LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120115\
Data File : BF083383.D
Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

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-BF113015.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	3.916	192	195	209	rBV	247886	507421	9.32%	1.028%
2	4.476	242	244	248	rBV	41385	84545	1.55%	0.171%
3	4.659	258	260	278	rVB	838845	1675385	30.79%	3.393%
4	5.139	299	302	316	rBV	4126681	4763014	87.53%	9.646%
5	6.224	394	397	399	rBV	4010040	5380685	98.88%	10.896%
6	6.327	403	406	408	rBV	4099200	4946447	90.90%	10.017%
7	6.544	423	425	428	rBV	932458	980872	18.02%	1.986%
8	6.704	437	439	442	rBV	3903518	3459233	63.57%	7.005%
9	7.116	473	475	478	rBV	2240105	3152895	57.94%	6.385%
10	7.276	486	489	495	rVB	120554	192350	3.53%	0.390%
11	7.836	536	538	541	rBV	1442147	1289336	23.69%	2.611%
12	8.922	630	633	635	rBV	4732466	5441810	100.00%	11.020%
13	9.322	666	668	670	rBV	1166638	1012273	18.60%	2.050%
14	9.539	685	687	689	rBV	93129	87776	1.61%	0.178%
15	9.585	689	691	693	rBV	1455627	1405652	25.83%	2.847%
16	10.042	729	731	733	rVB	177604	156128	2.87%	0.316%
17	10.259	747	750	753	rBV	87610	144731	2.66%	0.293%
18	10.373	758	760	763	rVV	2938941	3027536	55.63%	6.131%
19	10.453	766	767	771	rVV	81378	117792	2.16%	0.239%
20	10.522	771	773	777	rVB	171548	259861	4.78%	0.526%
21	11.013	814	816	818	rBV	119306	116530	2.14%	0.236%
22	11.116	823	825	827	rBV	964704	1405342	25.82%	2.846%
23	11.151	827	828	830	rVB	103298	87000	1.60%	0.176%
