LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093382.D
Acq On : 4 Mar 2017 2:02
Operator : SJ/MA
Sample : I2078-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-5

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-BF013017.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	3.218	96	99	108	rBV	33239	78416	1.68%	0.182%
2	4.258	187	190	209	rBV	2188511	3292989	70.40%	7.663%
3	4.944	247	250	252	rBV	2674669	3570781	76.34%	8.310%
4	5.379	286	288	304	rBV	2451570	2640715	56.46%	6.145%
5	6.430	377	380	388	rBV	3320972	3845157	82.21%	8.948%
6	6.556	388	391	393	rBV	2669235	3219616	68.84%	7.492%
7	6.784	408	411	413	rBV	1010347	1204385	25.75%	2.803%
8	6.853	415	417	419	rBV	103573	100100	2.14%	0.233%
9	6.933	422	424	427	rBV	2816621	3279867	70.12%	7.633%
10	7.127	438	441	444	rBV	36523	57282	1.22%	0.133%
11	7.356	458	461	463	rBV	2974557	2997658	64.09%	6.976%
12	7.836	500	503	511	rVB	32661	72661	1.55%	0.169%
13	8.065	521	523	526	rBV	1284980	1552245	33.19%	3.612%
14	9.150	615	618	620	rBV	4068278	4677263	100.00%	10.884%
