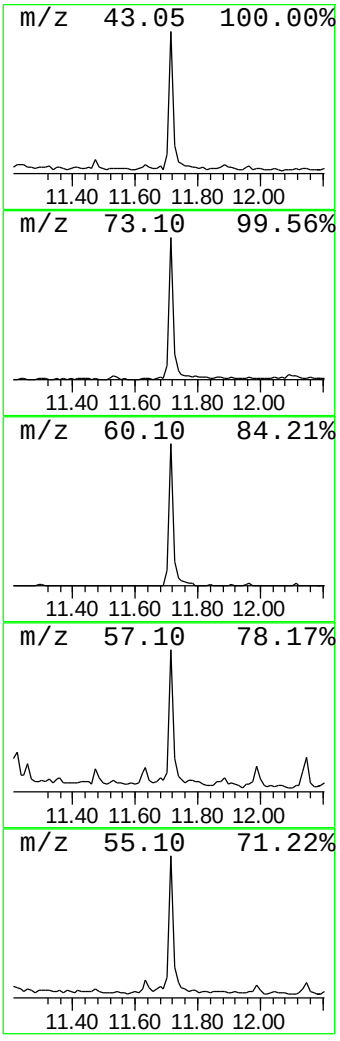
Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	5.18 ng	464861	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Amyl Nitrite	117	C5H11NO2	000110-46-3	38





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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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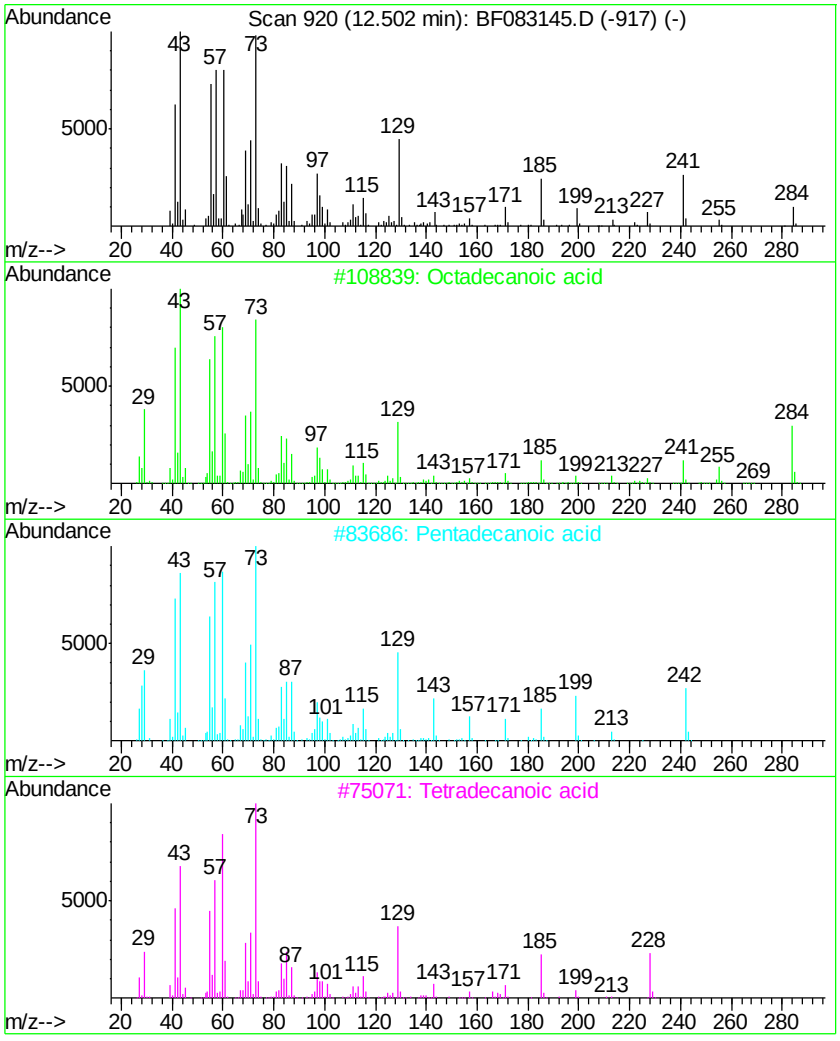
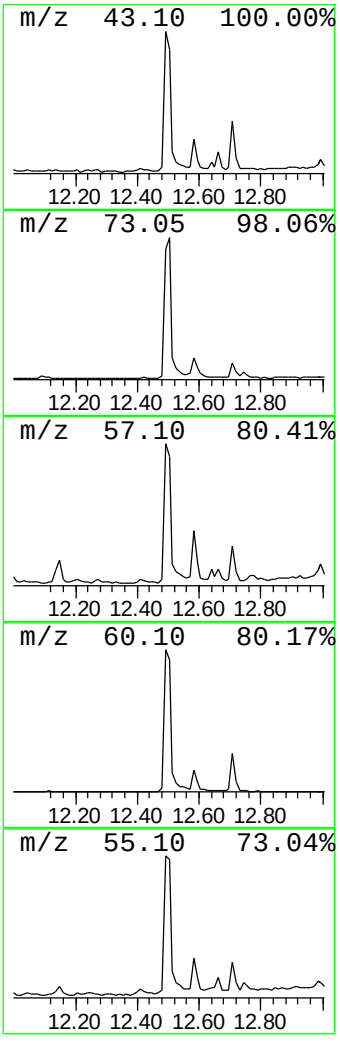
Peak Number 9 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	12.33 ng	1068830	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Eicosane	282	C20H42	000112-95-8	11





