LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092328.D
Acq On : 17 Jan 2017 20:58
Operator : UM/SJ
Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

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-BF122116.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	4.667	249	252	265	rBV	1222277	2132979	41.23%	4.477%
2	5.147	291	294	315	rBV	3565463	5051727	97.64%	10.603%
3	6.222	385	388	390	rBV	4542428	5173960	100.00%	10.860%
4	6.324	395	397	399	rBV	5003018	4725042	91.32%	9.918%
5	6.553	415	417	419	rBV	1104477	1053479	20.36%	2.211%
6	6.702	428	430	433	rBV	2822750	3714992	71.80%	7.798%
7	7.124	465	467	470	rBV	2836373	2908165	56.21%	6.104%
8	7.845	527	530	532	rBV	1076920	1400471	27.07%	2.940%
9	8.919	621	624	627	rBV	5062054	5130123	99.15%	10.768%
10	9.319	657	659	662	rBV	569106	511344	9.88%	1.073%
11	9.582	680	682	685	rBV	1591570	1643985	31.77%	3.451%
12	10.039	720	722	723	rVB	114334	107665	2.08%	0.226%
13	10.256	738	741	744	rBV	47095	73829	1.43%	0.155%
14	10.382	749	752	754	rBV2	2355197	3342687	64.61%	7.016%
15	10.508	761	763	767	rVB	182833	215447	4.16%	0.452%
16	10.953	800	802	803	rBV	187543	164198	3.17%	0.345%
17	11.056	809	811	814	rBV	1175326	1618268	31.28%	3.397%
18	11.376	837	839	842	rVB	144173	125748	2.43%	0.264%
19	11.616	858	860	864	rBV2	80470	116679	2.26%	0.245%
20	12.645	947	950	953	rBV	3480706	5095851	98.49%	10.696%
21	12.896	969	972	974	rBV	62669	66898	1.29%	0.140%
22	13.239	999	1002	1003	rBV	57883	64072	1.24%	0.134%
23	13.571	1028	1031	1039	rBV2	105343	336574	6.51%	0.706%
