LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

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-BF073015.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	2.132	3	4	8	rVB	19727	28888	1.01%	0.105%
2	2.224	8	12	16	rBV2	10854	33092	1.15%	0.120%
3	4.396	200	202	206	rBV	104591	128153	4.46%	0.465%
4	5.047	256	259	261	rBV	1994417	2539966	88.39%	9.216%
5	5.459	292	295	297	rBV	2686384	2873452	100.00%	10.426%
6	5.859	328	330	333	rVB	91665	94342	3.28%	0.342%
7	6.476	382	384	387	rBV	1930185	2513855	87.49%	9.121%
8	6.624	394	397	399	rBV	1964987	2601479	90.53%	9.439%
9	6.853	415	417	419	rBV	910405	752543	26.19%	2.730%
10	7.013	428	431	433	rBV	1812566	2015133	70.13%	7.312%
11	7.413	463	466	468	rBV	1885950	1709600	59.50%	6.203%
12	7.493	471	473	476	rVV	25244	32933	1.15%	0.119%
13	7.836	500	503	504	rBV	39969	49143	1.71%	0.178%
14	8.133	527	529	532	rBV	962216	829186	28.86%	3.009%
15	9.207	621	623	626	rBV	2280225	2405186	83.70%	8.727%
16	9.608	655	658	660	rBV	613334	563607	19.61%	2.045%
17	9.882	680	682	684	rVB	570612	693447	24.13%	2.516%
18	10.328	719	721	723	rVB	31311	33321	1.16%	0.121%
19	10.670	748	751	753	rBV	1103159	1029371	35.82%	3.735%
20	10.796	760	762	767	rBV	53450	68023	2.37%	0.247%
21	11.242	799	801	802	rBV	49892	42873	1.49%	0.156%
22	11.368	810	812	814	rBV	588218	517206	18.00%	1.877%
23	11.665	836	838	841	rBV	44728	42127	1.47%	0.153%
24	11.893	856	858	861	rBV	181264	209467	7.29%	0.760%
25	12.076	871	874	876	rBV	30565	29371	1.02%	0.107%
26	12.568	915	917	919	rBV3	25888	42635	1.48%	0.155%
27	12.682	925	927	930	rBV	32519	36183	1.26%	0.131%
28	12.796	933	937	939	rBV	23433	35010	1.22%	0.127%
29	12.945	948	950	953	rBV	1766381	1888446	65.72%	6.852%
30	13.322	979	983	985	rBV5	14525	34192	1.19%	0.124%
31	13.528	998	1001	1004	rVB4	21604	39744	1.38%	0.144%
32	13.711	1015	1017	1019	rBV	51647	52548	1.83%	0.191%
33	13.859	1027	1030	1031	rBV3	33686	46095	1.60%	0.167%
34	13.997	1039	1042	1044	rBV	1046071	1150865	40.05%	4.176%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

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-BF073015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.111	1049	1052	1053	rBV3	44156	77366	2.69%	0.281%
36	14.328	1069	1071	1073	rBV2	34656	72936	2.54%	0.265%
37	14.374	1073	1075	1081	rVV2	81271	156626	5.45%	0.568%
38	14.477	1081	1084	1086	rVV	84511	105010	3.65%	0.381%
39	14.751	1105	1108	1114	rBV4	77548	250589	8.72%	0.909%
40	14.842	1114	1116	1118	rVV	85322	98141	3.42%	0.356%
41	14.911	1121	1122	1124	rBV2	28364	29352	1.02%	0.106%
42	15.094	1135	1138	1141	rBV	180860	219357	7.63%	0.796%
43	15.414	1163	1166	1169	rVB	684417	812444	28.27%	2.948%
44	15.642	1184	1186	1190	rVB3	43178	73715	2.57%	0.267%
45	15.871	1203	1206	1209	rBV	84346	124737	4.34%	0.453%
46	18.328	1418	1421	1426	rVB6	29957	72751	2.53%	0.264%
47	18.454	1430	1432	1435	rBV4	18818	39036	1.36%	0.142%
48	19.151	1486	1493	1501	rBV10	55882	235123	8.18%	0.853%
49	19.540	1525	1527	1530	rBV4	13945	32046	1.12%	0.116%

Sum of corrected areas: 27560711

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Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
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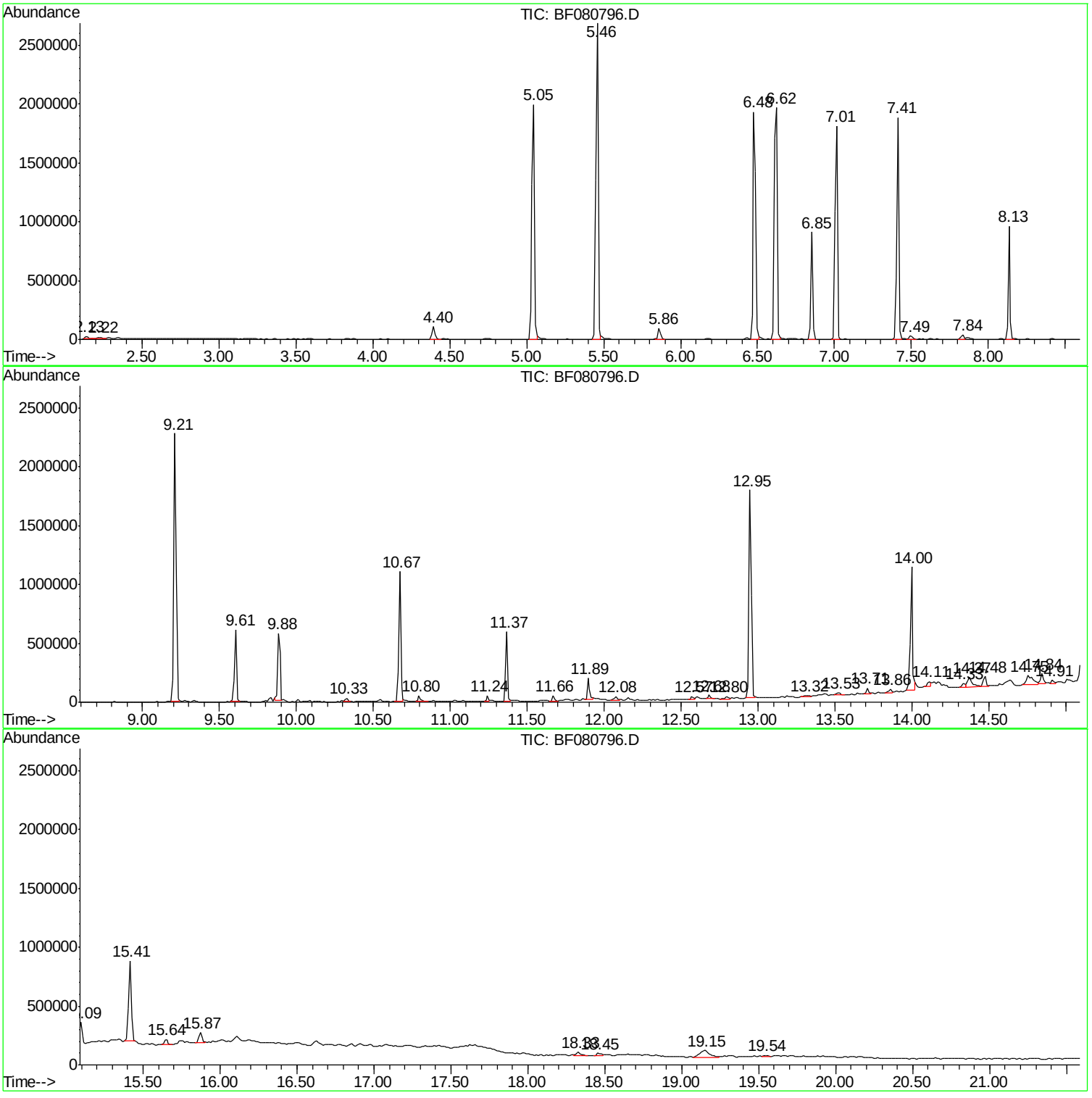
ALS Vial : 82 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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Data File : BF080796.D
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Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