15	9.219	622	624	626	rVB	46418	57529	1.23%	0.134%
16	9.539	650	652	656	rVB	404908	422610	9.04%	0.983%
17	9.756	669	671	673	rBV	84779	125703	2.69%	0.293%
18	9.825	674	677	679	rVV	1362206	1571338	33.60%	3.657%
19	10.248	713	714	716	rVB	165552	123874	2.65%	0.288%
20	10.465	731	733	736	rBV	53505	83877	1.79%	0.195%
21	10.613	743	746	751	rVB	376802	466630	9.98%	1.086%
22	10.716	754	755	760	rVB	163489	242240	5.18%	0.564%
23	11.162	792	794	796	rBV	113403	143214	3.06%	0.333%
24	11.299	804	806	810	rBV	1353397	1549010	33.12%	3.605%
25	11.356	810	811	815	rVB3	68694	83894	1.79%	0.195%
26	11.596	829	832	834	rBV	64509	83583	1.79%	0.195%
27	11.859	854	855	858	rVB	270207	279269	5.97%	0.650%
28	11.928	858	861	864	rVB	89630	119672	2.56%	0.278%
29	12.236	886	888	890	rBV	44902	53349	1.14%	0.124%
30	12.351	895	898	900	rBV2	29969	48658	1.04%	0.113%
31	12.511	911	912	915	rBV	92471	133016	2.84%	0.310%
32	12.705	927	929	930	rBV	75474	77824	1.66%	0.181%
33	12.751	930	933	935	rVB	74156	131577	2.81%	0.306%
34	12.888	942	945	947	rBV	3397377	3220022	68.84%	7.493%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093382.D