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Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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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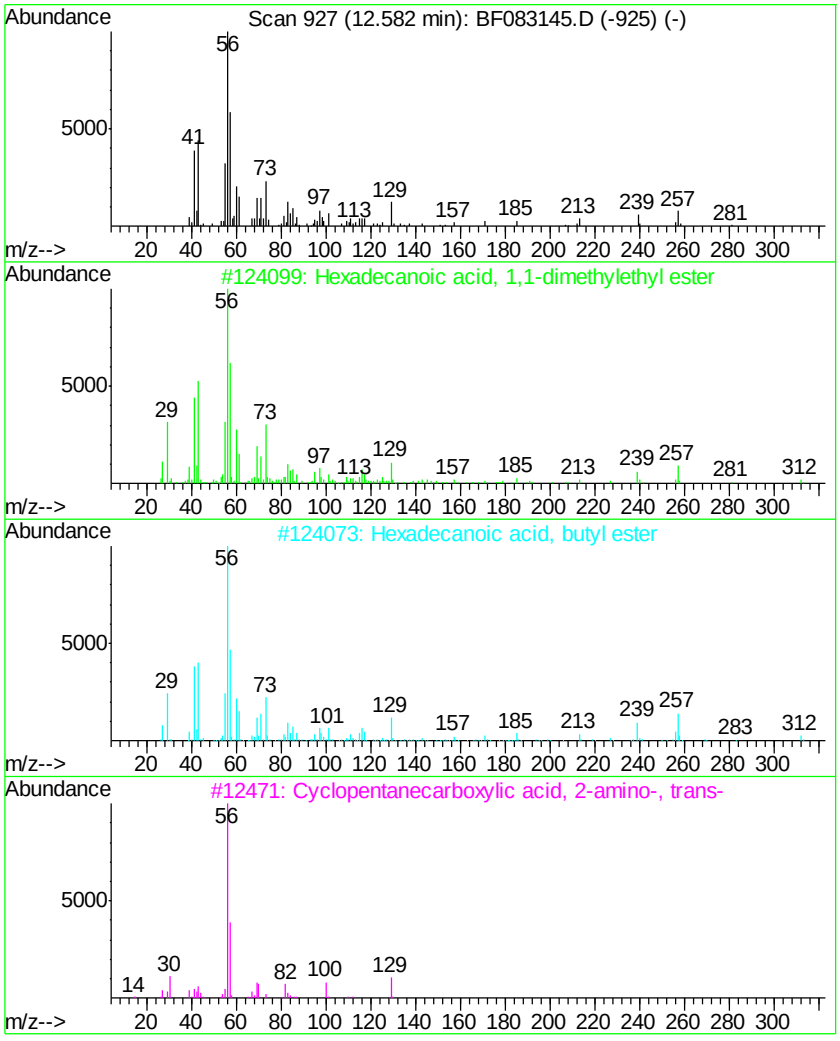
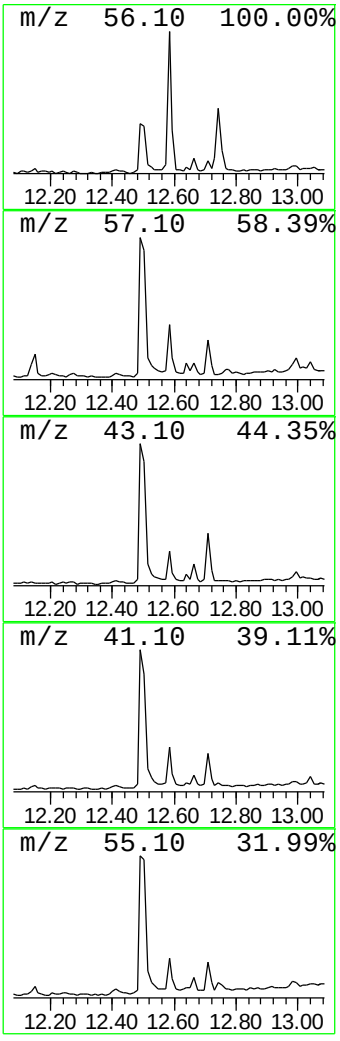
Peak Number 10 Hexadecanoic acid, 1,1-dime... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	2.44 ng	211246	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	47
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	37