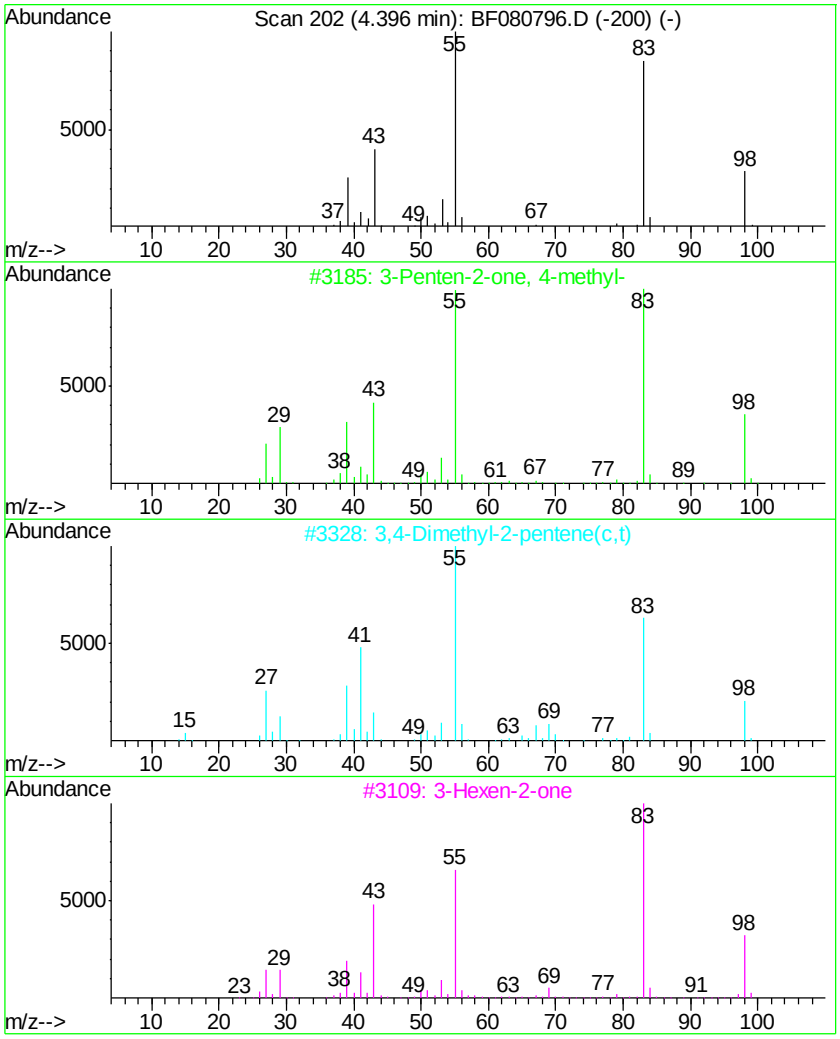
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

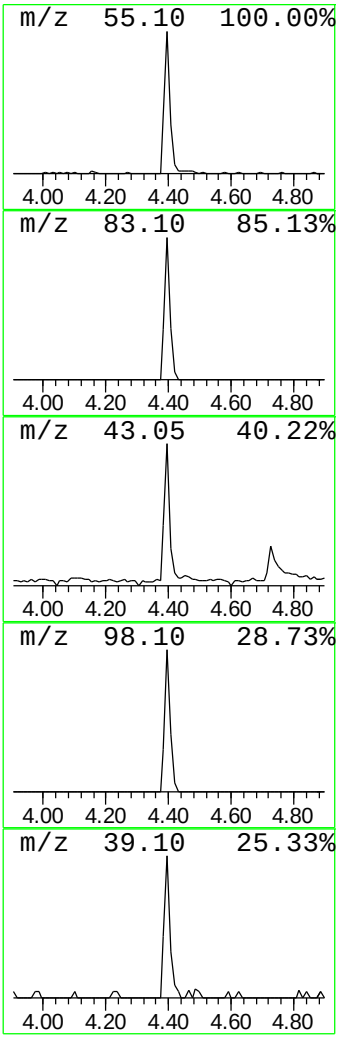
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	3.41 ng	128153	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3	3-Hexen-2-one	98	C6H10O	000763-93-9	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

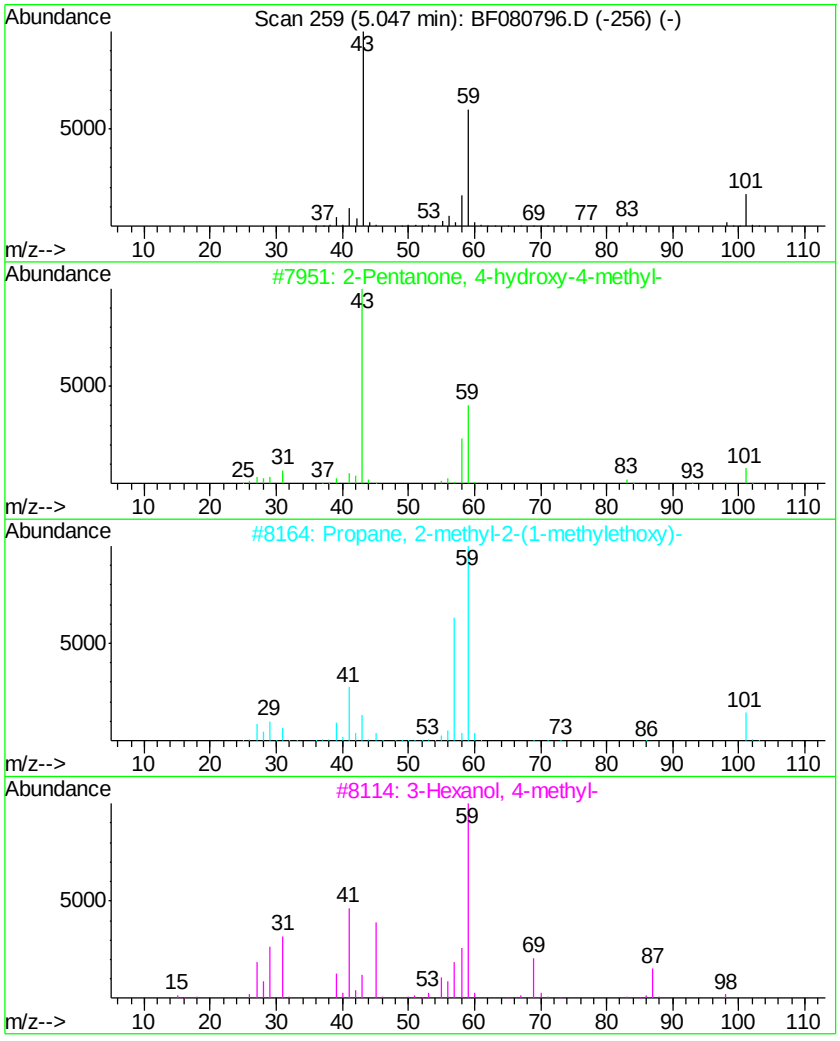
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