Acq On : 4 Mar 2017 2:02
Operator : SJ/MA
Sample : I2078-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-5

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.311	980	982	985	rBV4	18995	48975	1.05%	0.114%
36	13.448	992	994	996	rBV2	36074	52431	1.12%	0.122%
37	13.779	1020	1023	1028	rVB2	242797	386195	8.26%	0.899%
38	13.939	1035	1037	1042	rVB	1064008	1101086	23.54%	2.562%
39	14.099	1049	1051	1055	rBV	45199	71164	1.52%	0.166%
40	14.408	1076	1078	1083	rBV	64731	133406	2.85%	0.310%
41	14.694	1101	1103	1106	rVB2	56664	85244	1.82%	0.198%
42	15.357	1158	1161	1164	rBV	792199	1025081	21.92%	2.385%
43	15.757	1193	1196	1198	rBV	95886	143028	3.06%	0.333%
44	16.214	1233	1236	1241	rVB	90055	171065	3.66%	0.398%
45	16.751	1280	1283	1287	rVB2	78051	148177	3.17%	0.345%

Sum of corrected areas: 42971876

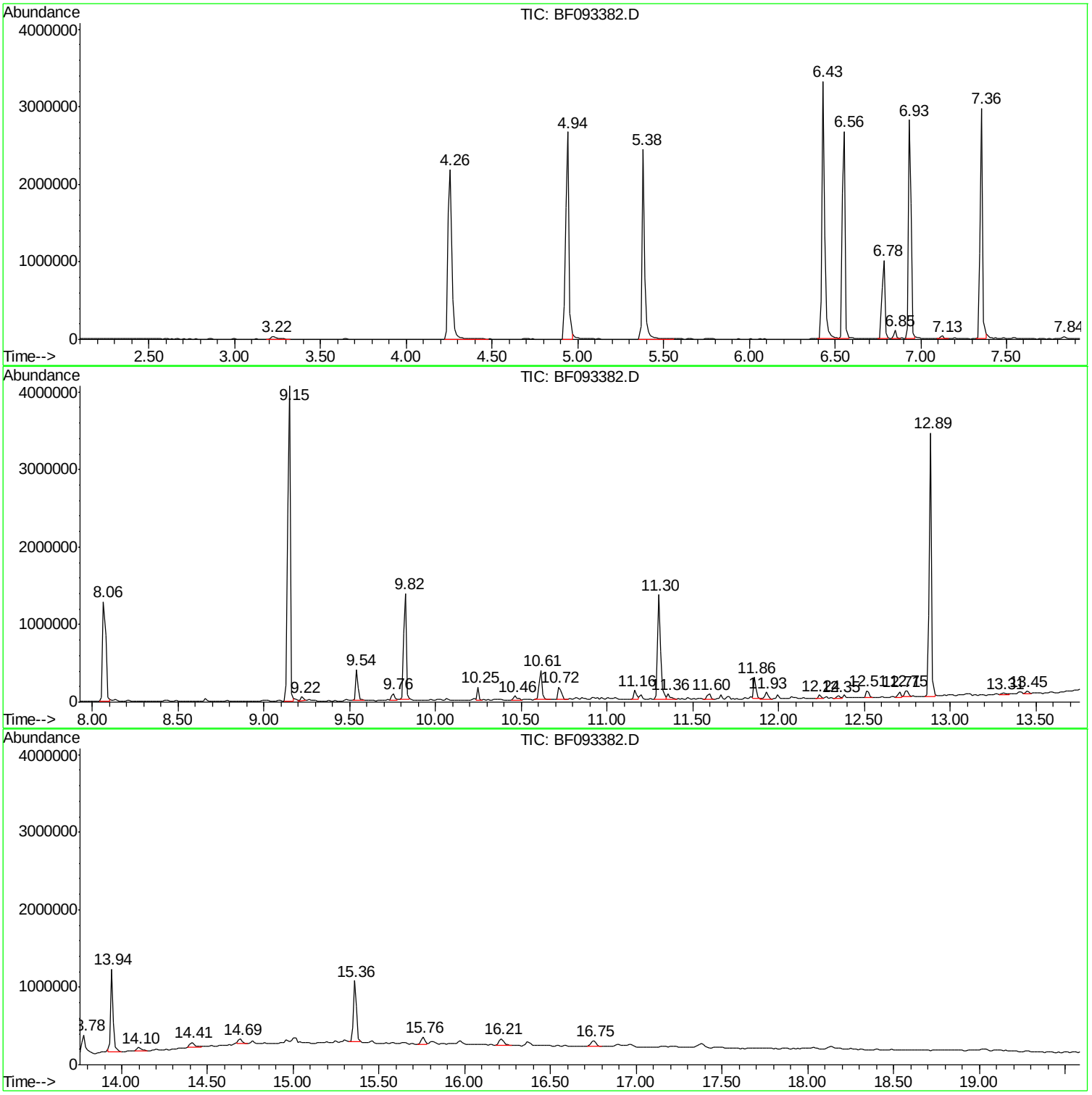
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093382.D
Acq On : 4 Mar 2017 2:02
Operator : SJ/MA