24	11.436	849	853	858	rBV3	27687	74806	1.37%	0.151%
25	11.528	858	861	864	rVB	52560	74090	1.36%	0.150%
26	11.734	874	879	881	rBV4	34355	71774	1.32%	0.145%
27	11.825	885	887	890	rBV2	271575	378536	6.96%	0.767%
28	12.465	940	943	946	rBV2	54655	69636	1.28%	0.141%
29	12.659	958	960	963	rVB	159512	187989	3.45%	0.381%
30	12.899	979	981	983	rBV	79962	119187	2.19%	0.241%
31	12.968	983	987	989	rVB2	152508	245928	4.52%	0.498%
32	13.219	1006	1009	1012	rBV	3589943	4580923	84.18%	9.277%
33	14.671	1133	1136	1140	rBV2	77652	199620	3.67%	0.404%
34	14.740	1140	1142	1145	rVV	656521	1115408	20.50%	2.259%

LSC Area Percent Report

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Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

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-BF113015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.785	1145	1146	1150	rVB	60422	73553	1.35%	0.149%
36	14.865	1150	1153	1155	rBV	54094	69503	1.28%	0.141%
37	15.677	1221	1224	1233	rVB3	26975	72622	1.33%	0.147%
38	16.305	1276	1279	1280	rBV	50486	76325	1.40%	0.155%
39	16.340	1280	1282	1287	rVB	111140	163980	3.01%	0.332%
40	16.614	1302	1306	1307	rBV	51082	87446	1.61%	0.177%
41	16.671	1307	1311	1315	rVB3	41348	120606	2.22%	0.244%
42	16.808	1320	1323	1330	rVB	526103	852389	15.66%	1.726%
43	17.254	1357	1362	1365	rVB	69668	102505	1.88%	0.208%
44	17.494	1380	1383	1385	rBV	85415	152210	2.80%	0.308%
45	17.940	1418	1422	1428	rBV8	15771	60411	1.11%	0.122%