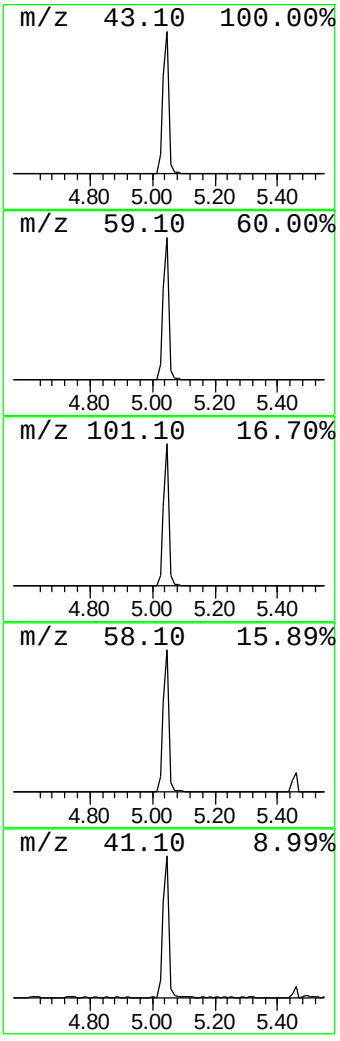
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	67.50 ng	2539970	1,4-Dichlorobenzene-d4	6.85