Sample : I2078-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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\BF030317\
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Acq On : 4 Mar 2017 2:02
Operator : SJ/MA
Sample : I2078-09
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Instrument : BNA_F
ClientSampleId : C-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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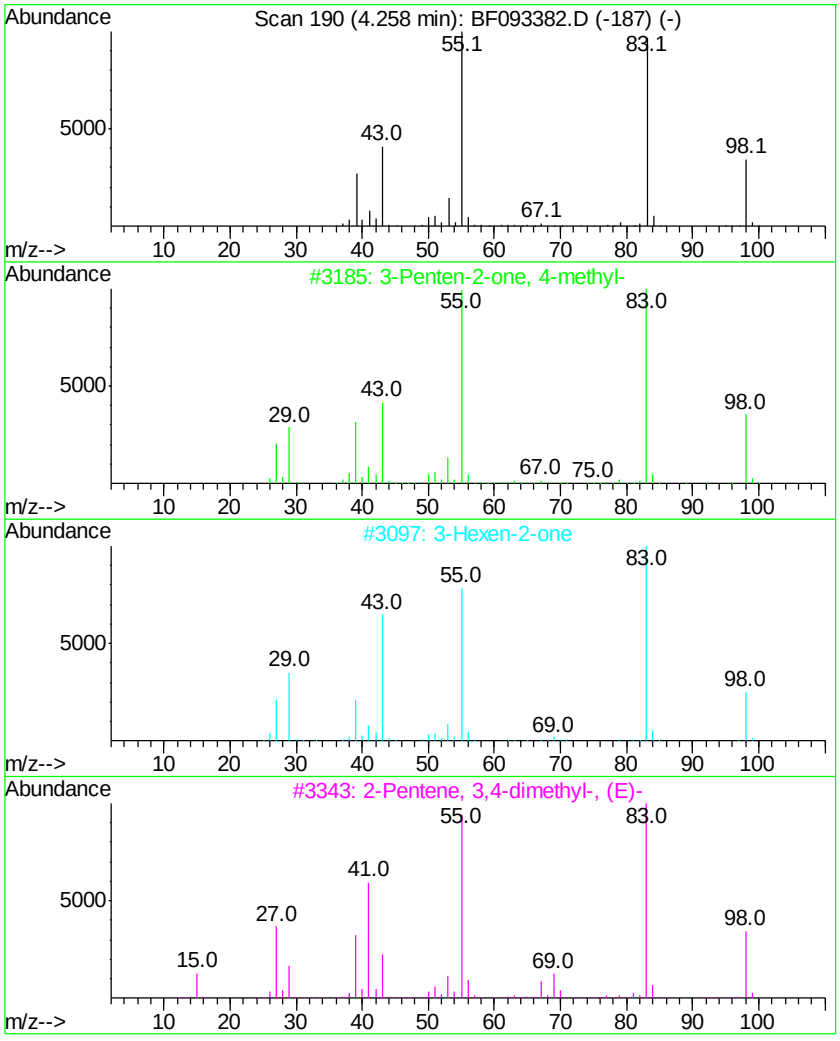
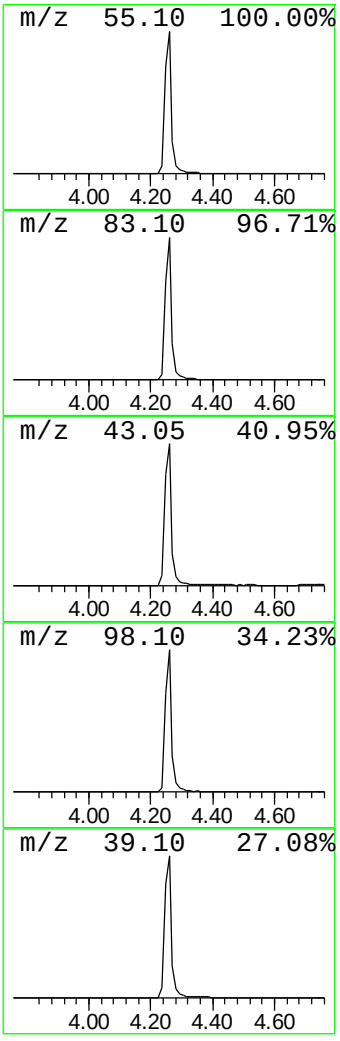
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.26	54.68 ng	3292990	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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Acq On : 4 Mar 2017 2:02
Operator : SJ/MA
Sample : I2078-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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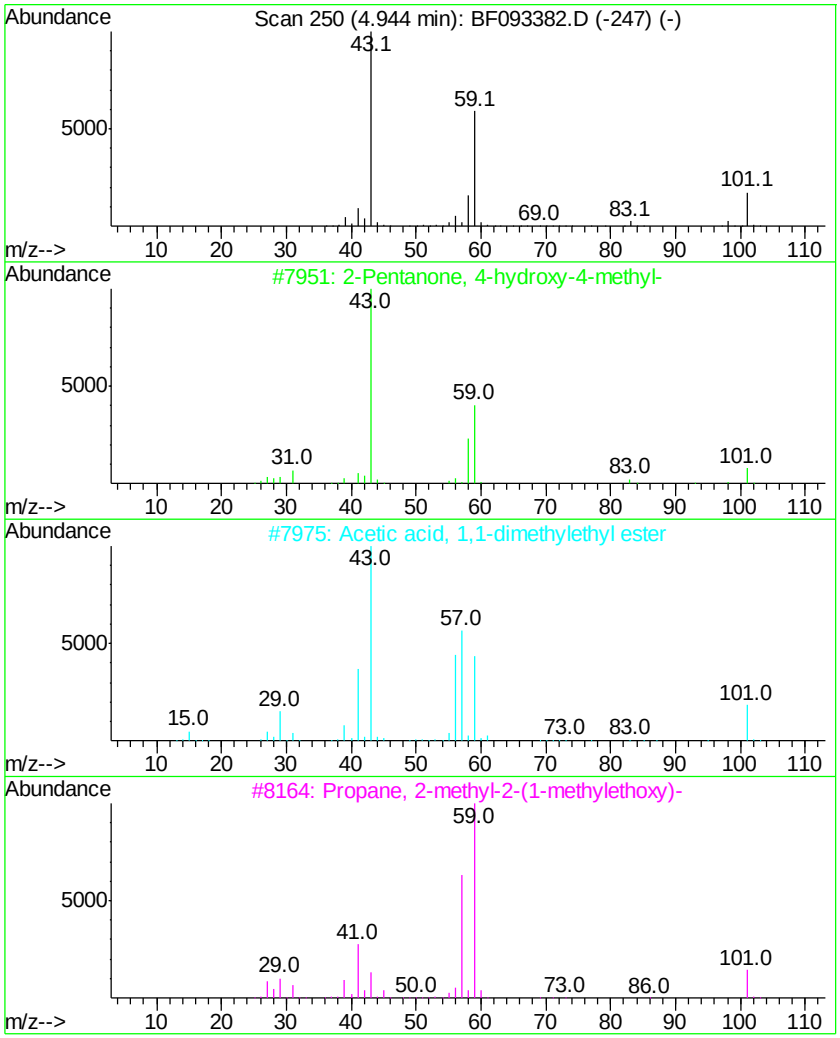
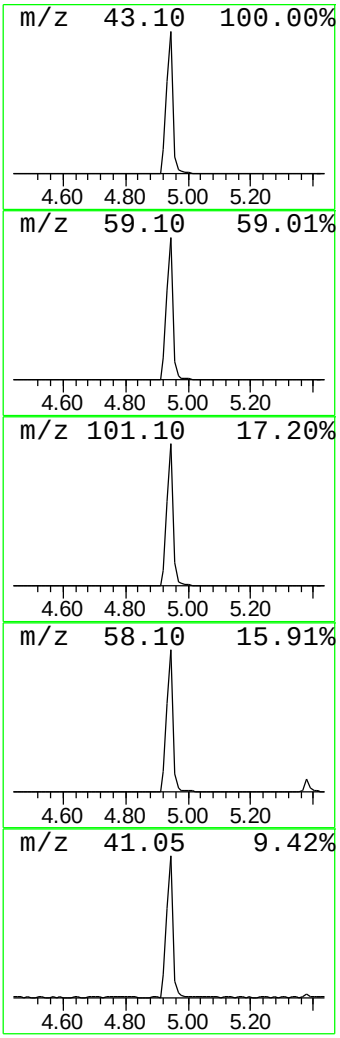
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	59.30 ng	3570780	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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Acq On : 4 Mar 2017 2:02