46	18.180	1439	1443	1450	rBV3	128278	299077	5.50%	0.606%
47	18.443	1462	1466	1469	rBV2	38730	80834	1.49%	0.164%
48	18.511	1469	1472	1475	rBV4	36031	88785	1.63%	0.180%
49	18.580	1475	1478	1484	rVB2	37901	107125	1.97%	0.217%
50	18.751	1488	1493	1499	rBV8	21409	86580	1.59%	0.175%
51	19.369	1543	1547	1552	rVB4	33927	73900	1.36%	0.150%

Sum of corrected areas: 49380362

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Instrument : BNA_F
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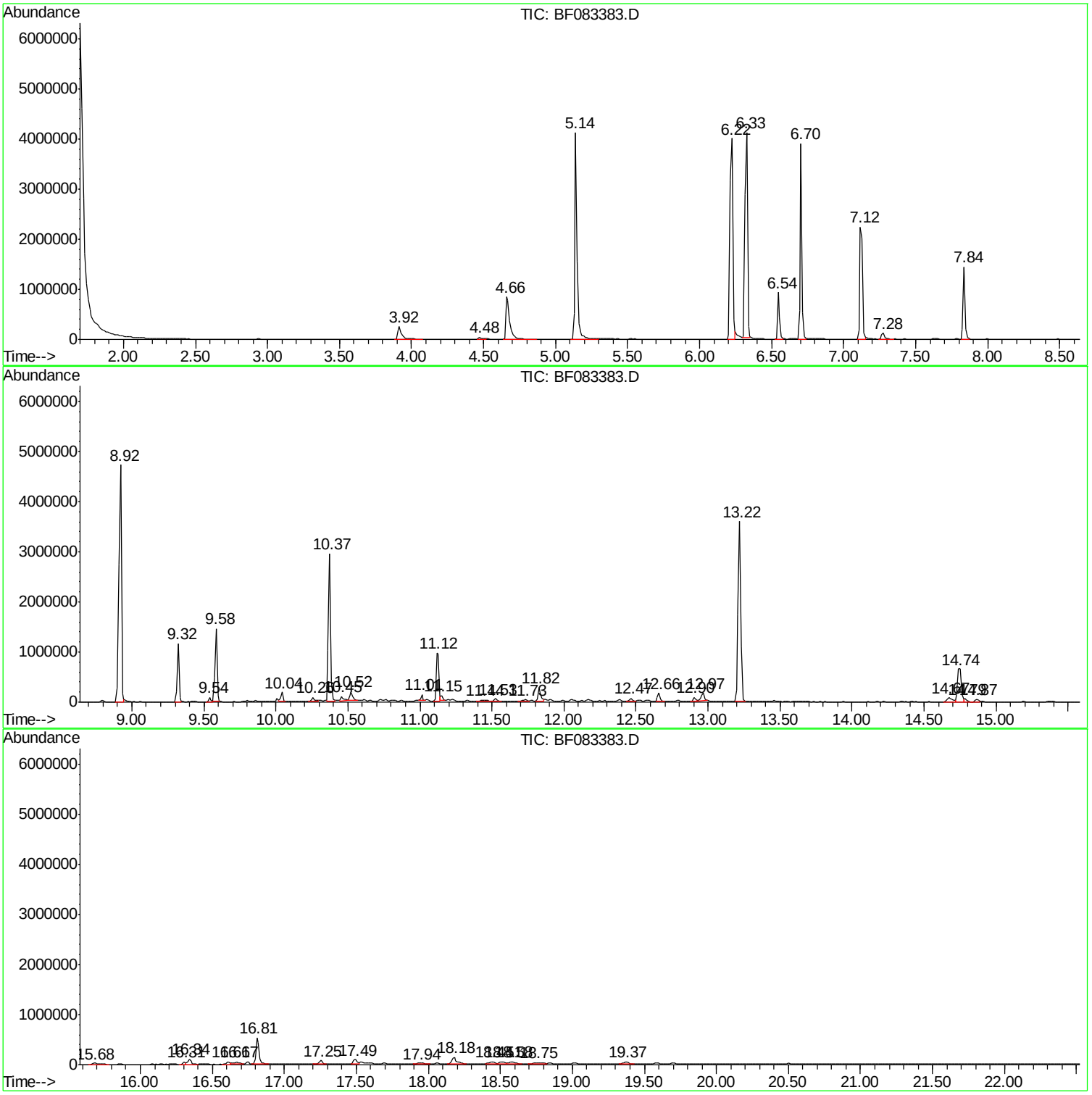
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

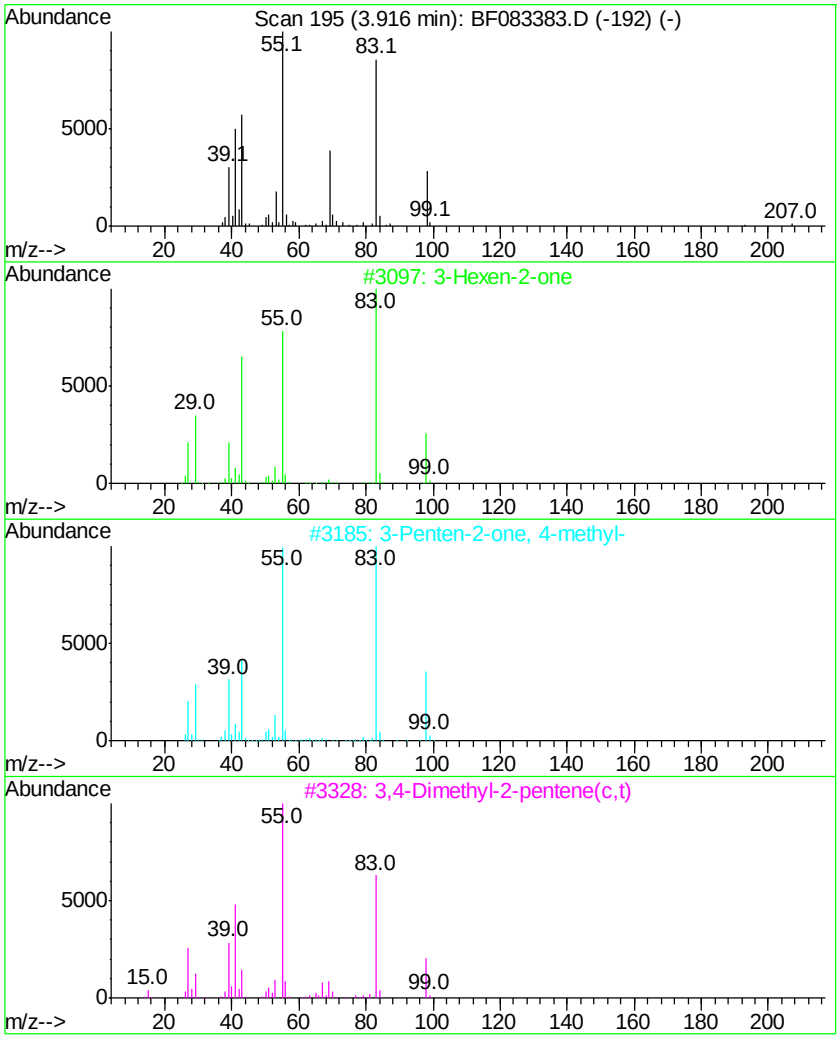
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

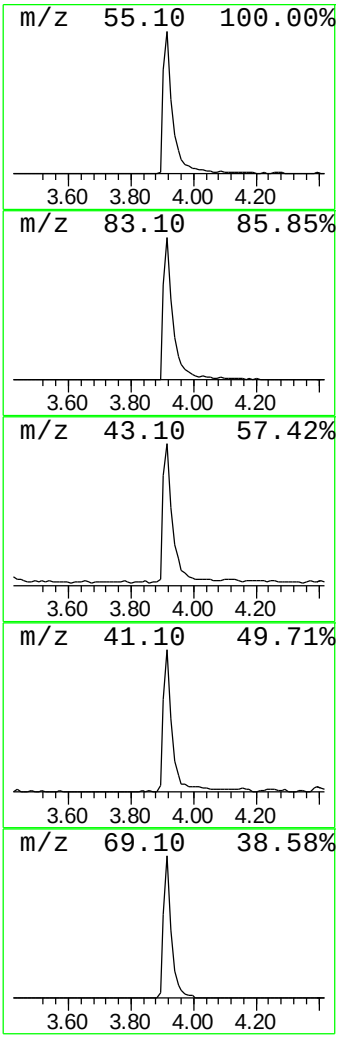
****

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	10.35 ng	507421	1,4-Dichlorobenzene-d4	6.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	87
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
3	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120115\
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Sample : G4593-03
Misc :
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Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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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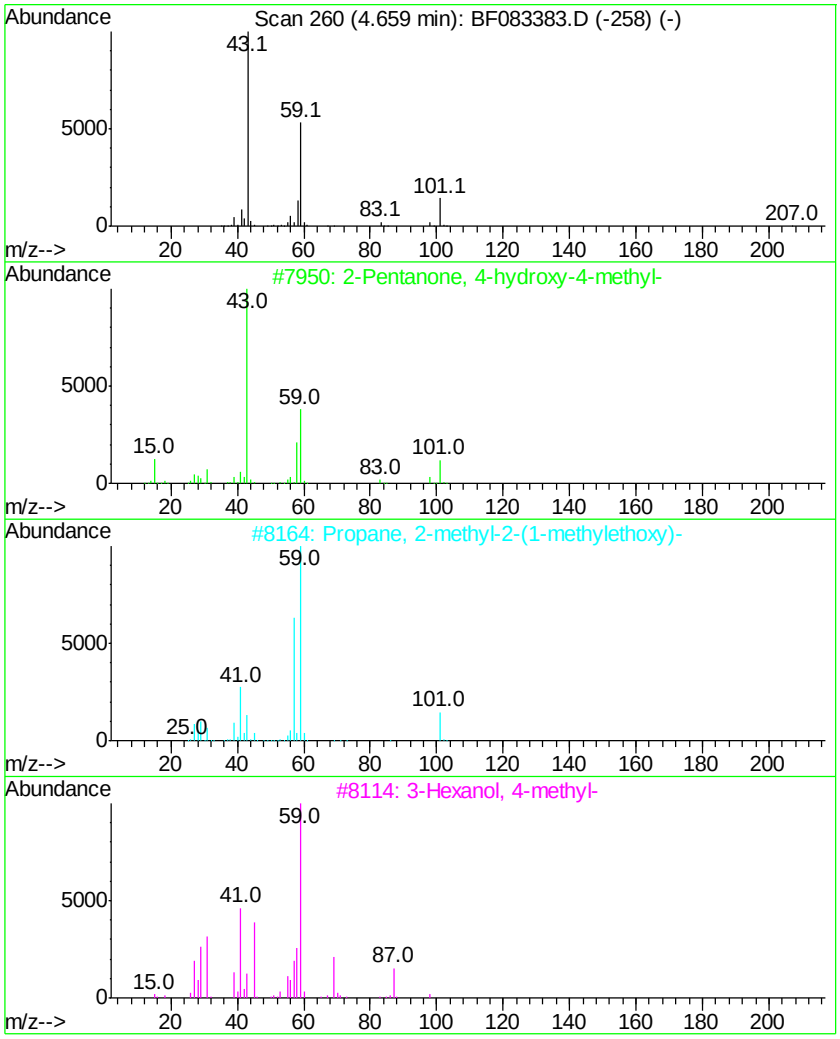
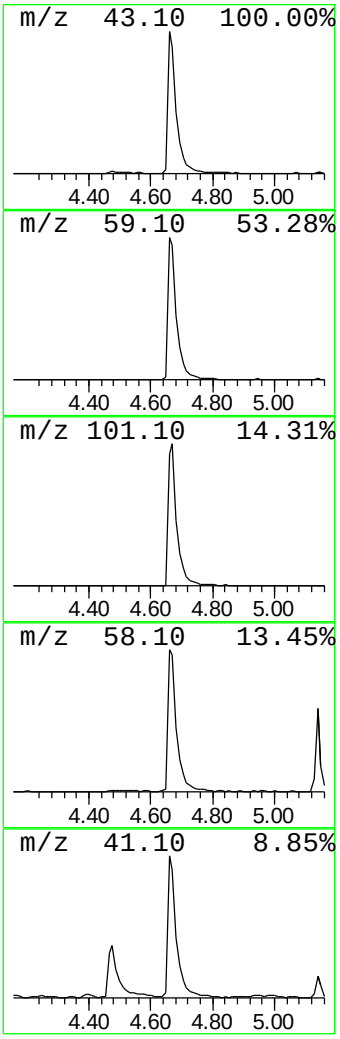
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	34.16 ng	1675390	1,4-Dichlorobenzene-d4	6.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120115\