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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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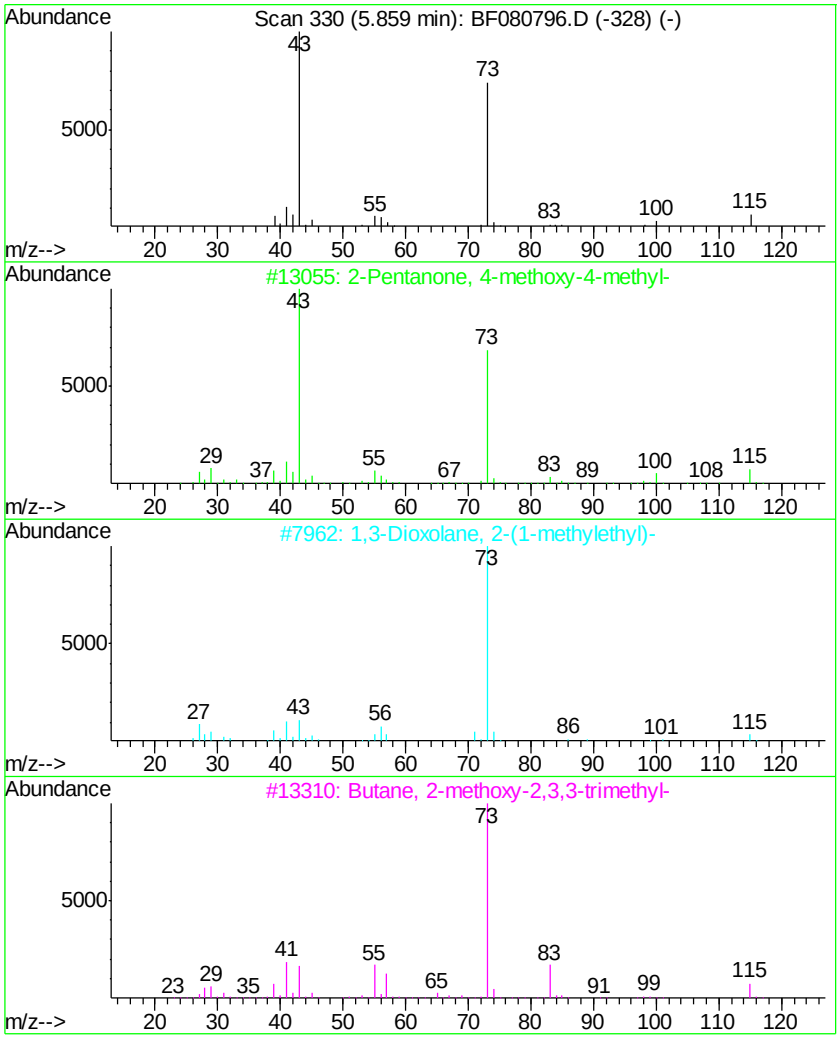
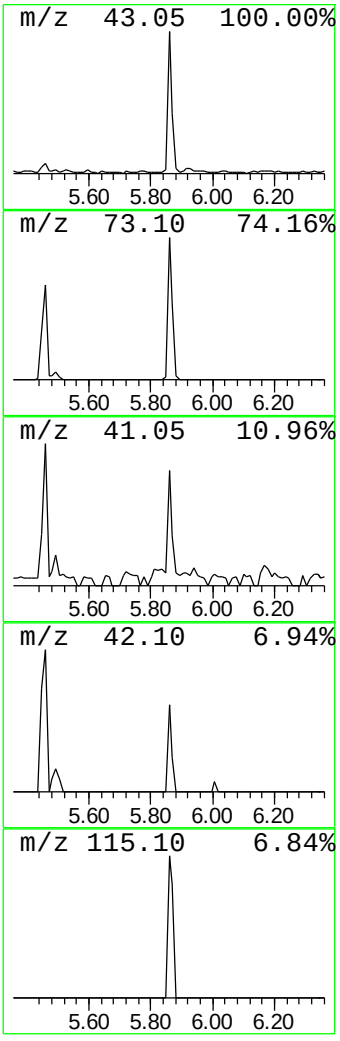
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	2.51 ng	94342	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	17
3	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	17
4	Pentane, 2-methoxy-2,4,4-trimethyl-	144	C9H20O	062108-41-2	12
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
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Sample : G3125-13
Misc :
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Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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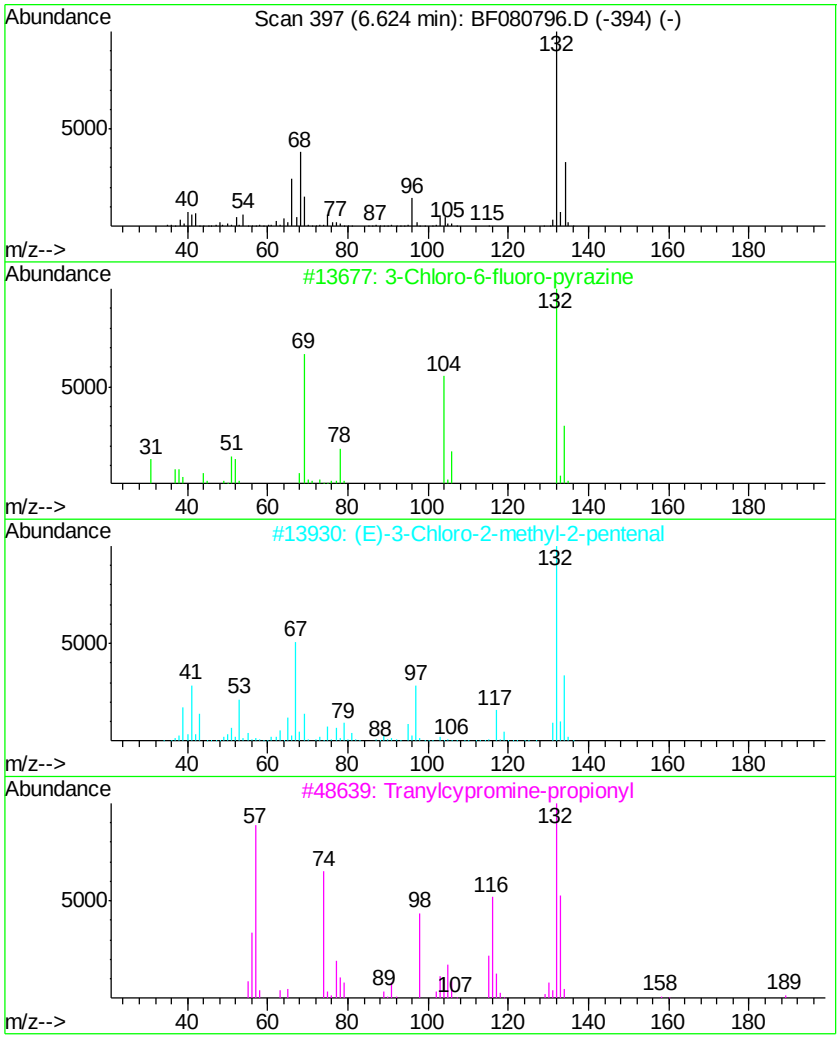
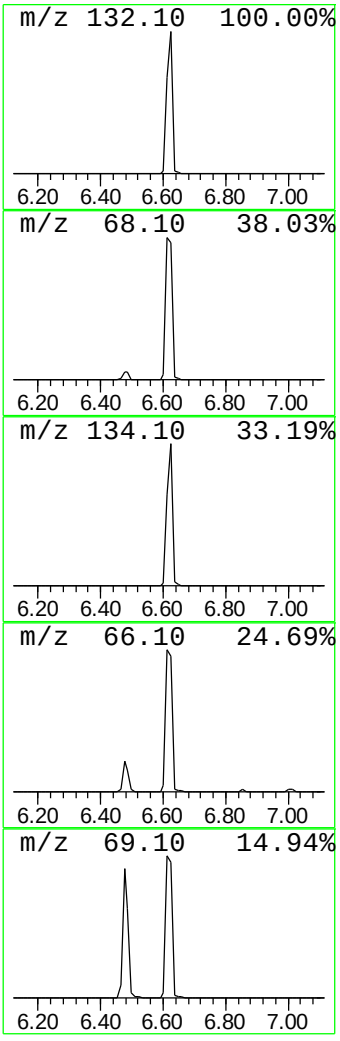
Peak Number 4 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	69.14 ng	2601480	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Misc :
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Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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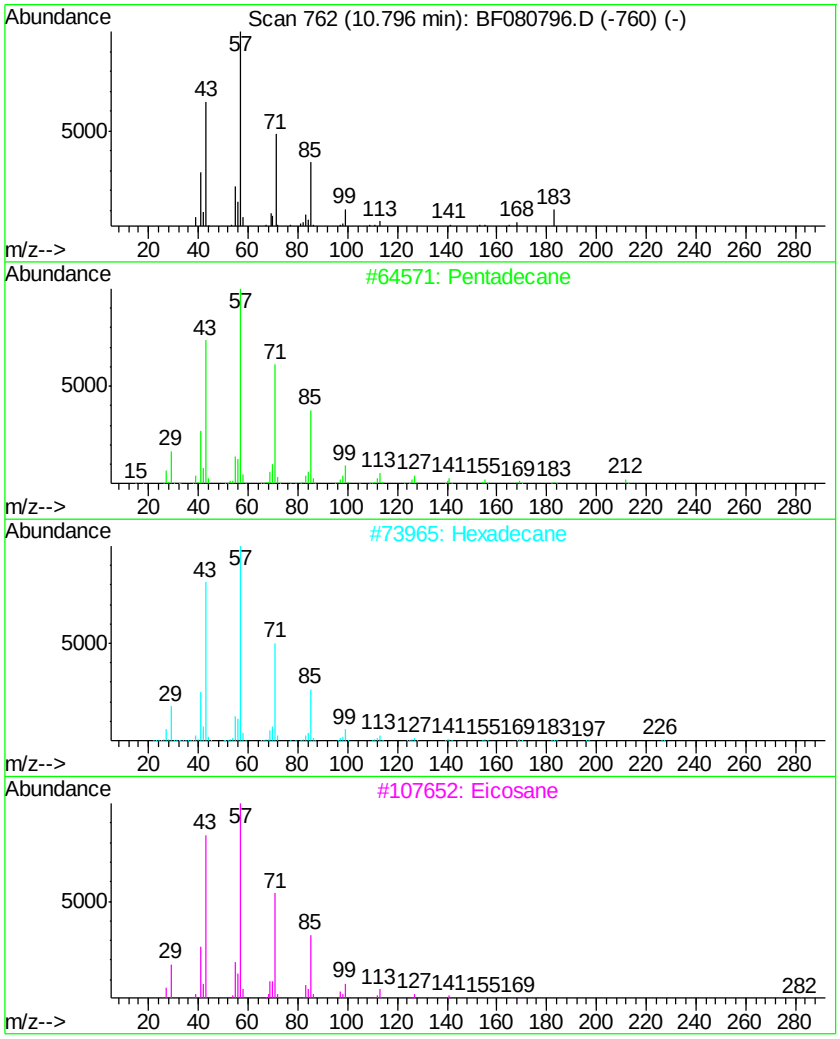
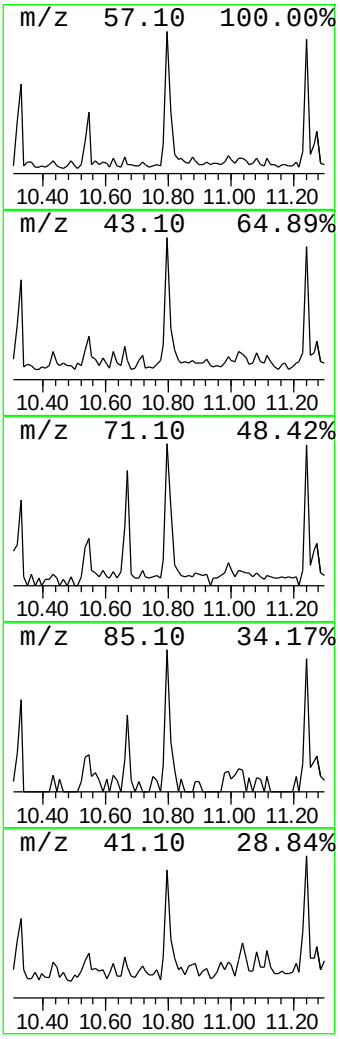
Peak Number 6 Pentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.63 ng	68023	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	80
2	Hexadecane	226	C16H34	000544-76-3	80
3	Eicosane	282	C20H42	000112-95-8	72
4	Tetradecane	198	C14H30	000629-59-4	72
5	Tetracosane	338	C24H50	000646-31-1	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
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Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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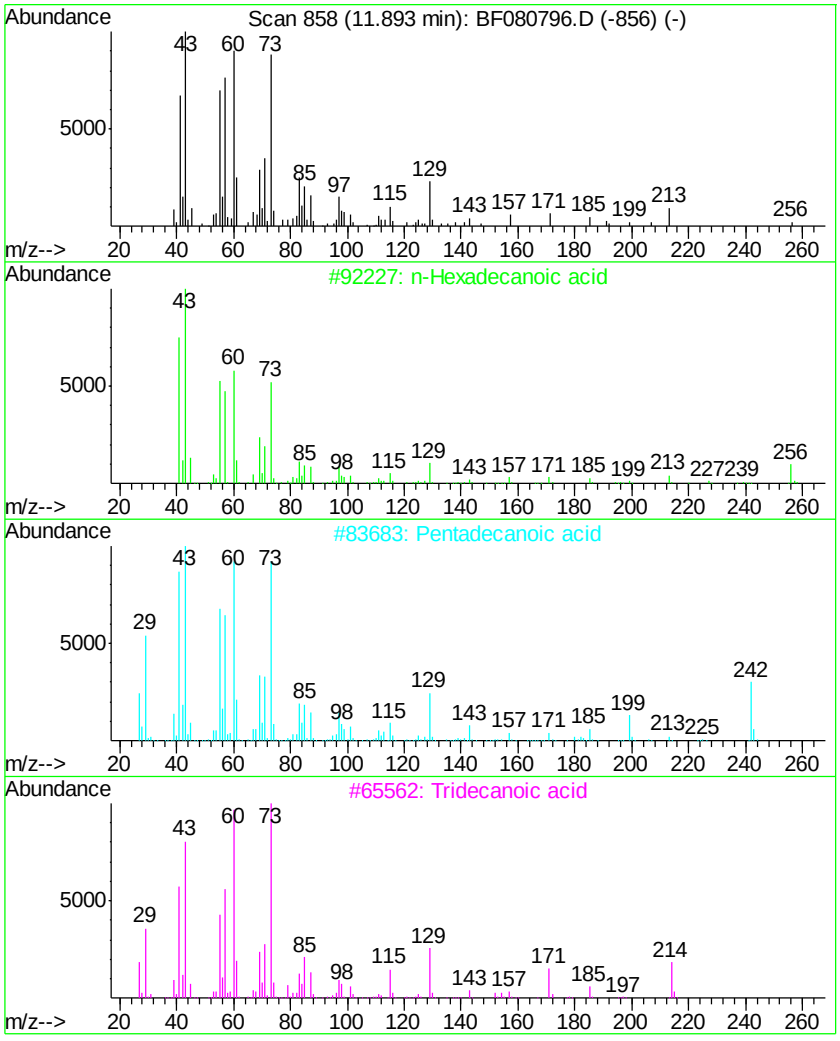
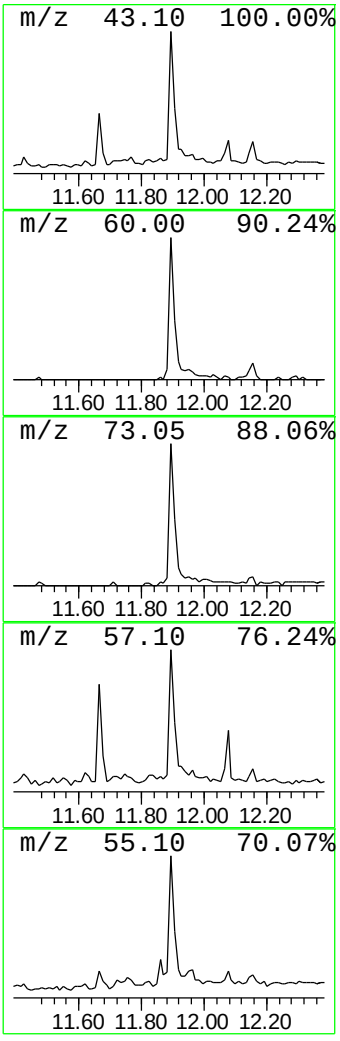
Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	8.10 ng	209467	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Misc :
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Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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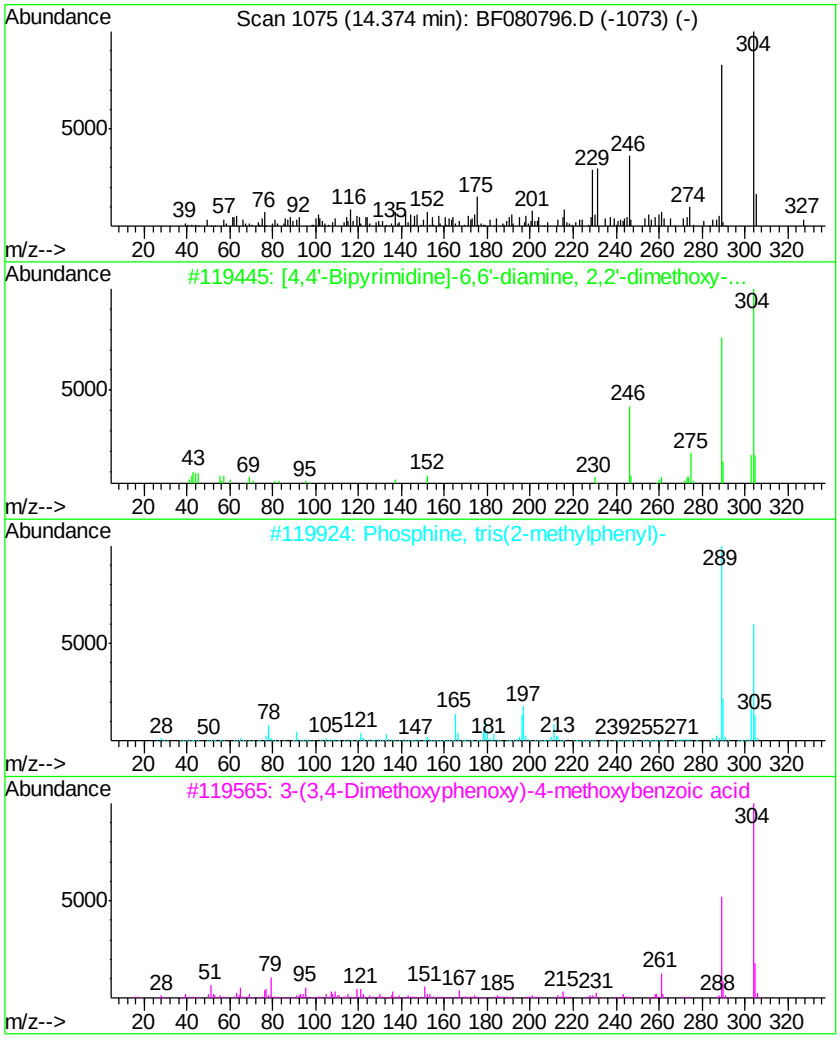
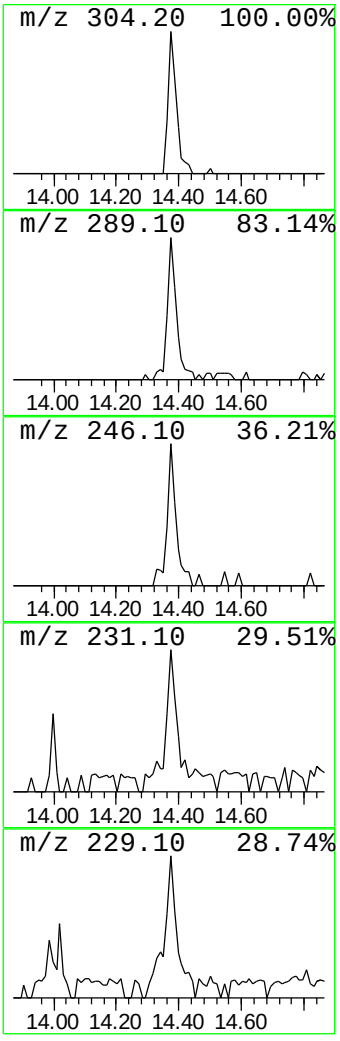
Peak Number 8 [4,4'-Bipyrimidine]-6,6'-di... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	2.72 ng	156626	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[4,4'-Bipyrimidine]-6,6'-diamine...	304	C14H20N6O2	062880-75-5	90
2	Phosphine, tris(2-methylphenyl)-	304	C21H21P	006163-58-2	50
3	3-(3,4-Dimethoxyphenoxy)-4-metho...	304	C16H16O6	1000243-56-7	42
4	p-Diphosphorinane, 1,4-diphenyl-...	304	C16H18O2P2	109501-46-4	35
5	Androstan-2-one, oxime, (5.alpha.)-	289	C19H31NO	014614-11-0	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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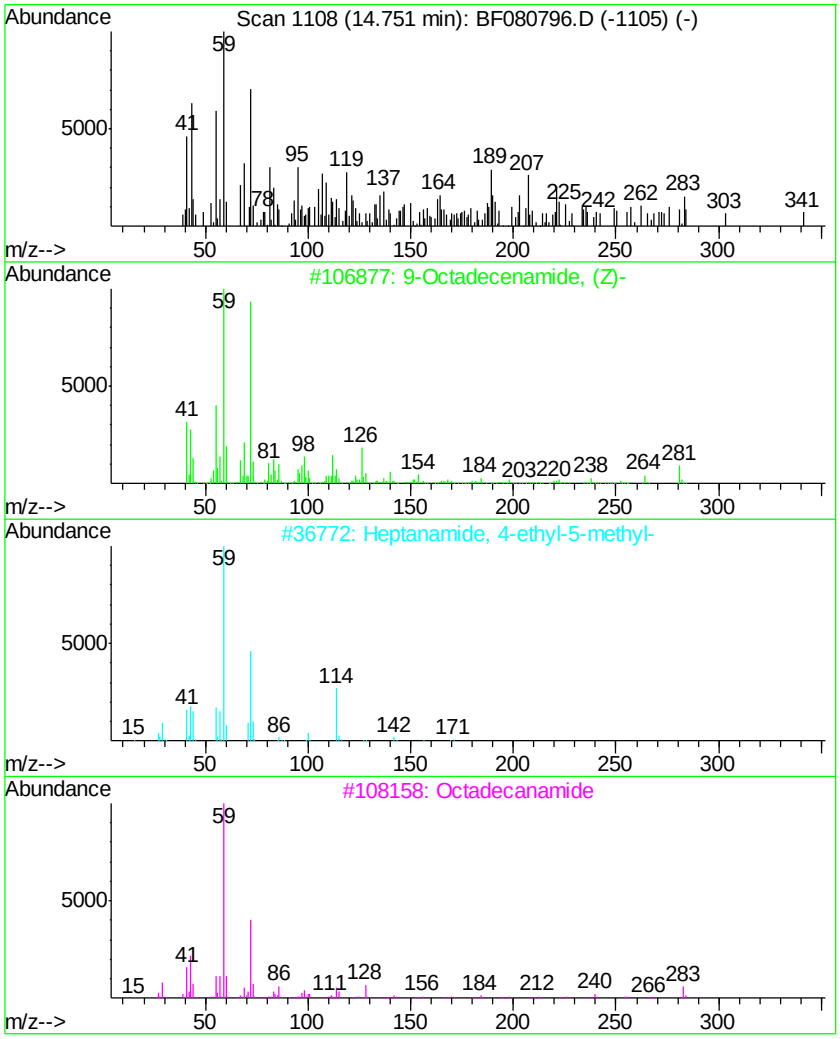
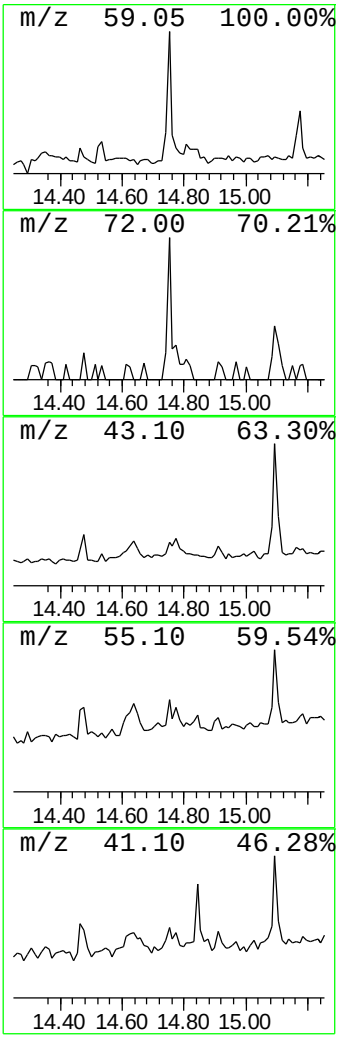
Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	6.17 ng	250589	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	55
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	49
3	Octadecanamide	283	C18H37NO	000124-26-5	46
4	Decanamide-	171	C10H21NO	002319-29-1	46
5	Tetradecanamide	227	C14H29NO	000638-58-4	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080115\
Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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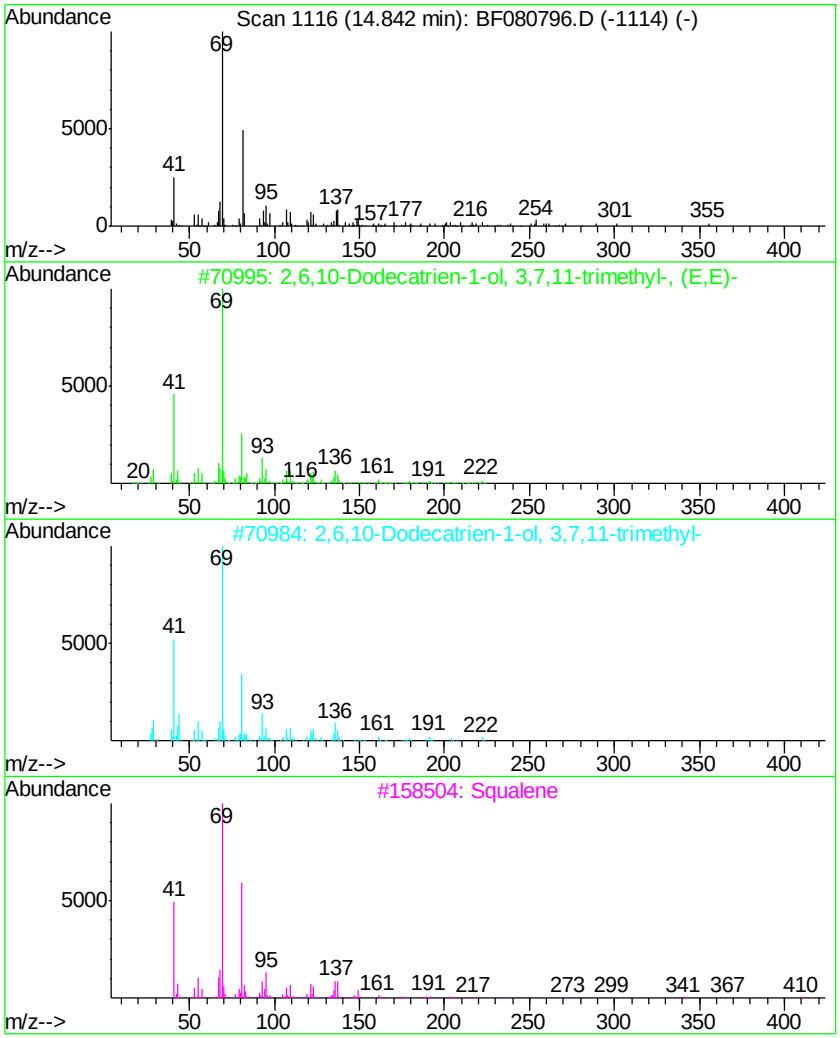
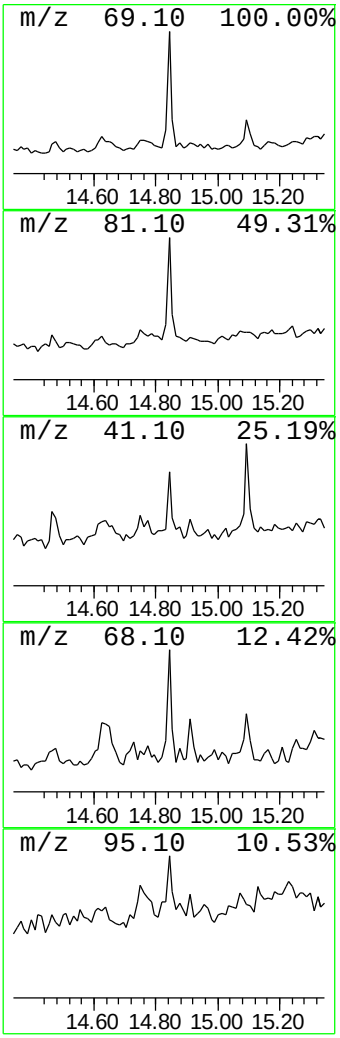
Peak Number 10 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.42 ng	98141	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	81
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
3	Squalene	410	C30H50	007683-64-9	64
4	1-Propyne, 3-(2-bromoethoxy)-	162	C5H7BrO	018668-74-1	64
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64