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Sample : I2078-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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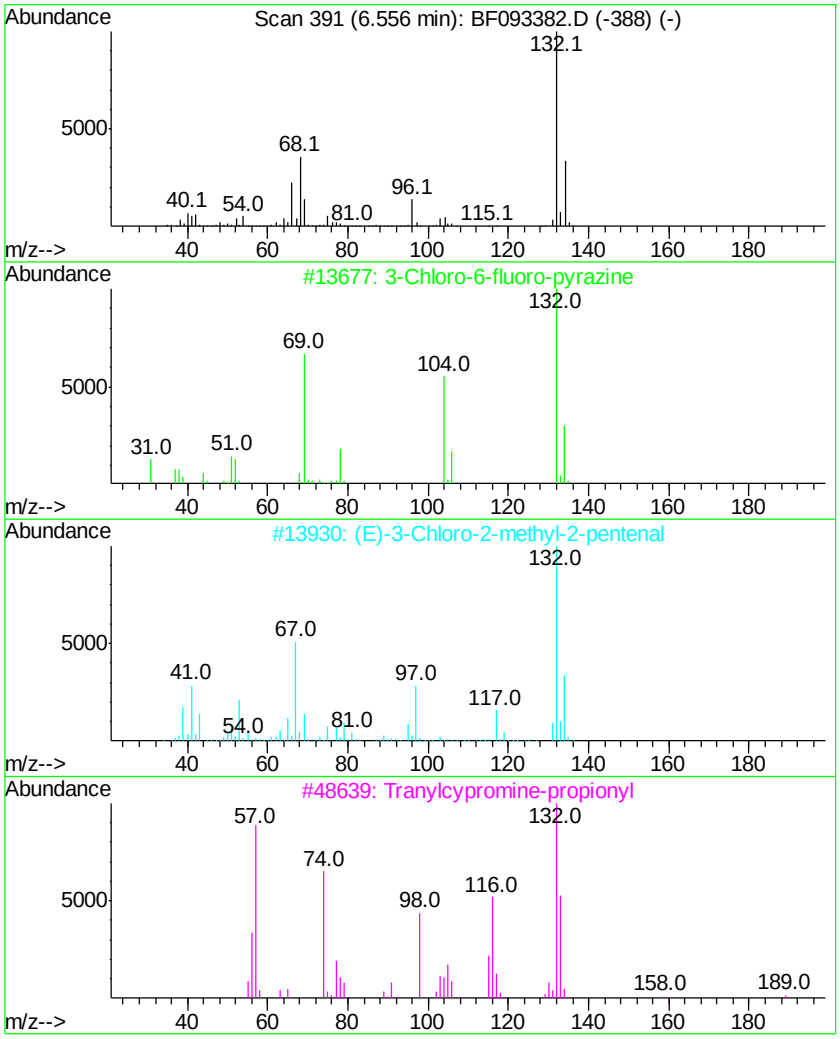
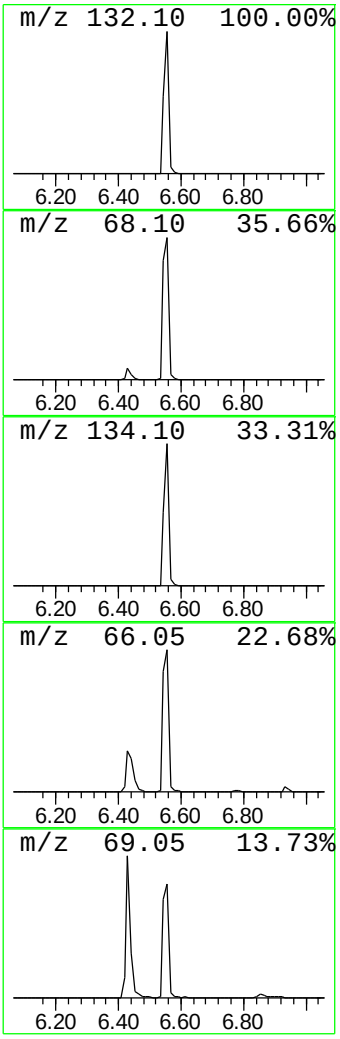
Peak Number 3 unknown6.56 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	53.46 ng	3219620	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
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Acq On : 4 Mar 2017 2:02
Operator : SJ/MA
Sample : I2078-09
Misc :
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Instrument : BNA_F
ClientSampleId : C-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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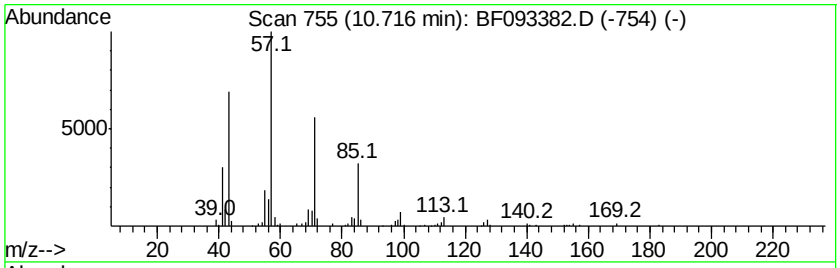
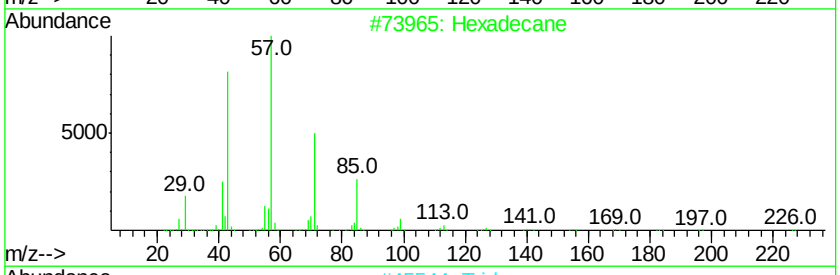
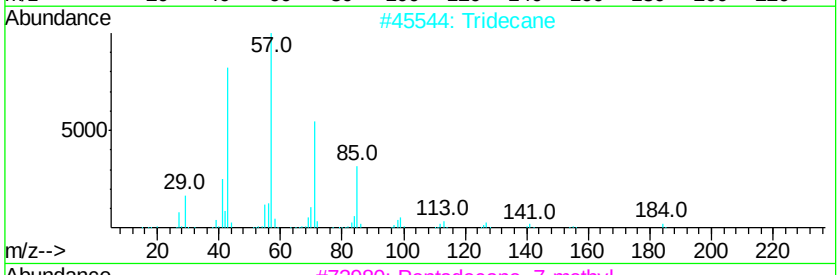
Peak Number 5 Hexadecane Concentration Rank 7

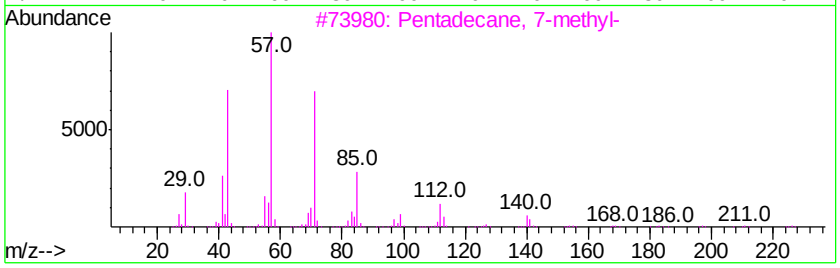
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	3.13 ng	242240	Phenanthrene-d10	11.30