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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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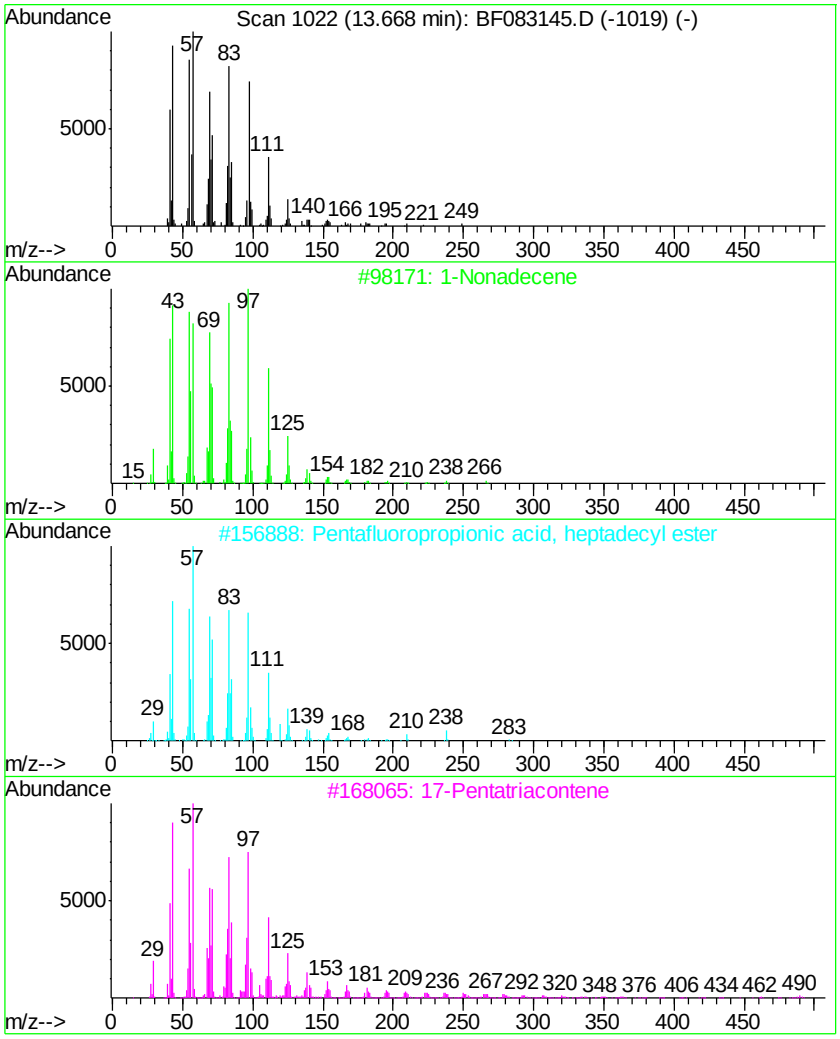
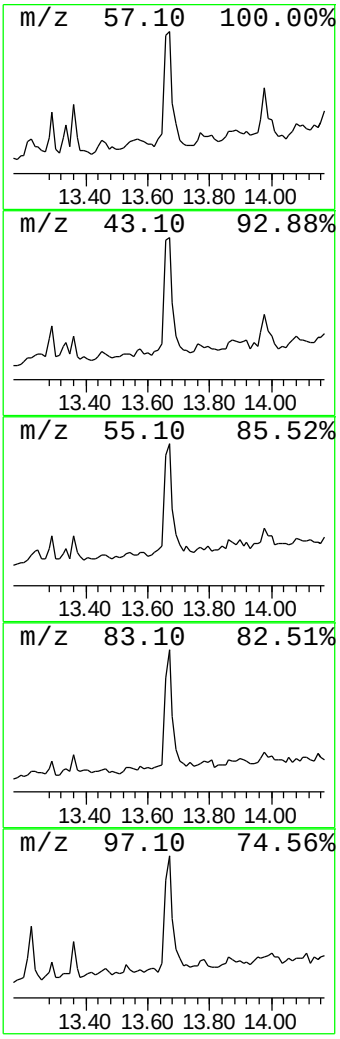
Peak Number 11 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	6.14 ng	532355	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
3	17-Pentatriacontene	491	C35H70	006971-40-0	86
4	1-Nonadecanol	284	C19H40O	001454-84-8	74
5	1-Docosene	308	C22H44	001599-67-3	74