Data File : BF083383.D
Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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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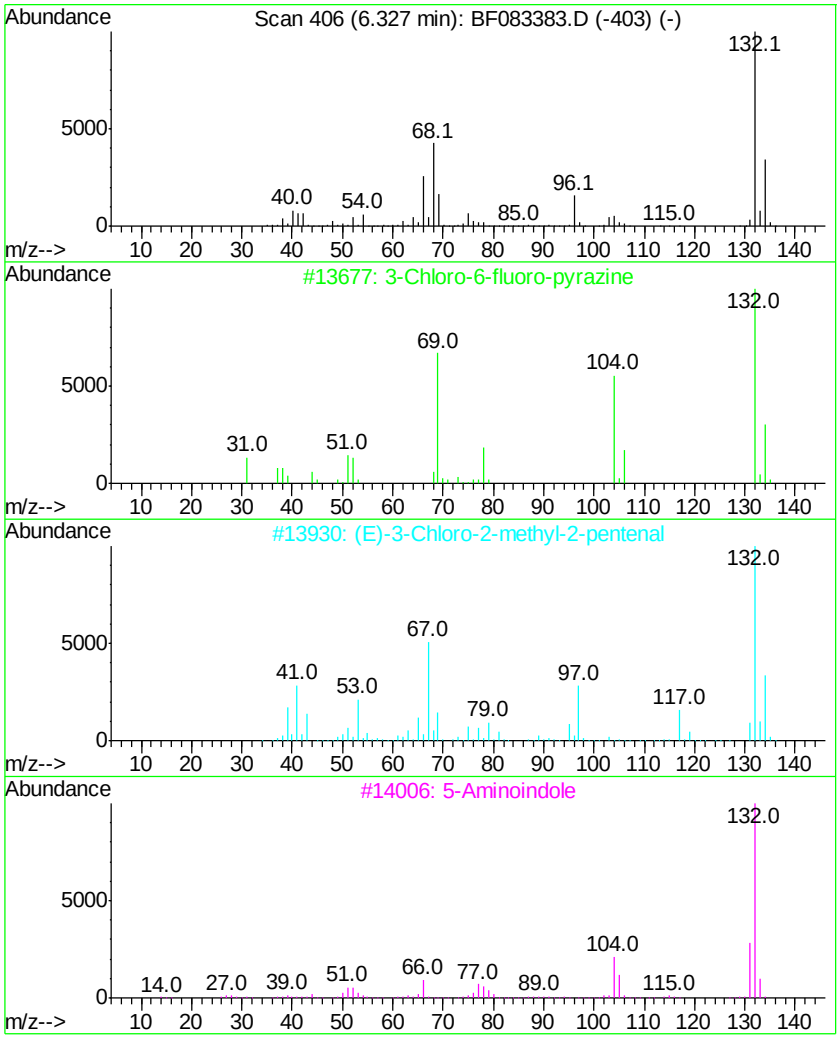
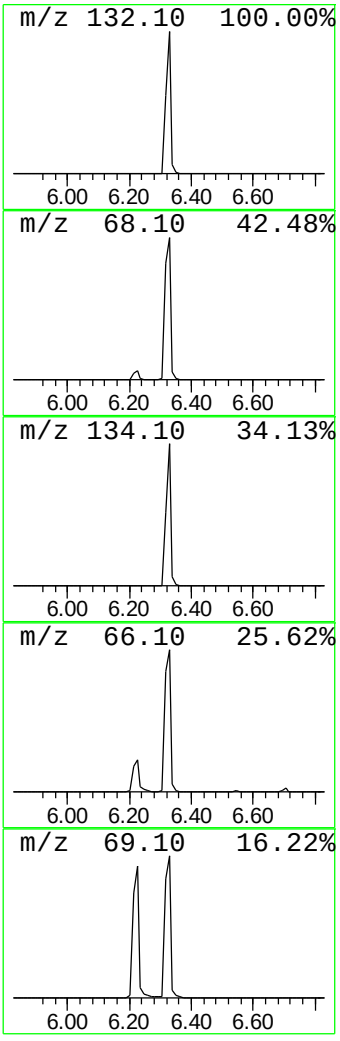
Peak Number 3 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	100.86 ng	4946450	1,4-Dichlorobenzene-d4	6.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Sample : G4593-03
Misc :
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Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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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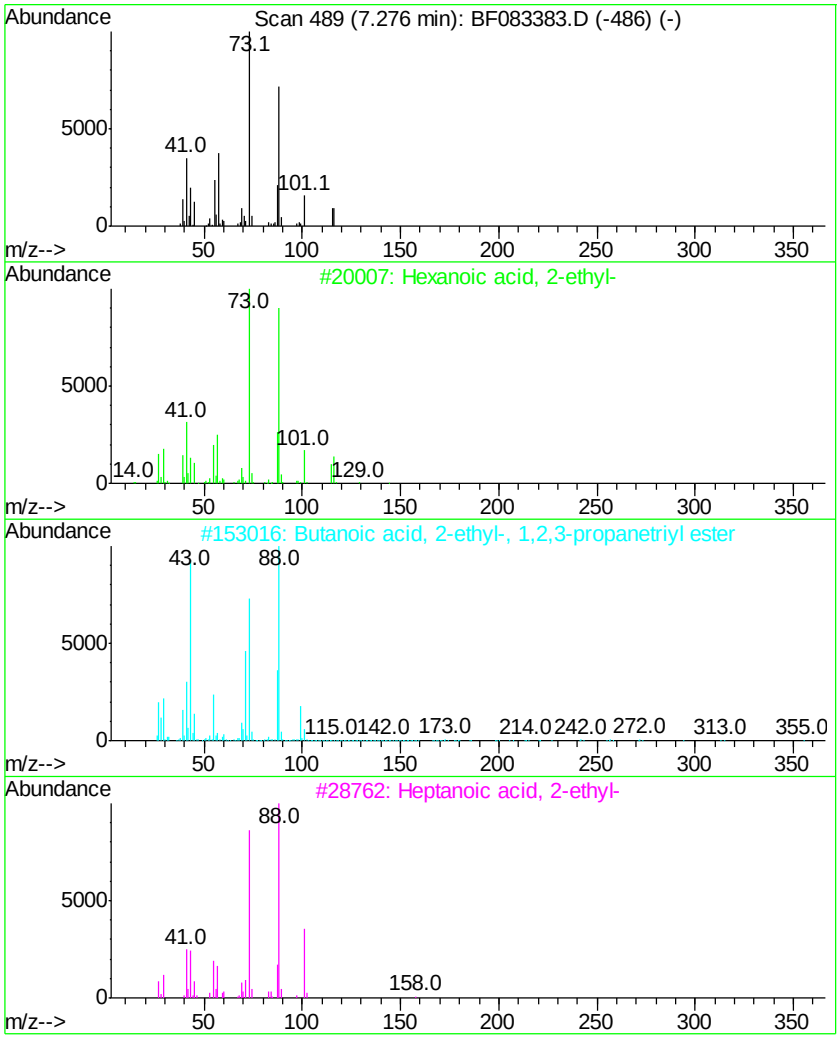
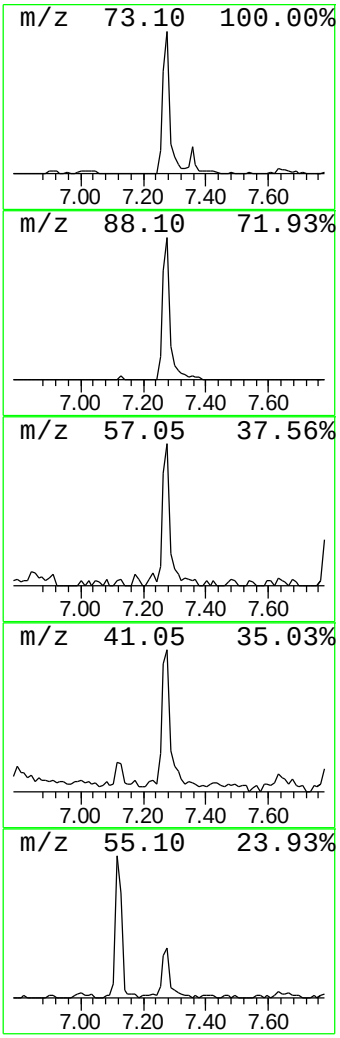
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	2.98 ng	192350	Naphthalene-d8	7.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	38
4	1,4-Dioxane	88	C4H8O2	000123-91-1	35
5	Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	33





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120115\
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Operator : UM/IZ
Sample : G4593-03
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Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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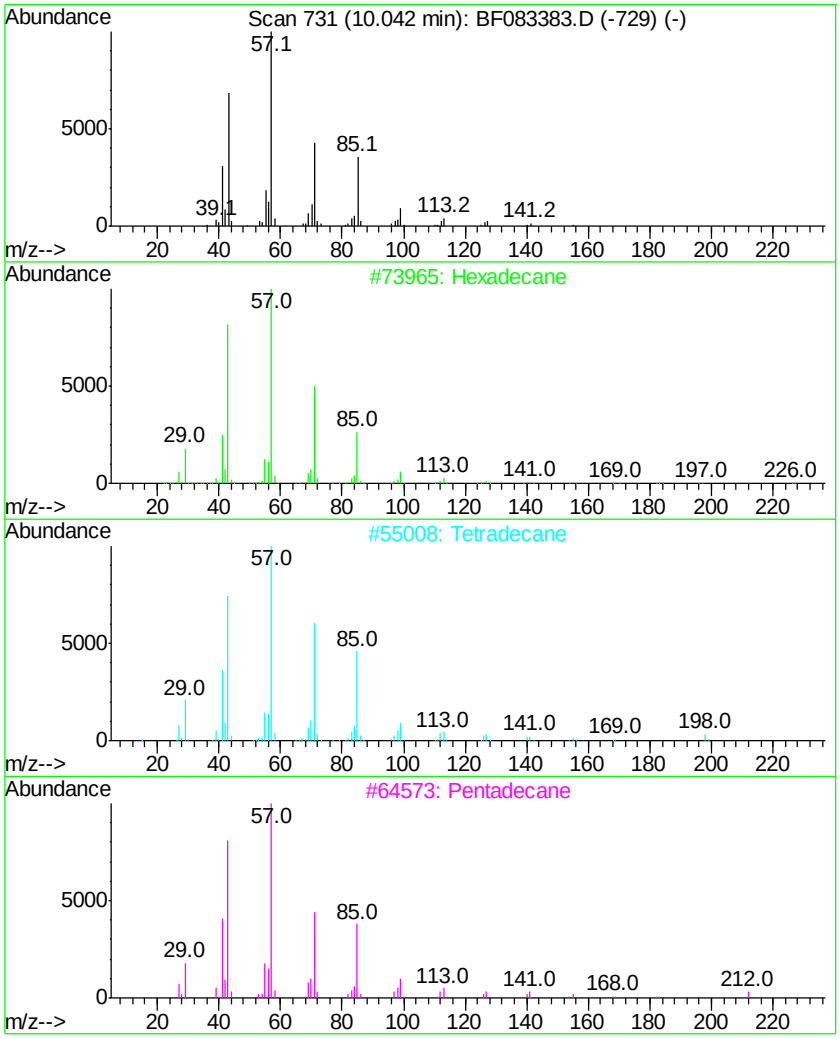
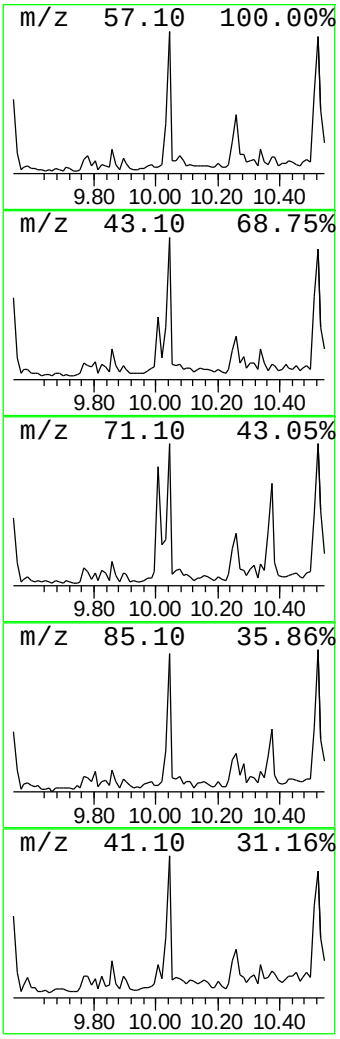