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Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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TIC Integration Parameters: LSCINT.P

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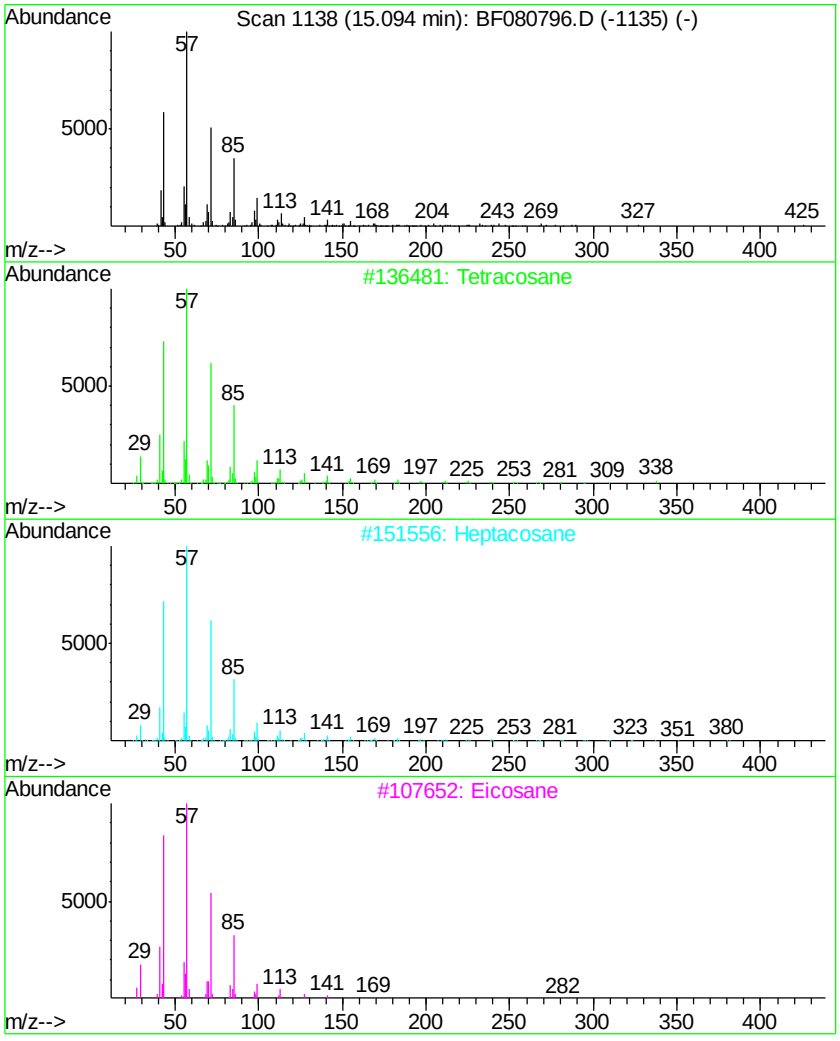
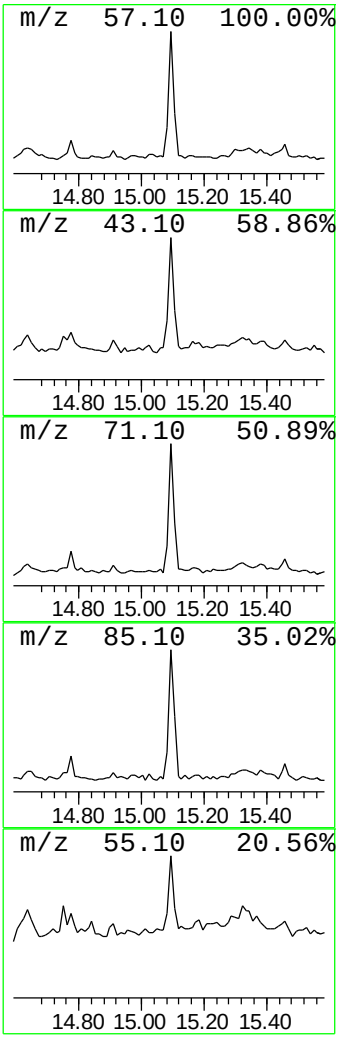
Peak Number 11 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	5.40 ng	219357	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Heptacosane	380	C27H56	000593-49-7	87
3	Eicosane	282	C20H42	000112-95-8	86
4	Pentacosane	352	C25H52	000629-99-2	86
5	Heneicosane	296	C21H44	000629-94-7	81