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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

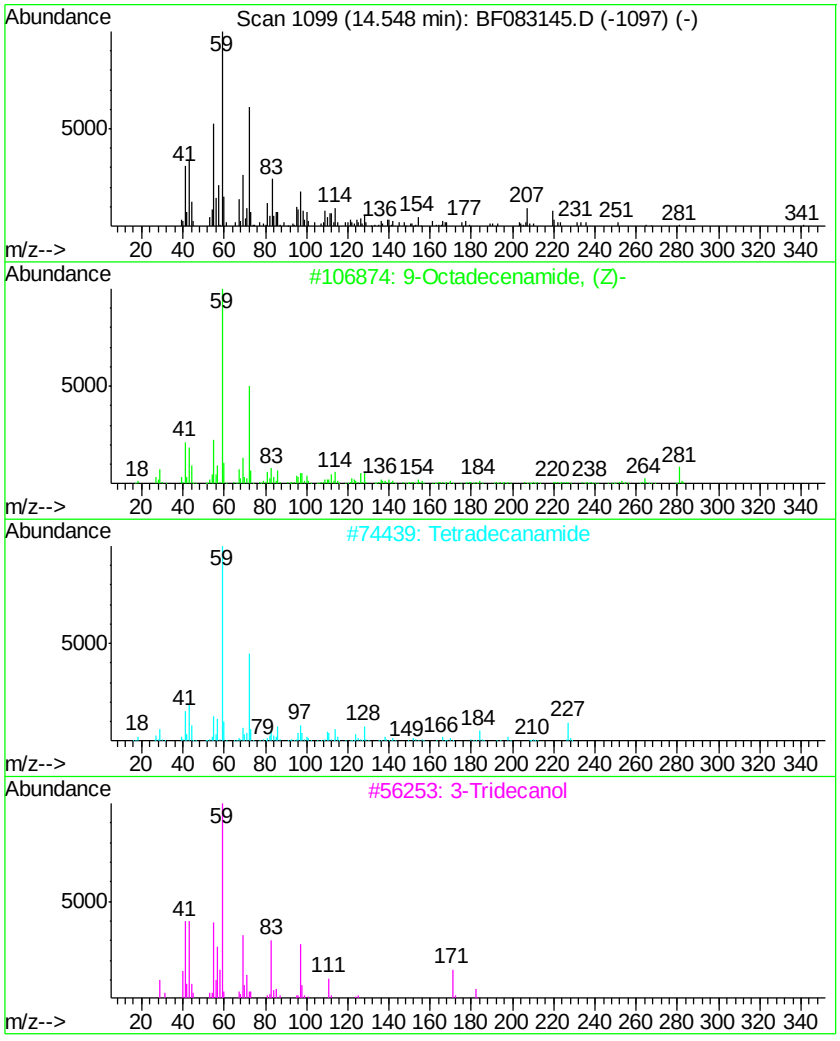
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