Peak Number 6 Hexadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.04	2.22 ng	156128	Acenaphthene-d10	9.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Tetracosane	338	C24H50	000646-31-1	78





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Misc :
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Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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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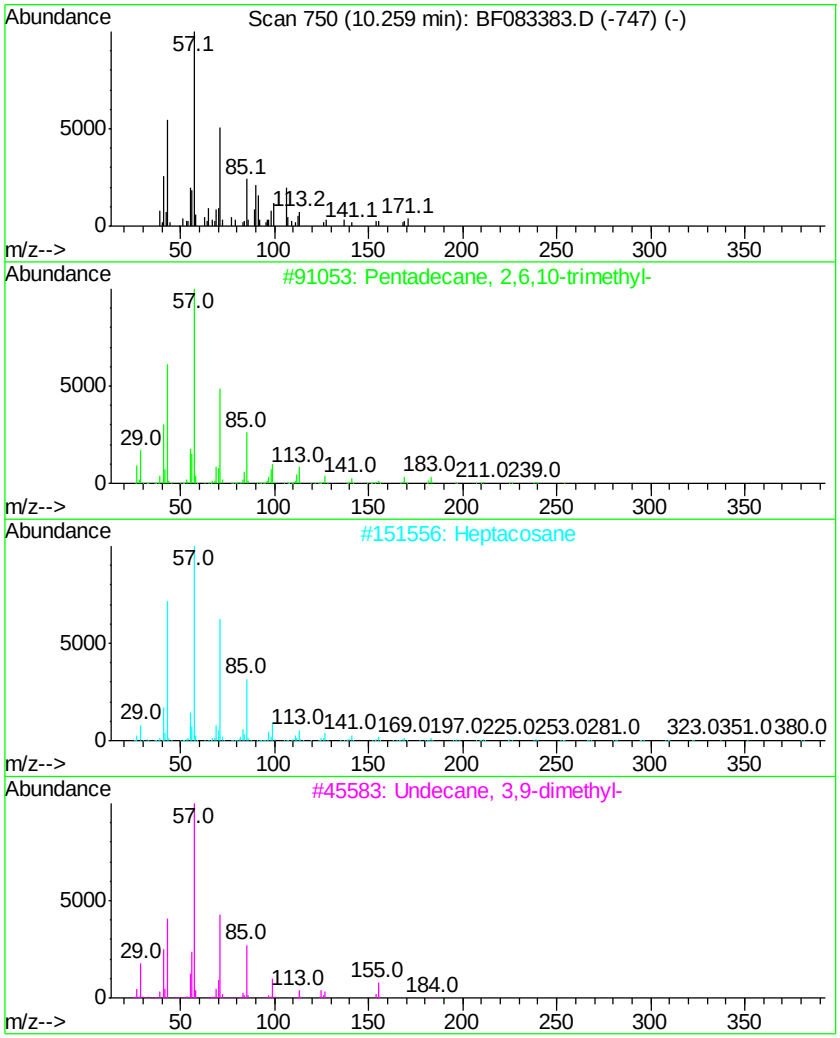
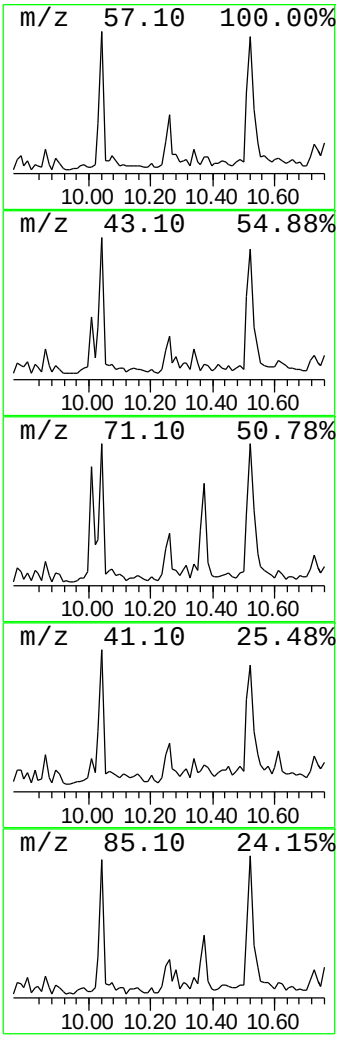
Peak Number 7 Pentadecane, 2,6,10-trimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	2.06 ng	144731	Acenaphthene-d10	9.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	53
2	Heptacosane	380	C27H56	000593-49-7	52
3	Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	50
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	43
5	Pentadecane	212	C15H32	000629-62-9	43





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : S12-15

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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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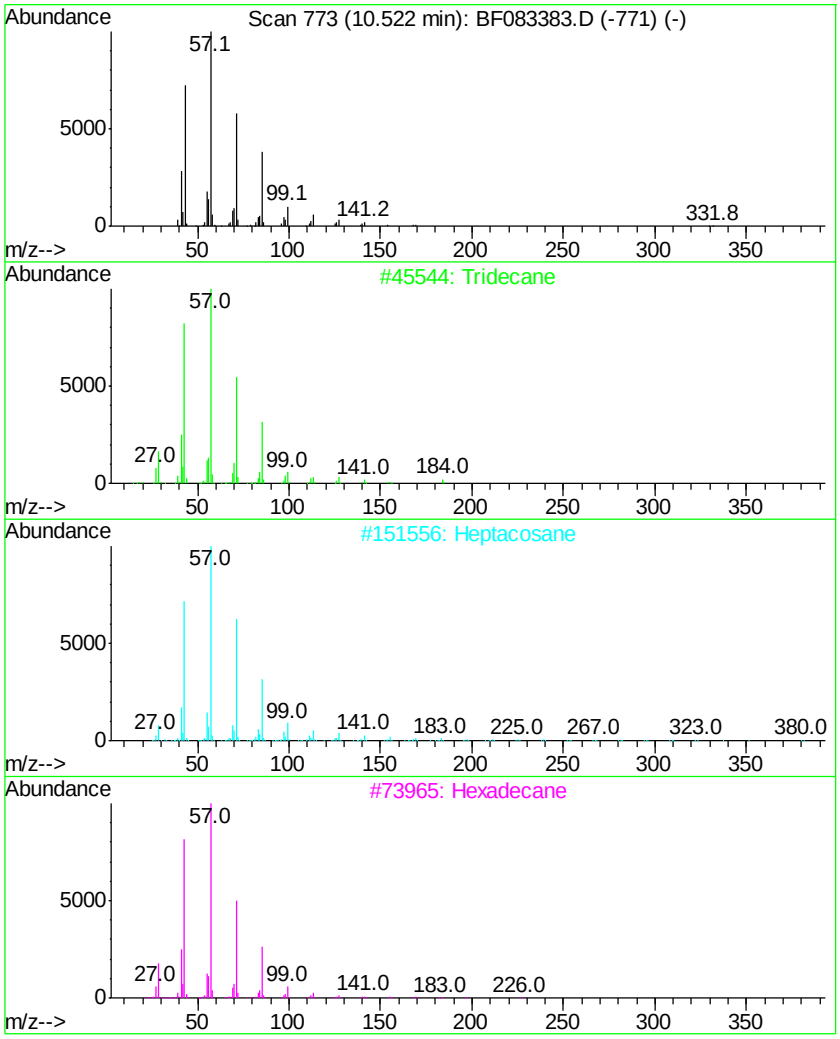
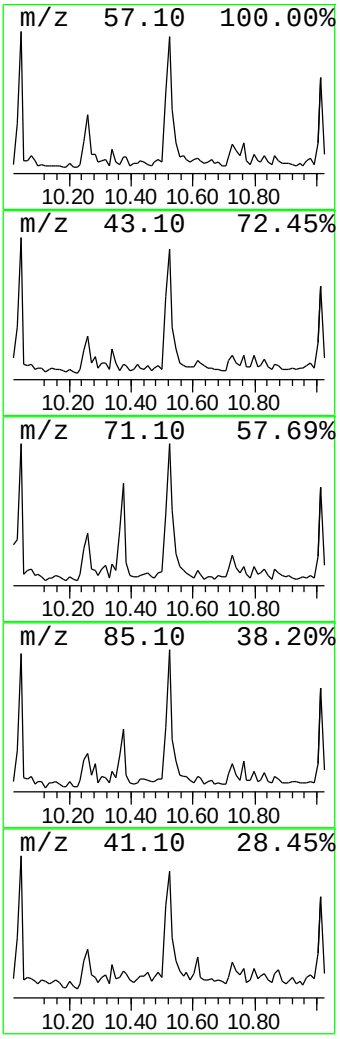
Peak Number 8 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	3.70 ng	259861	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Pentadecane	212	C15H32	000629-62-9	86
5	Octadecane	254	C18H38	000593-45-3	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120115\