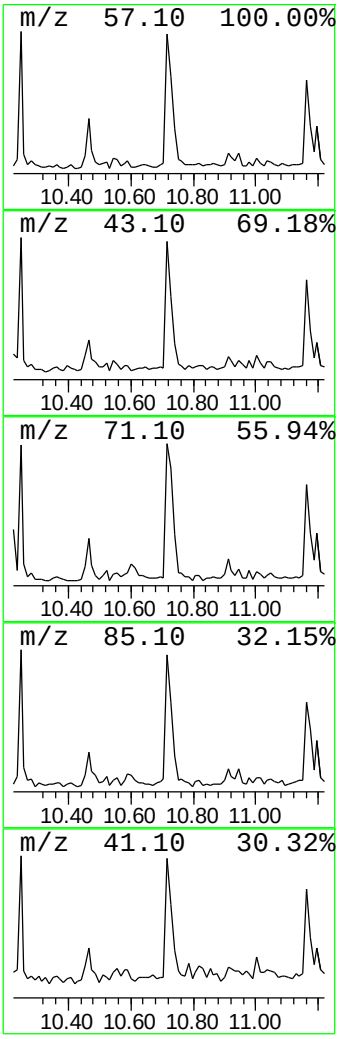
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tridecane	184	C13H28	000629-50-5	86
3	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83











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Operator : SJ/MA
Sample : I2078-09
Misc :
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Instrument : BNA_F
ClientSampleId : C-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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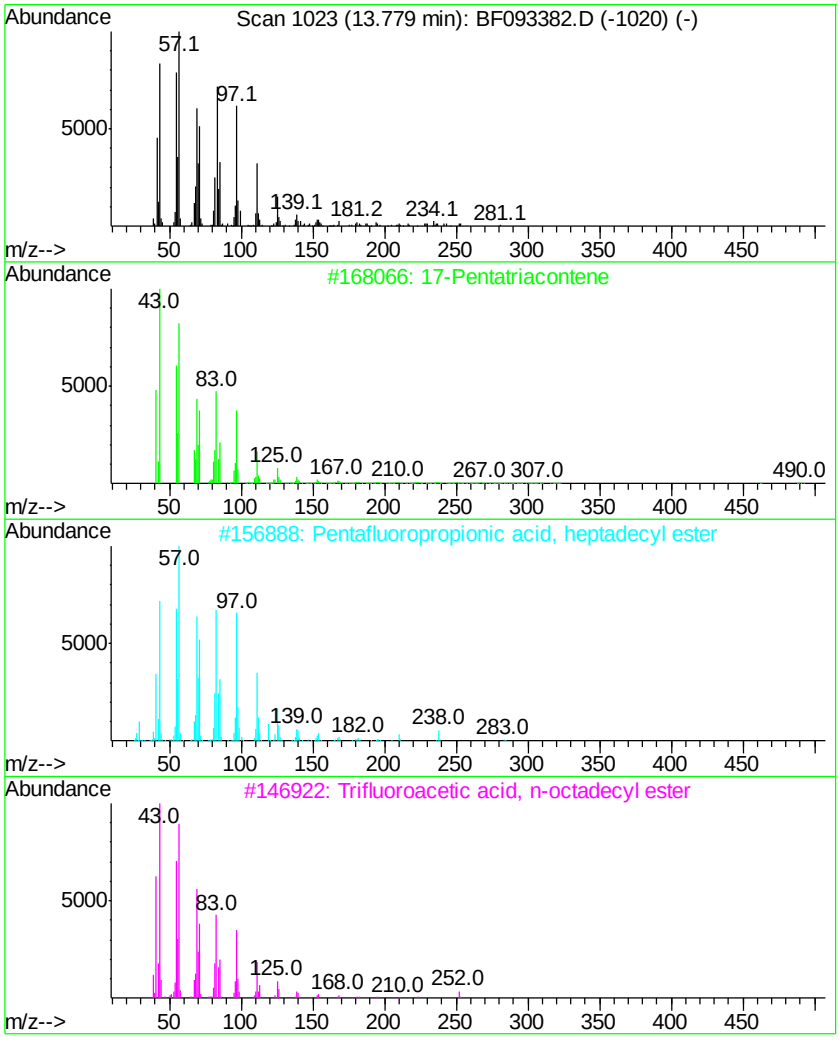
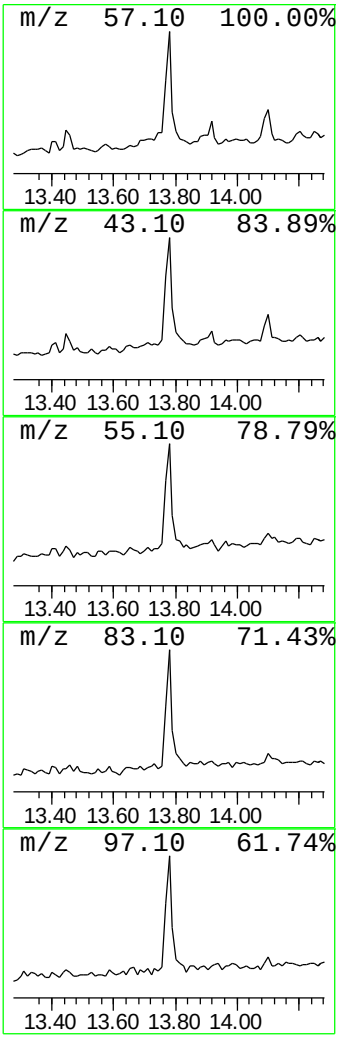
Peak Number 7 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	7.01 ng	386195	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	86
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	86
5	1-Octadecanol	270	C18H38O	000112-92-5	83





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

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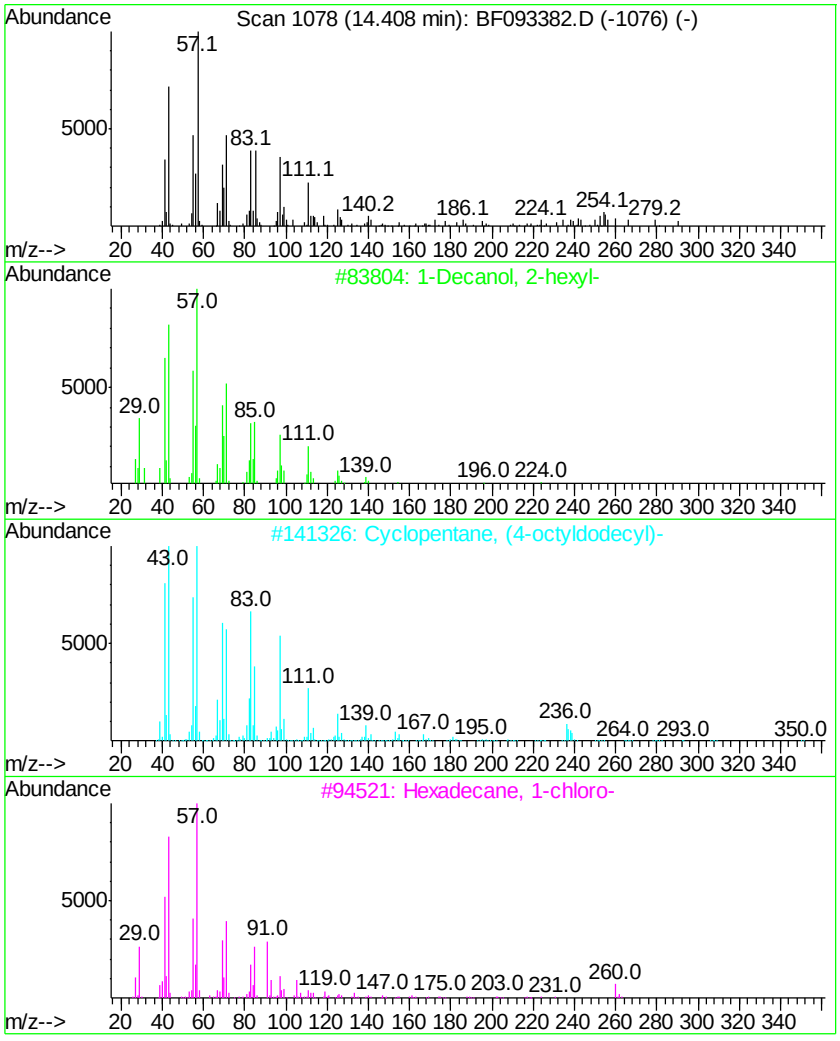
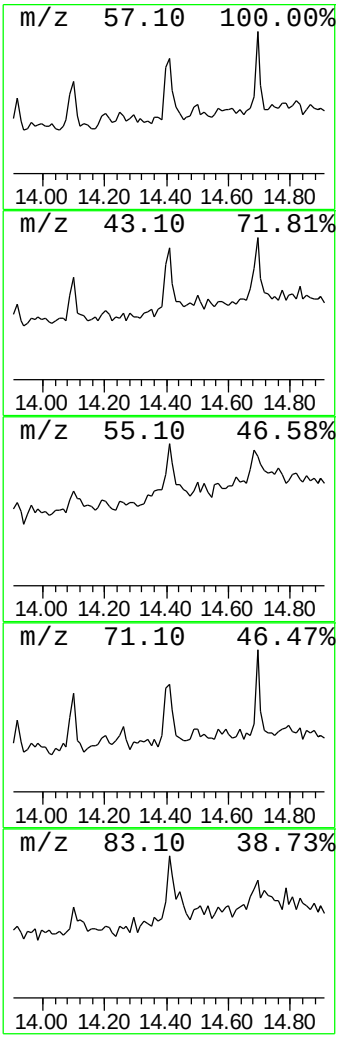