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Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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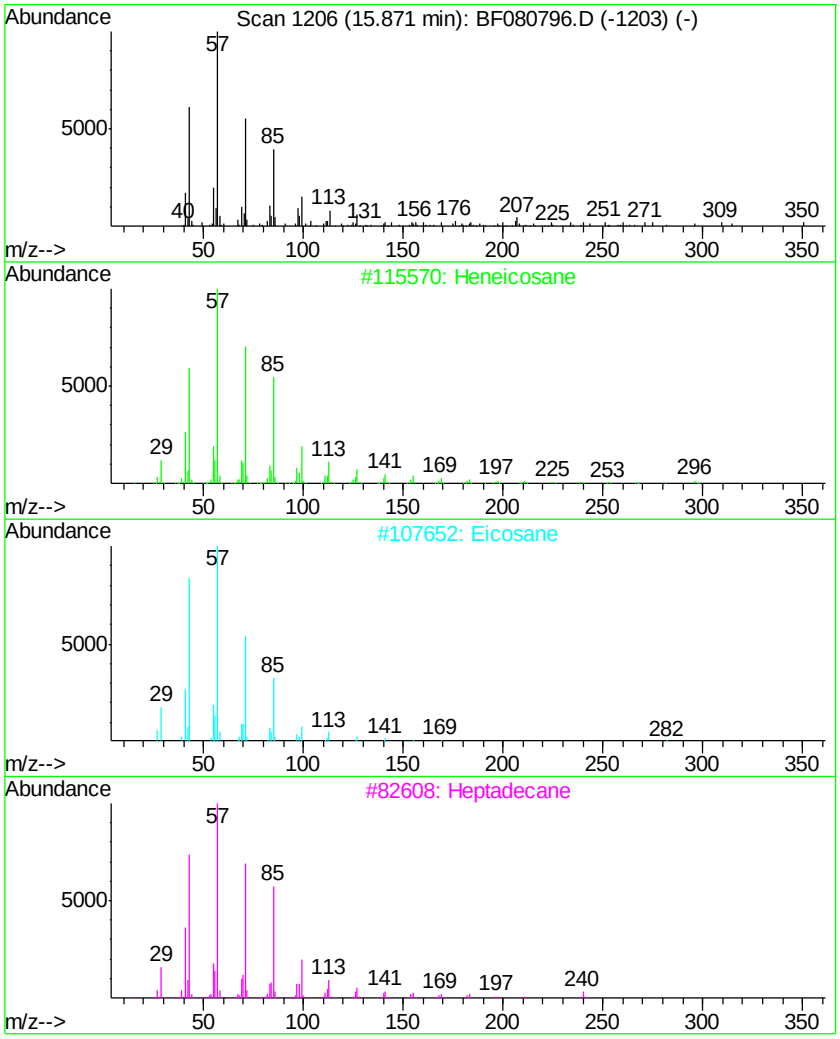
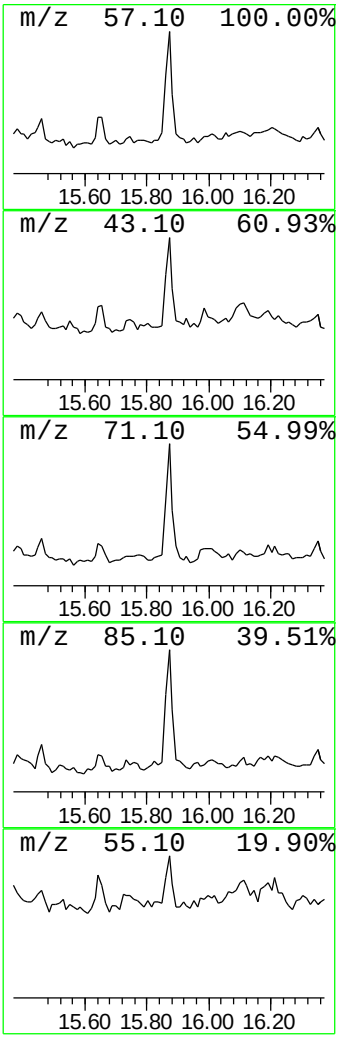
Peak Number 12 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	3.07 ng	124737	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Eicosane	282	C20H42	000112-95-8	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86