Data File : BF083383.D
Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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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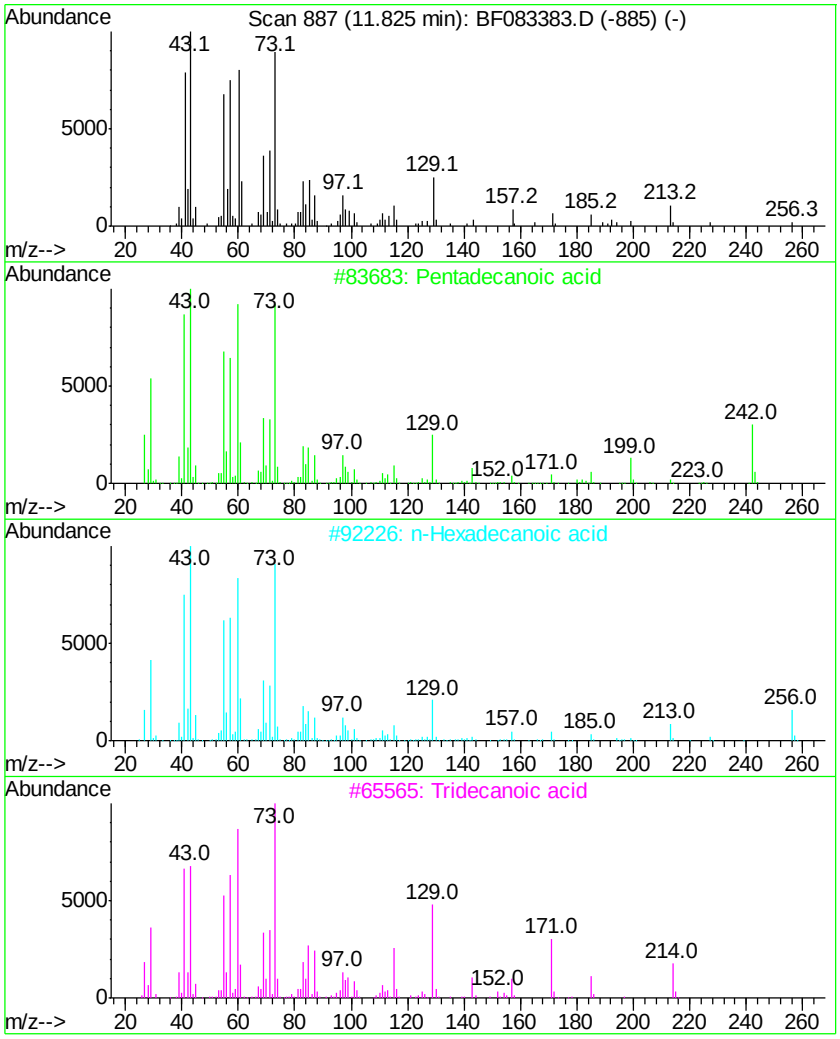
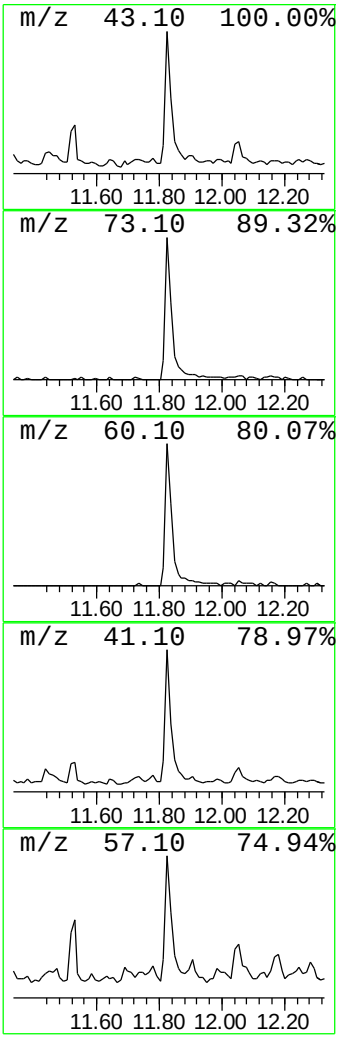
Peak Number 9 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	5.39 ng	378536	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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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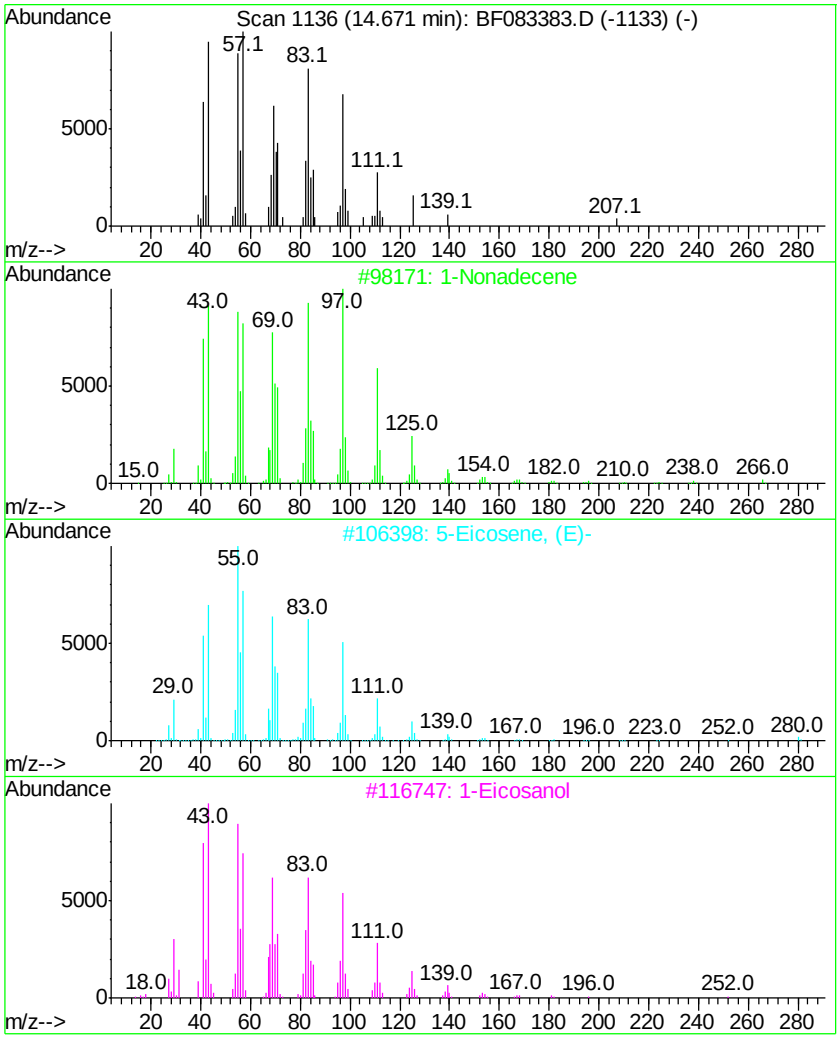
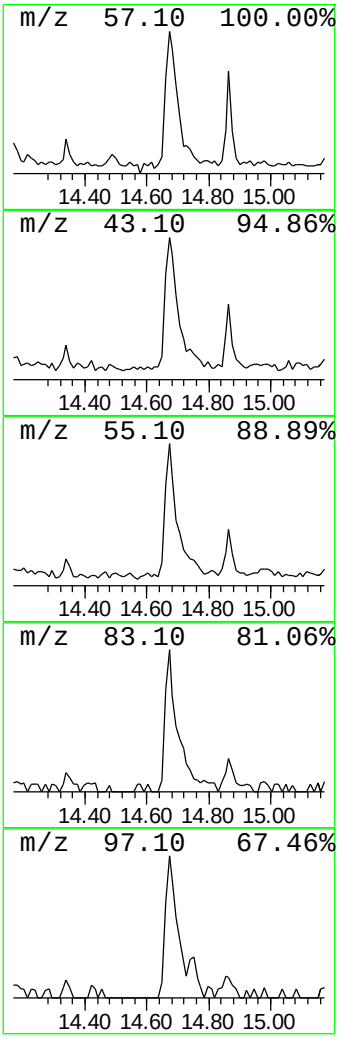
Peak Number 10 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	3.58 ng	199620	Chrysene-d12	14.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	1-Eicosanol	298	C20H42O	000629-96-9	90
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	87
5	1-Tetracosanol	354	C24H50O	000506-51-4	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120115\
Data File : BF083383.D
Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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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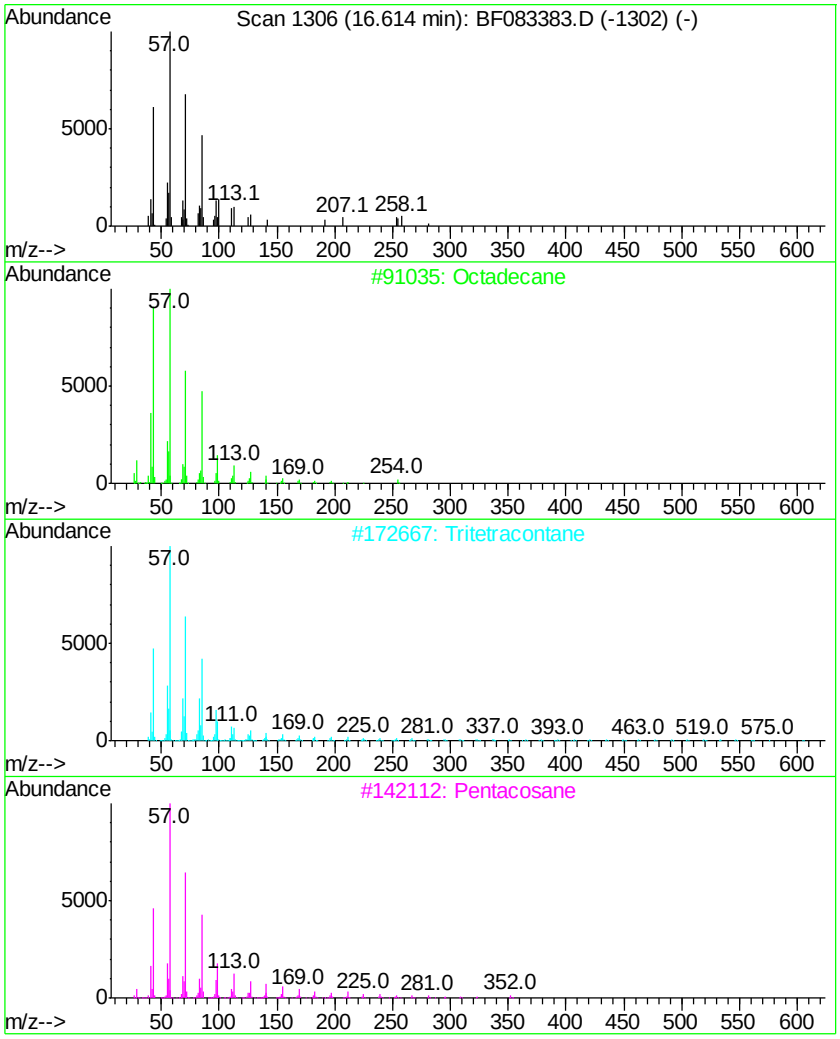
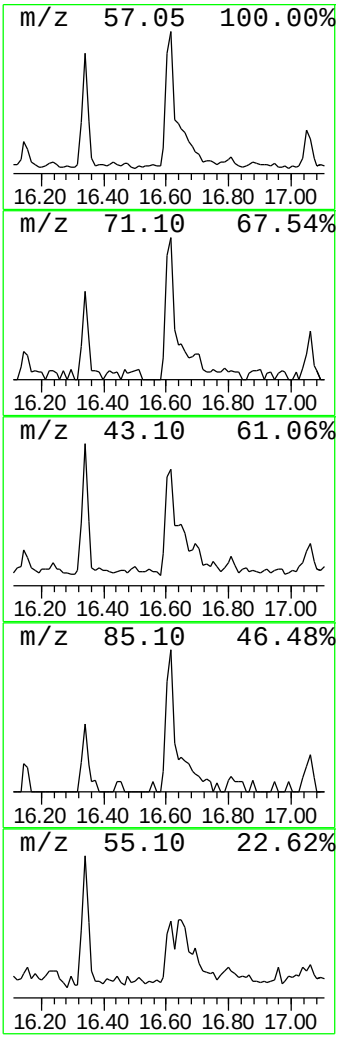
Peak Number 12 Octadecane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	2.05 ng	87446	Perylene-d12	16.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Tritetracontane	605	C43H88	007098-21-7	86
3	Pentacosane	352	C25H52	000629-99-2	86