Peak Number 8 1-Decanol, 2-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	2.42 ng	133406	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	86
2	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	58
3	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	52
4	Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	46
5	Octadecane	254	C18H38	000593-45-3	45





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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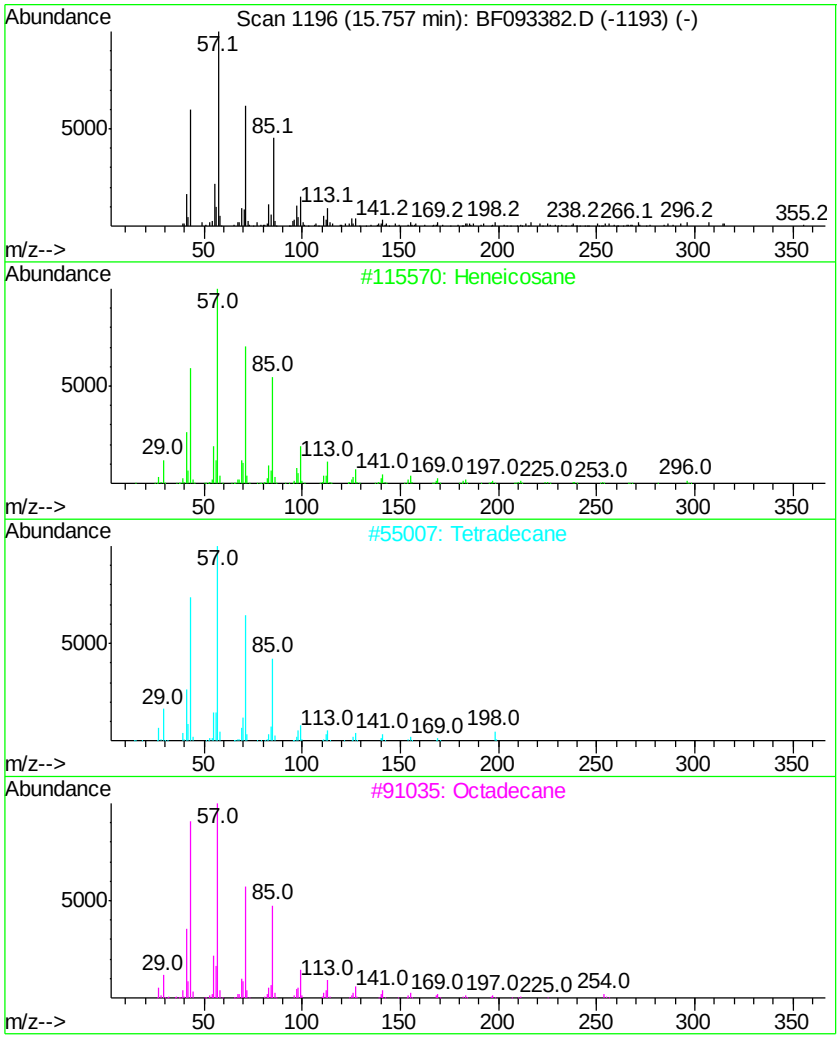
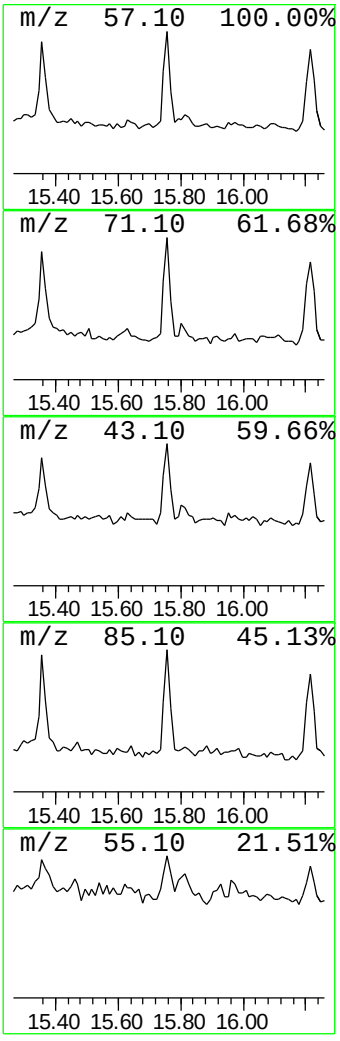
Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	2.79 ng	143028	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Tetradecane	198	C14H30	000629-59-4	93
3	Octadecane	254	C18H38	000593-45-3	90
4	Heptacosane	380	C27H56	000593-49-7	87
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093382.D
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Sample : I2078-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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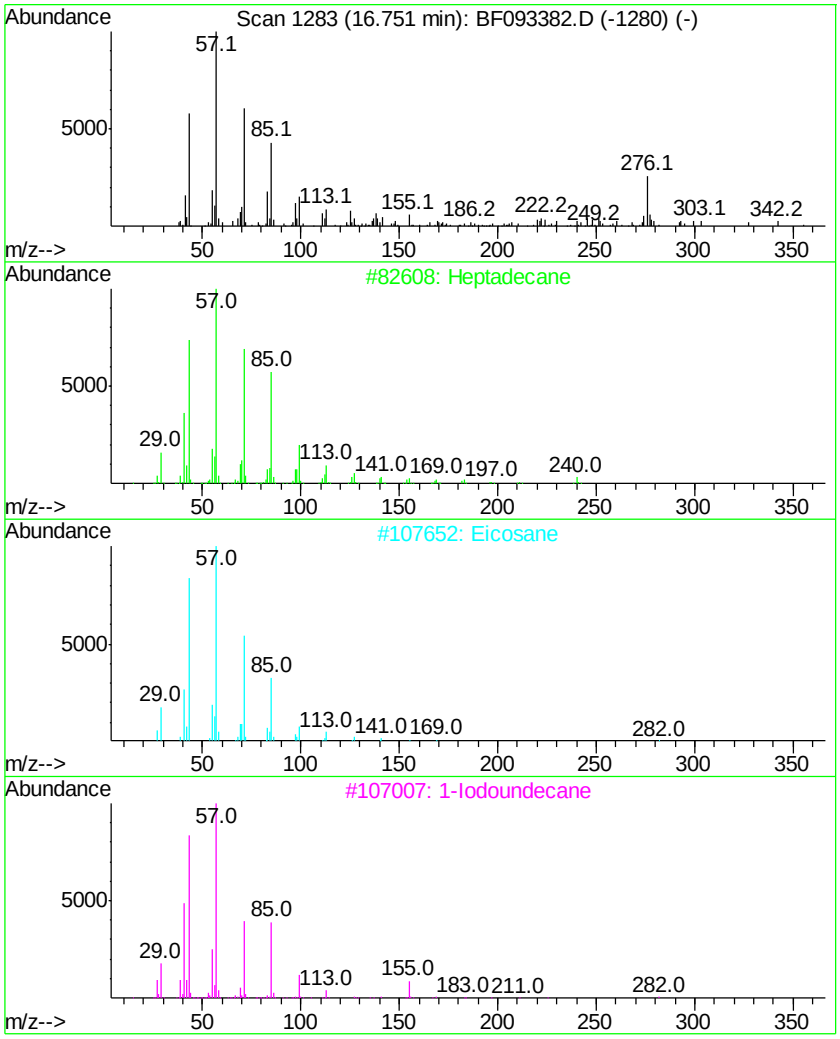