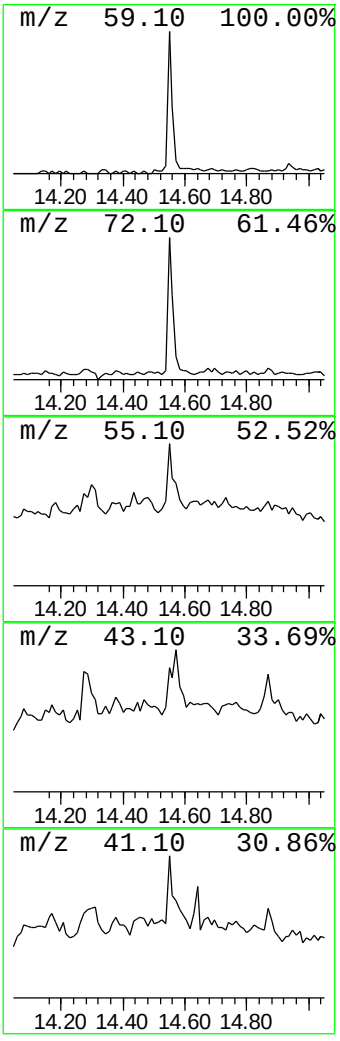
****

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	4.72 ng	324037	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	59
2	Tetradecanamide	227	C14H29NO	000638-58-4	59
3	3-Tridecanol	200	C13H28O	010289-68-6	47
4	Octadecanamide	283	C18H37NO	000124-26-5	47
5	Dodecanamide	199	C12H25NO	001120-16-7	47





Tentatively Identified Compound (LSC) summary

Data Path : V:\HPCHEM1\BNA_F\DATA\BF112115\
Data File : BF083145.D
Acq On : 22 Nov 2015 8:27
Operator : UM/IZ
Sample : G4505-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-22(1-2.2)

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...	4.82	57.9	ng	3578280	1	6.65	1236070	20.0
unknown6.42	6.42	97.6	ng	6033150	1	6.65	1236070	20.0
Tetradecane	9.63	2.3	ng	207903	3	9.69	1796640	20.0
Hexadecane	10.14	3.1	ng	279418	3	9.69	1796640	20.0
Eicosane	10.60	3.6	ng	322133	4	11.16	1793590	20.0
n-Hexadecanoic acid	11.71	5.2	ng	464861	4	11.16	1793590	20.0
Octadecanoic acid	12.50	12.3	ng	1068830	5	13.78	1733100	20.0
Hexadecanoic acid...	12.58	2.4	ng	211246	5	13.78	1733100	20.0
1-Nonadecene	13.67	6.1	ng	532355	5	13.78	1733100	20.0
9-Octadecenamide,...	14.55	4.7	ng	324037	6	15.15	1372380	20.0