24	13.685	1039	1041	1044	rBV	1217082	1337234	25.85%	2.807%
25	13.879	1055	1058	1060	rBV	72950	71174	1.38%	0.149%
26	14.177	1083	1084	1087	rBV	43551	58897	1.14%	0.124%
27	14.474	1108	1110	1113	rVB	59774	54140	1.05%	0.114%
28	14.542	1113	1116	1118	rBV	88043	118390	2.29%	0.248%
29	14.760	1133	1135	1139	rVB	49753	65263	1.26%	0.137%
30	15.045	1157	1160	1162	rBV	709832	987555	19.09%	2.073%
31	15.434	1192	1194	1197	rBV	42981	59710	1.15%	0.125%
32	15.845	1227	1230	1233	rVB	36442	59316	1.15%	0.125%
33	16.325	1268	1272	1278	rVB	25174	56238	1.09%	0.118%

LSC Area Percent Report

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Acq On : 17 Jan 2017 20:58
Operator : UM/SJ
Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 47642100

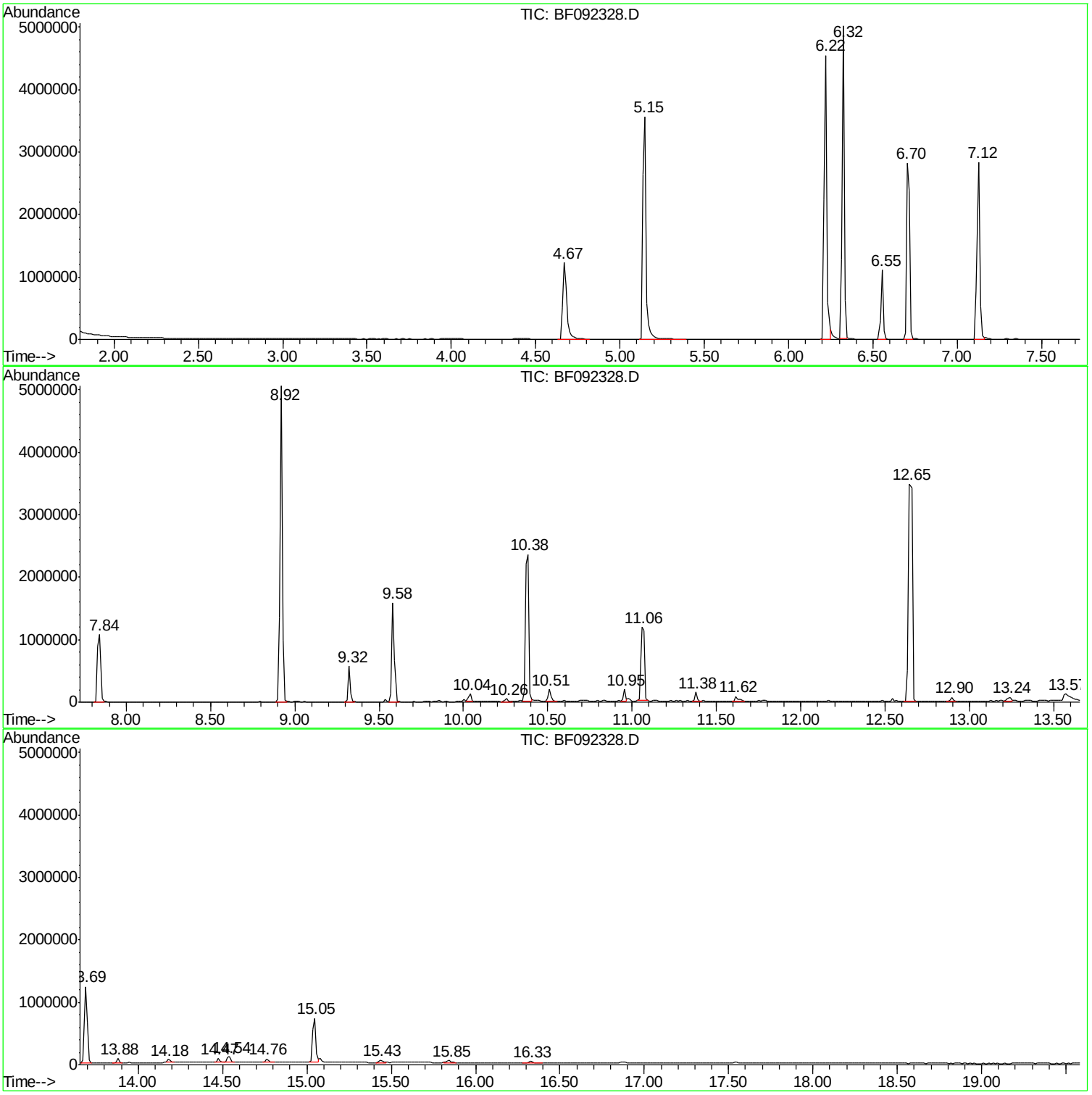