4	Octacosane	394	C28H58	000630-02-4	83
5	Heneicosane	296	C21H44	000629-94-7	83





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Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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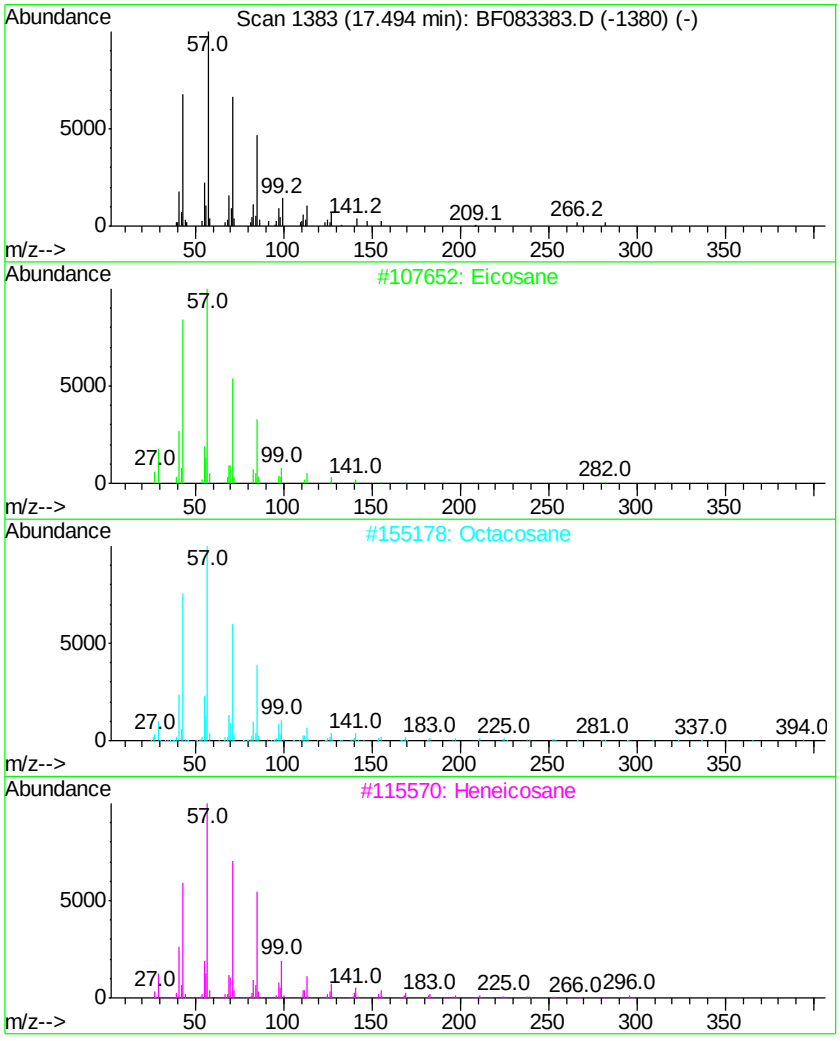
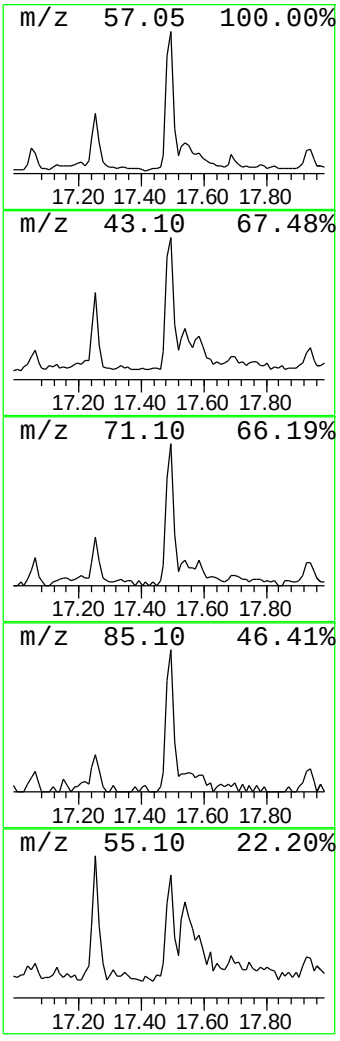
Peak Number 15 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.49	3.57 ng	152210	Perylene-d12	16.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
5	Tetracosane	338	C24H50	000646-31-1	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120115\
Data File : BF083383.D
Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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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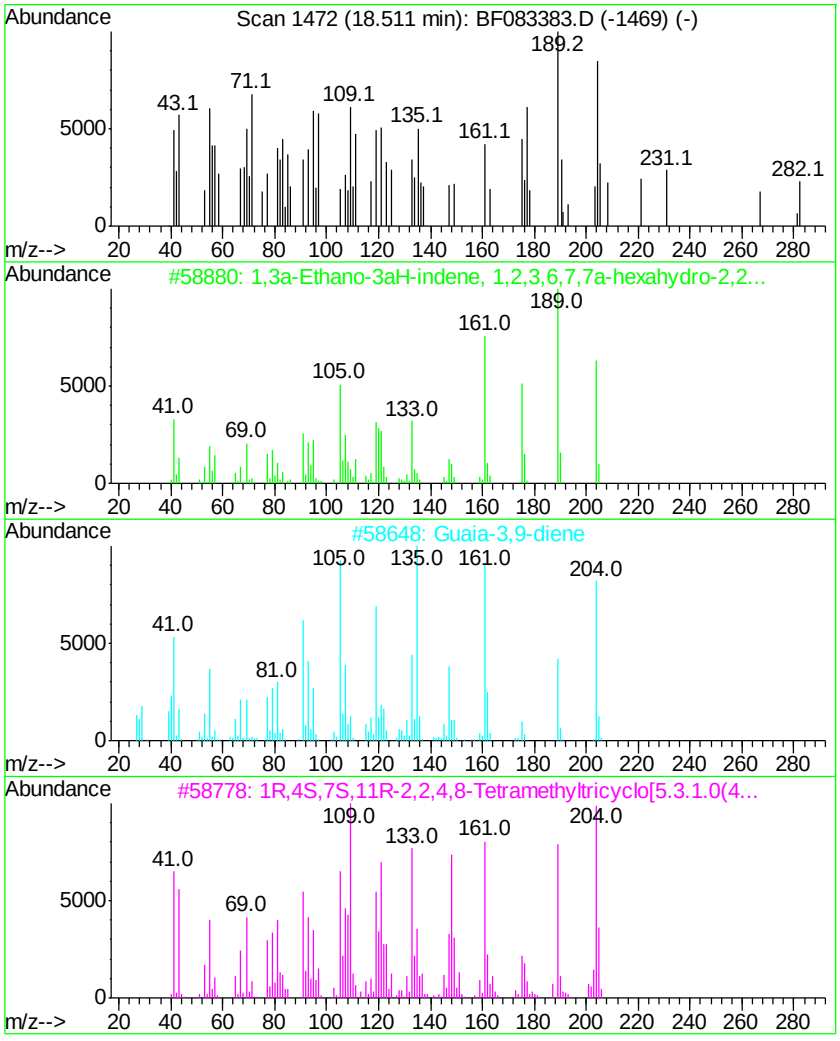
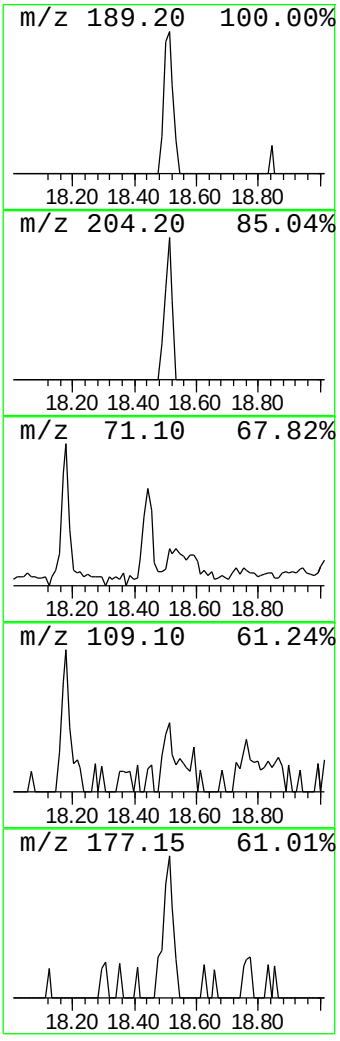
Peak Number 17 1,3a-Ethano-3aH-indene, 1,2... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.51	2.08 ng	88785	Perylene-d12	16.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	53
2	Guaia-3,9-diene	204	C15H24	000489-83-8	43
3	1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1000140-07-6	38
4	6-Chloro-2-acetonaphthone	204	C12H9ClO	042036-59-9	35
5	1-Naphthalenol, decahydro-1,4a-d...	222	C15H26O	000473-04-1	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120115\
Data File : BF083383.D
Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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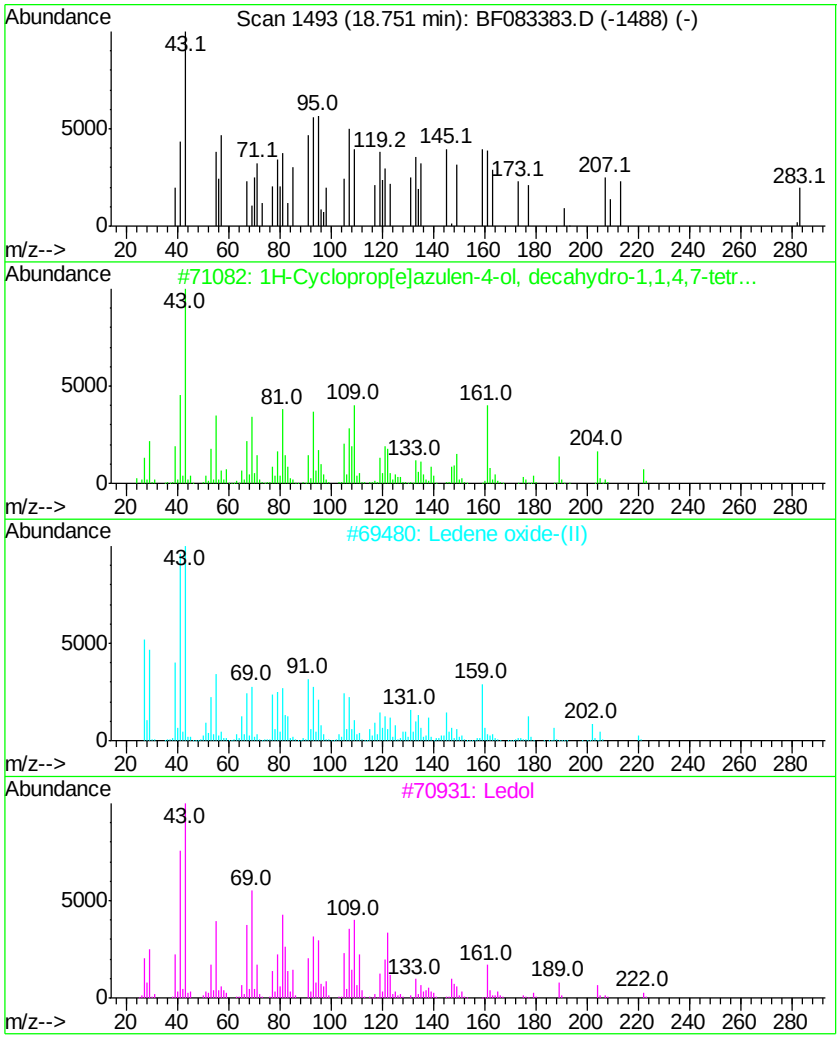