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Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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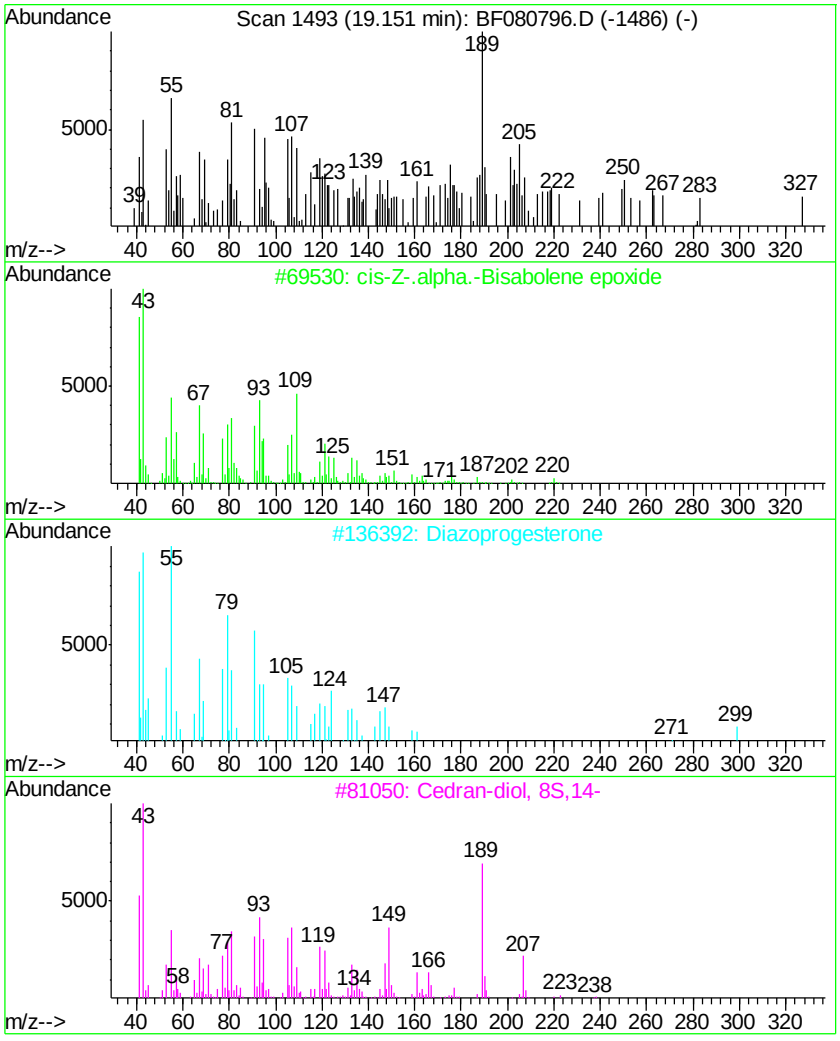
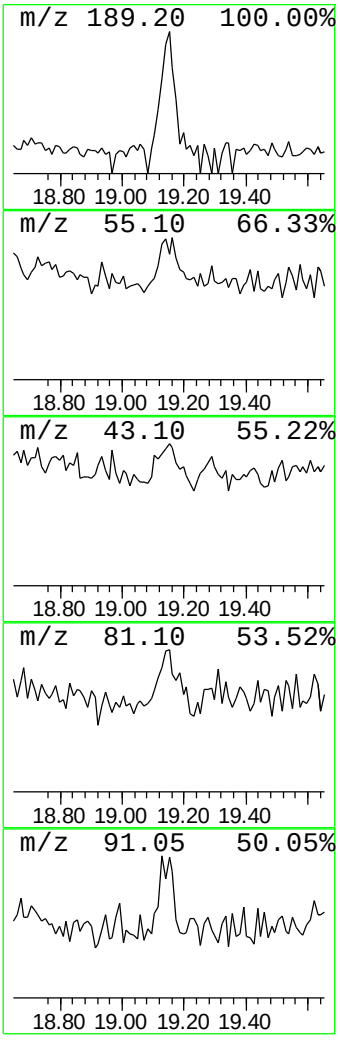
Peak Number 13 unknown19.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	5.79 ng	235123	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Z-.alpha.-Bisabolene epoxide	220	C15H24O	1000131-71-2	32
2	Diazoprogesterone	338	C21H30N4	1000255-30-9	32
3	Cedran-diol, 8S,14-	238	C15H26O2	062600-05-9	25
4	Benz[e]azulene-3,8-dione, 5-[(ac...	348	C19H24O6	025536-74-7	25
5	2-(4-Bromobutyl)-furan	202	C8H11BrO	066356-49-8	22





Tentatively Identified Compound (LSC) summary

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Data File : BF080796.D
Acq On : 1 Aug 2015 23:08
Operator : TP/UM
Sample : G3125-13
Misc :
ALS Vial : 82 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WEST-ABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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-one, 4...	4.40	3.4	ng	128153	1	6.85	752543	20.0
2-Pentanone, 4-hy...	5.05	67.5	ng	2539970	1	6.85	752543	20.0
2-Pentanone, 4-me...	5.86	2.5	ng	94342	1	6.85	752543	20.0
unknown6.62	6.62	69.1	ng	2601480	1	6.85	752543	20.0
Pentadecane	10.80	2.6	ng	68023	4	11.37	517206	20.0
n-Hexadecanoic acid	11.89	8.1	ng	209467	4	11.37	517206	20.0
[4,4'-Bipyrimidin...	14.37	2.7	ng	156626	5	14.00	1150870	20.0
9-Octadecenamide,...	14.75	6.2	ng	250589	6	15.41	812444	20.0
2,6,10-Dodecatrie...	14.84	2.4	ng	98141	6	15.41	812444	20.0
Tetracosane	15.09	5.4	ng	219357	6	15.41	812444	20.0
Heneicosane	15.87	3.1	ng	124737	6	15.41	812444	20.0
unknown19.15	19.15	5.8	ng	235123	6	15.41	812444	20.0