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092328.D
Acq On : 17 Jan 2017 20:58
Operator : UM/SJ
Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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 : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092328.D
Acq On : 17 Jan 2017 20:58
Operator : UM/SJ
Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

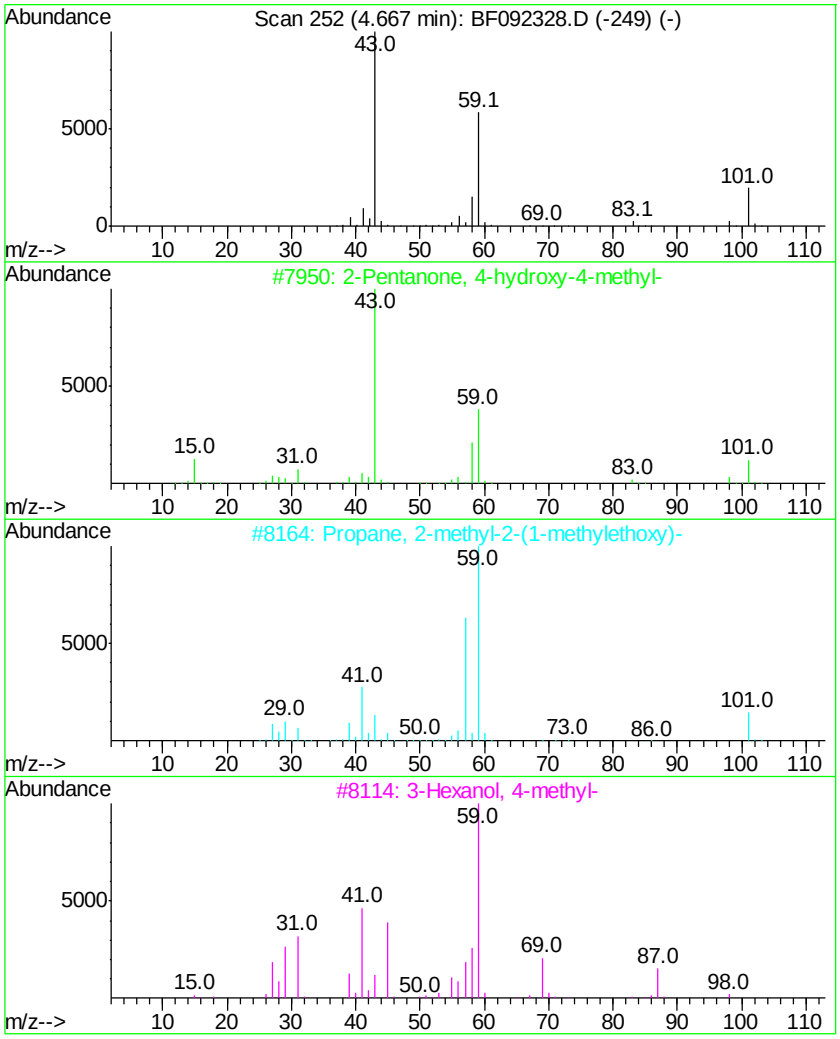
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

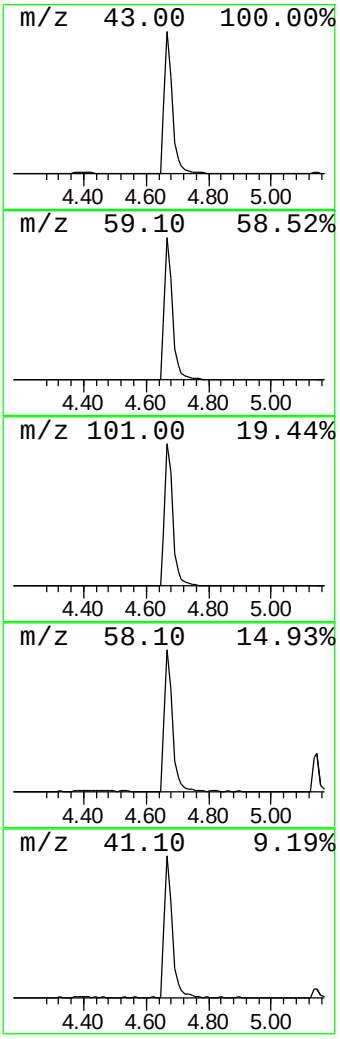
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	40.49 ng	2132980	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092328.D
Acq On : 17 Jan 2017 20:58
Operator : UM/SJ
Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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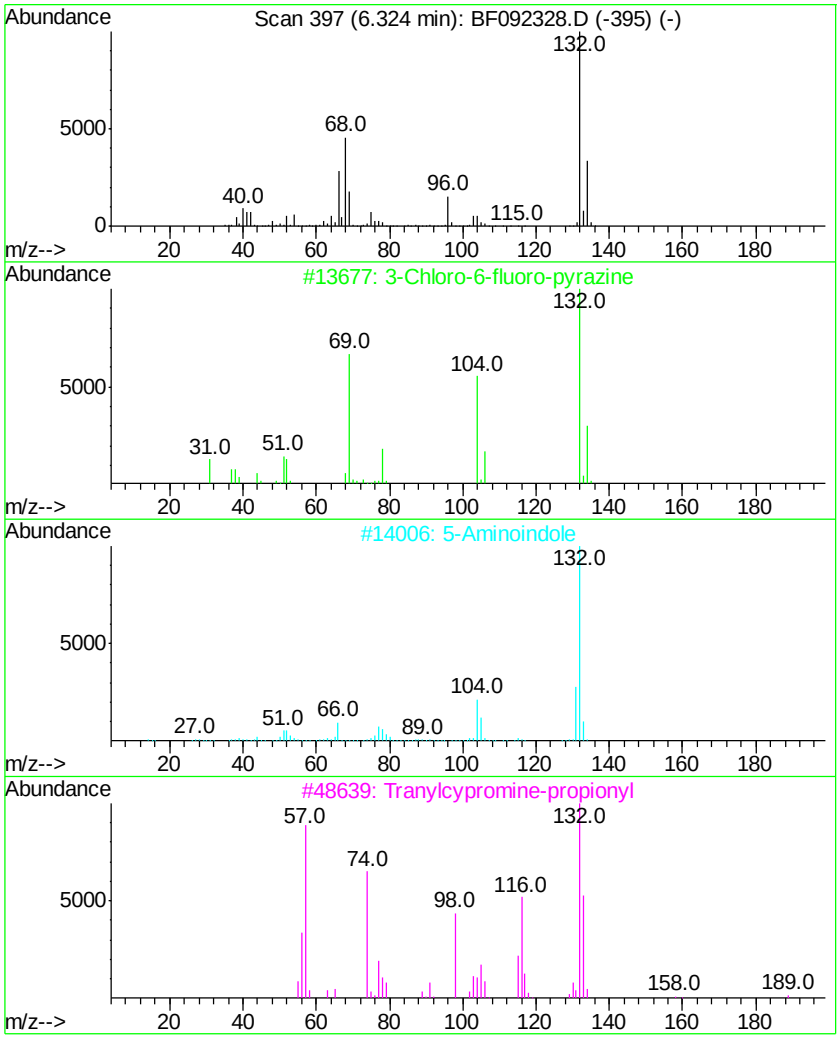
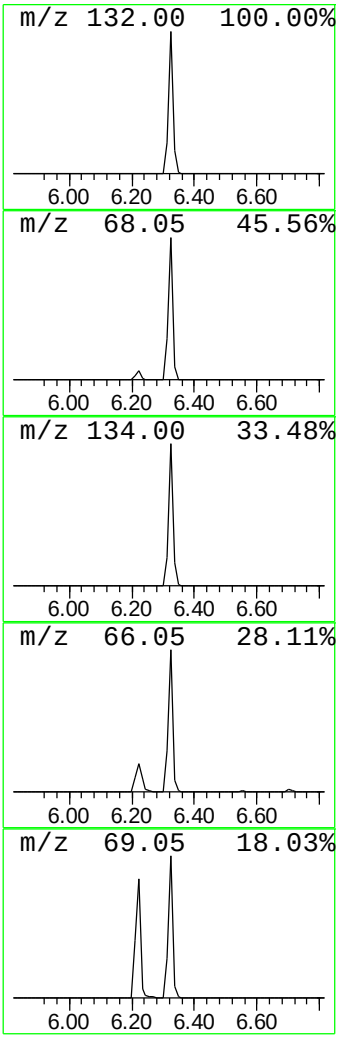
Peak Number 2 unknown6.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	89.70 ng	4725040	1,4-Dichlorobenzene-d4	6.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092328.D
Acq On : 17 Jan 2017 20:58
Operator : UM/SJ
Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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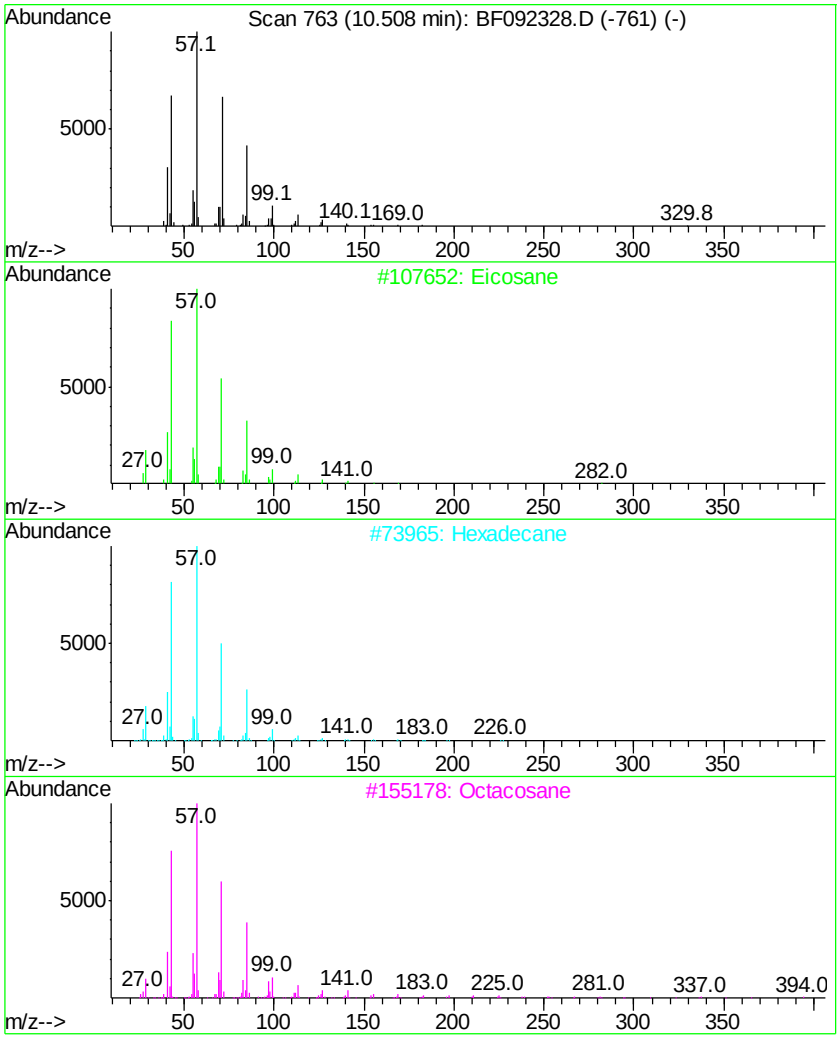
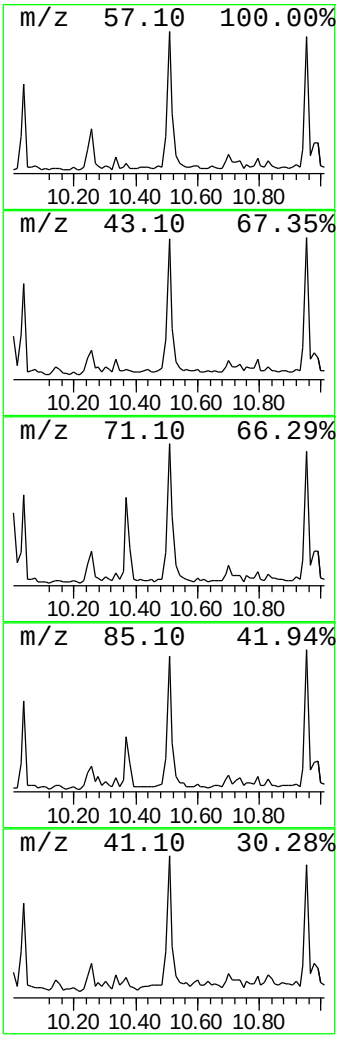
Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	2.66 ng	215447	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Pentadecane	212	C15H32	000629-62-9	90
5	Nonadecane	268	C19H40	000629-92-5	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011717\