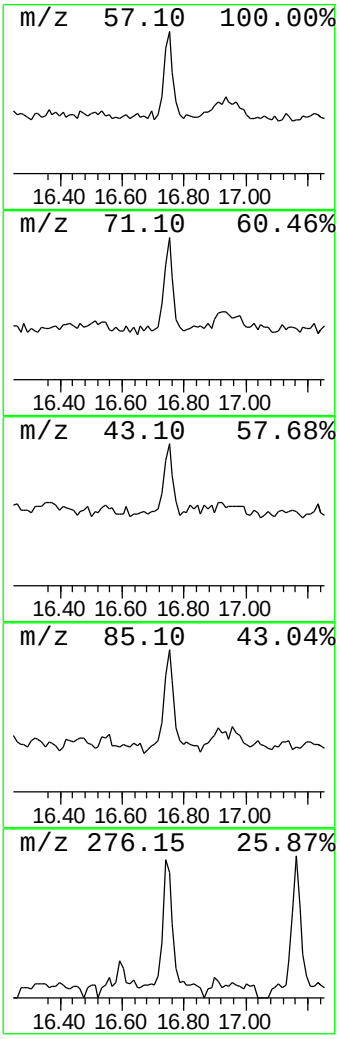
Peak Number 11 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.75	2.89 ng	148177	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Eicosane	282	C20H42	000112-95-8	64
3	1-Iodoundecane	282	C11H23I	004282-44-4	53
4	Nonadecane	268	C19H40	000629-92-5	52
5	Heptacosane	380	C27H56	000593-49-7	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
Data File : BF093382.D
Acq On : 4 Mar 2017 2:02
Operator : SJ/MA
Sample : I2078-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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...	4.26	54.7	ng	3292990	1	6.78	1204390	20.0
2-Pentanone, 4-hy...	4.94	59.3	ng	3570780	1	6.78	1204390	20.0
unknown6.56	6.56	53.5	ng	3219620	1	6.78	1204390	20.0
Hexadecane	10.72	3.1	ng	242240	4	11.30	1549010	20.0
17-Pentatriacontene	13.78	7.0	ng	386195	5	13.94	1101090	20.0
1-Decanol, 2-hexyl-	14.41	2.4	ng	133406	5	13.94	1101090	20.0
Heneicosane	15.76	2.8	ng	143028	6	15.36	1025080	20.0
Heptadecane	16.75	2.9	ng	148177	6	15.36	1025080	20.0