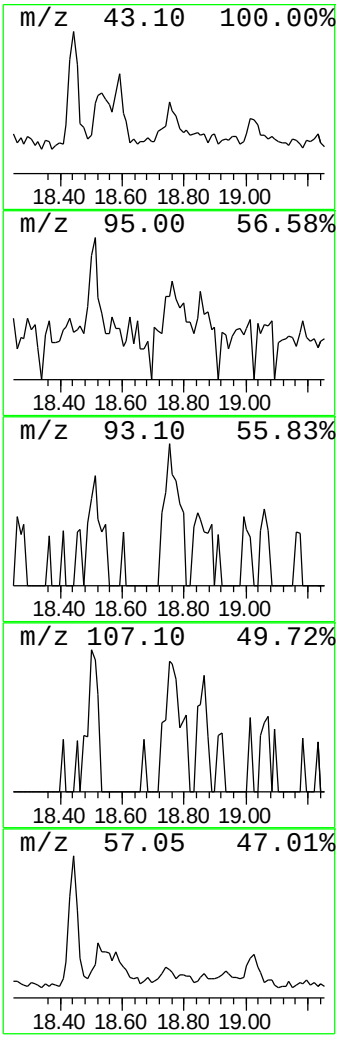
Peak Number 19 unknown18.75 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.75	2.03 ng	86580	Perylene-d12	16.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	22
2	Ledene oxide-(II)	220	C15H24O	1000159-36-7	16
3	Ledol	222	C15H26O	000577-27-5	10
4	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	000079-77-6	10
5	9,12,15-Octadecatrienoic acid, 2...	436	C25H40O6	055320-01-9	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120115\
Data File : BF083383.D
Acq On : 1 Dec 2015 20:27
Operator : UM/IZ
Sample : G4593-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S12-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113015.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-Hexen-2-one	3.92	10.4	ng	507421	1	6.54	980872	20.0
2-Pentanone, 4-hy...	4.66	34.2	ng	1675390	1	6.54	980872	20.0
unknown6.33	6.33	100.9	ng	4946450	1	6.54	980872	20.0
Hexanoic acid, 2-...	7.28	3.0	ng	192350	2	7.84	1289340	20.0
Hexadecane	10.04	2.2	ng	156128	3	9.58	1405650	20.0
Pentadecane, 2,6,...	10.26	2.1	ng	144731	3	9.58	1405650	20.0
Tridecane	10.52	3.7	ng	259861	4	11.13	1405340	20.0
Pentadecanoic acid	11.83	5.4	ng	378536	4	11.13	1405340	20.0
1-Nonadecene	14.67	3.6	ng	199620	5	14.75	1115410	20.0
Octadecane	16.61	2.0	ng	87446	6	16.81	852389	20.0
Eicosane	17.49	3.6	ng	152210	6	16.81	852389	20.0
1,3a-Ethano-3aH-i...	18.51	2.1	ng	88785	6	16.81	852389	20.0
unknown18.75	18.75	2.0	ng	86580	6	16.81	852389	20.0