Data File : BF092328.D
Acq On : 17 Jan 2017 20:58
Operator : UM/SJ
Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
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TIC Library : C:\DATABASE\NIST02.L
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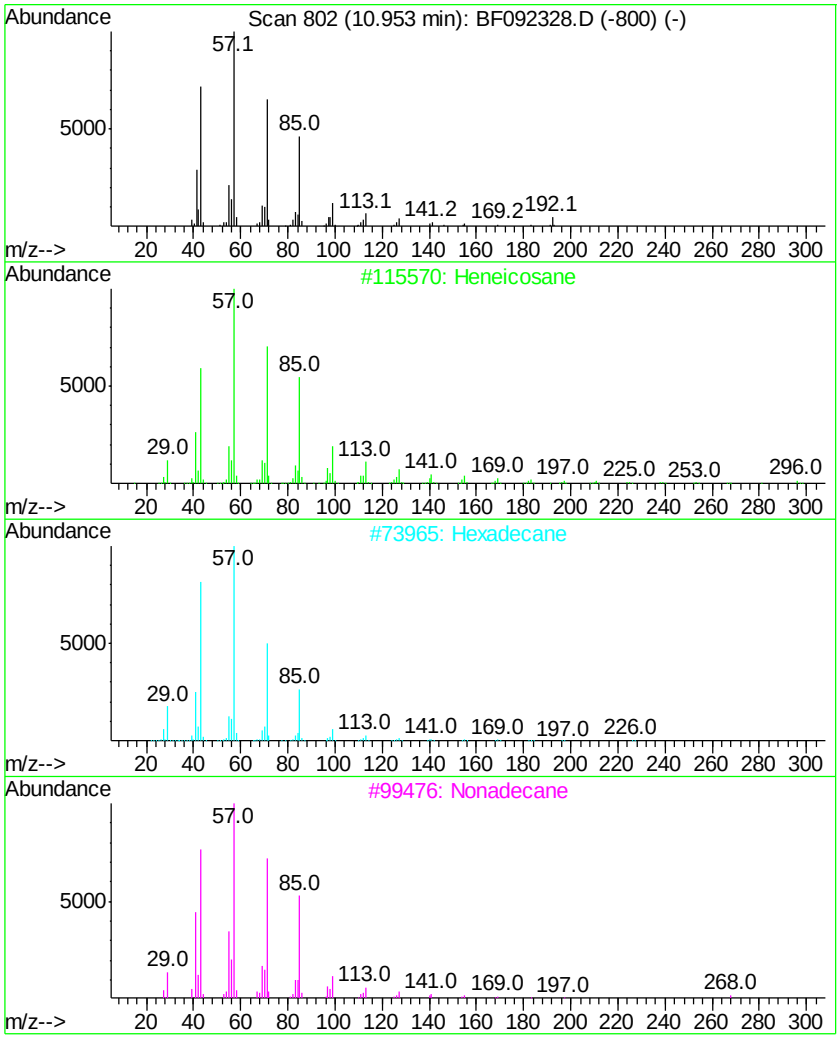
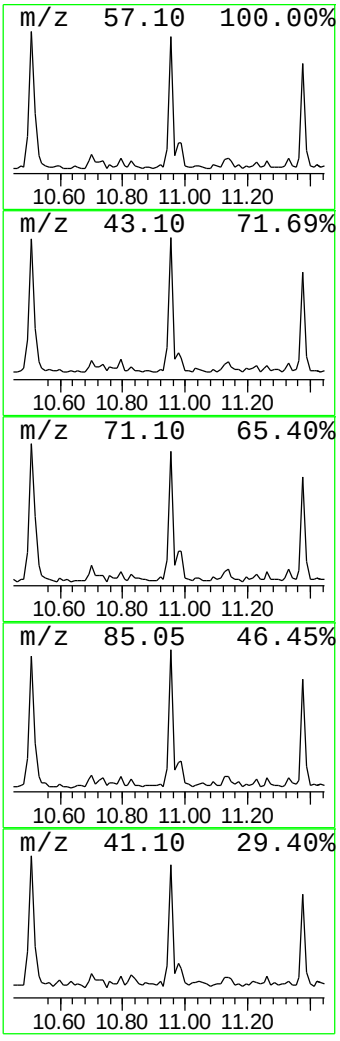
Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.03 ng	164198	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Tetradecane	198	C14H30	000629-59-4	87
5	Heptadecane	240	C17H36	000629-78-7	87





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Data File : BF092328.D
Acq On : 17 Jan 2017 20:58
Operator : UM/SJ
Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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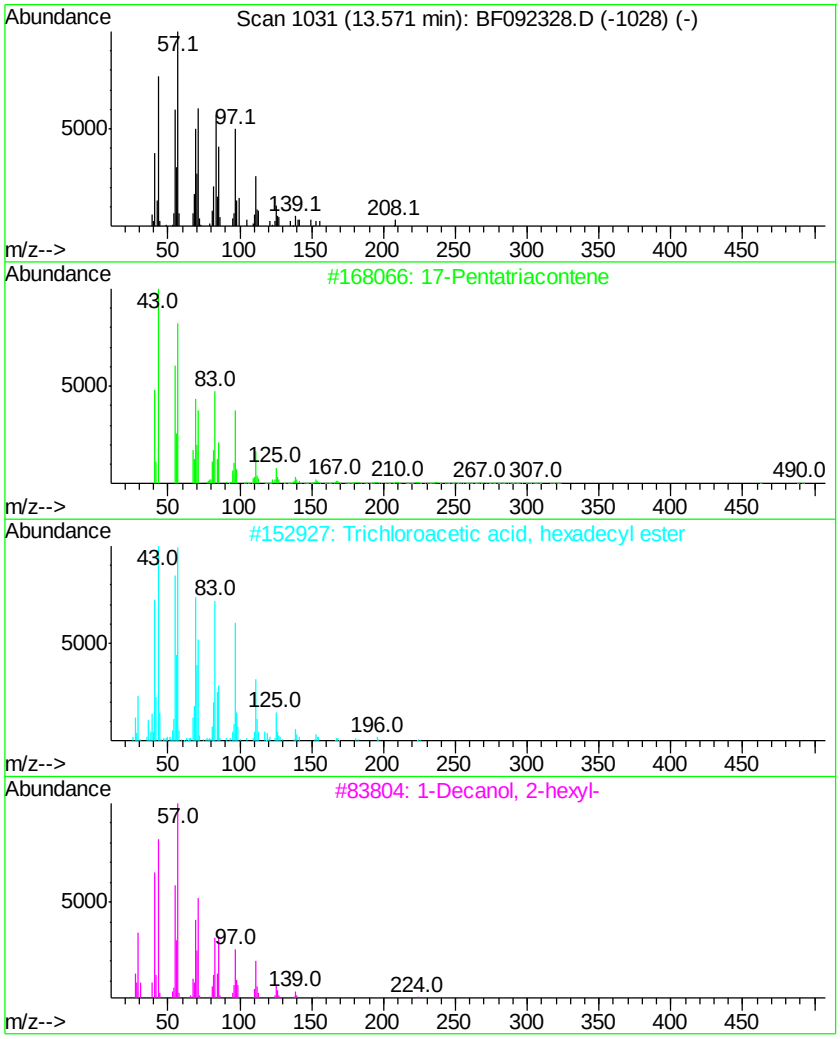
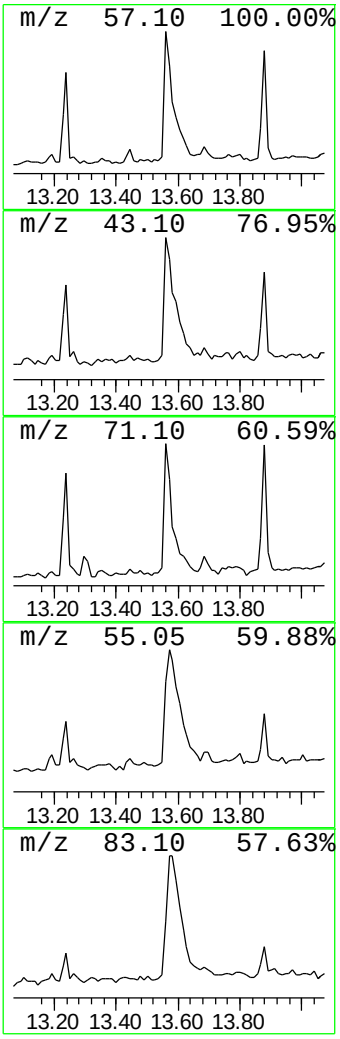
Peak Number 6 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	5.03 ng	336574	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	87
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	68
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	60
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	46





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Acq On : 17 Jan 2017 20:58
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Sample : I1243-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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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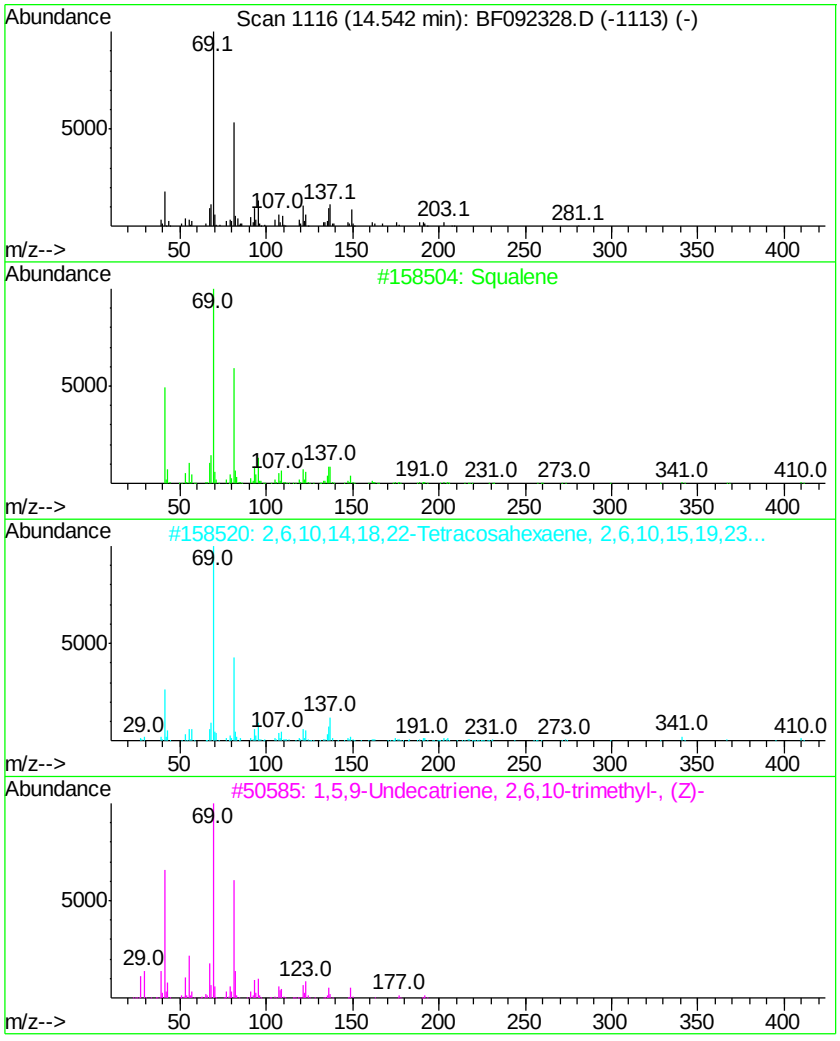
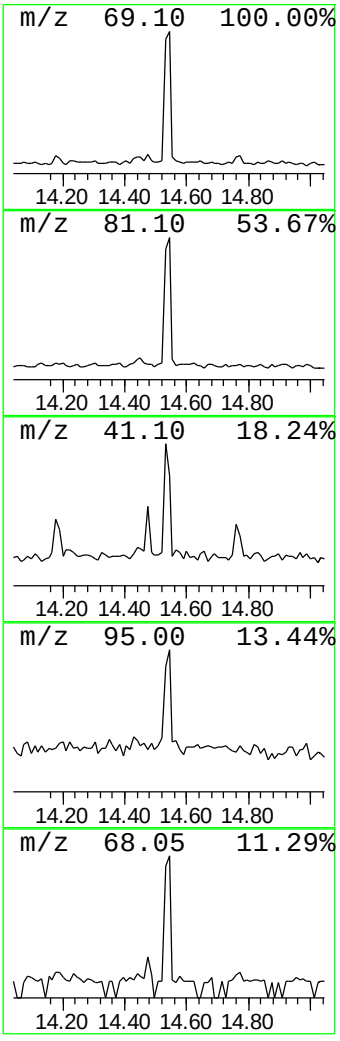
Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.40 ng	118390	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011717\
Data File : BF092328.D
Acq On : 17 Jan 2017 20:58
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Sample : I1243-01
Misc :
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Instrument : BNA_F
ClientSampleId : PHOENIX-BPM

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.67	40.5	ng	2132980	1	6.55	1053480	20.0
unknown6.32	6.32	89.7	ng	4725040	1	6.55	1053480	20.0
Eicosane	10.51	2.7	ng	215447	4	11.07	1618270	20.0
Heneicosane	10.95	2.0	ng	164198	4	11.07	1618270	20.0
17-Pentatriacontene	13.57	5.0	ng	336574	5	13.69	1337230	20.0
Squalene	14.54	2.4	ng	118390	6	15.05	987555	20.0