LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
Data File : BF093769.D
Acq On : 20 Mar 2017 17:35
Operator : SJ/MA
Sample : I2263-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

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-BF032017.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	2.161	22	24	27	rBV	74723	92046	1.42%	0.244%
2	5.019	271	274	276	rBV	584541	834373	12.87%	2.212%
3	5.430	308	310	313	rBV	1198292	1149423	17.73%	3.047%
4	6.447	397	399	402	rBV	642191	807662	12.46%	2.141%
5	6.596	409	412	414	rBV	2589747	2260910	34.87%	5.993%
6	6.836	430	433	435	rBV	1269418	1175591	18.13%	3.116%
7	6.996	444	447	449	rVB	3896632	4265756	65.79%	11.308%
8	7.396	479	482	484	rBV	3216807	3445417	53.14%	9.133%
9	8.116	542	545	548	rBV	1692774	1575018	24.29%	4.175%
10	9.202	636	640	642	rBV	5369240	6483684	100.00%	17.187%
11	9.865	696	698	701	rVB	1447851	1787925	27.58%	4.740%
12	10.379	741	743	745	rVB	87955	75631	1.17%	0.200%
13	10.653	764	767	769	rBV	1720400	1782316	27.49%	4.725%
14	11.351	825	828	830	rVB	1643236	1907446	29.42%	5.056%
15	12.939	963	967	969	rBV	4559265	5945314	91.70%	15.760%
16	13.968	1055	1057	1060	rBV	1718562	1649940	25.45%	4.374%
17	14.757	1124	1126	1129	rVB	64427	72706	1.12%	0.193%
18	15.077	1152	1154	1158	rBV	99337	126990	1.96%	0.337%
19	15.374	1177	1180	1183	rBV	982393	1372856	21.17%	3.639%
20	15.443	1183	1186	1192	rVB	136341	209703	3.23%	0.556%
21	15.854	1218	1222	1226	rBV	113087	206087	3.18%	0.546%
22	16.323	1259	1263	1270	rBV	105105	203760	3.14%	0.540%
23	16.883	1308	1312	1316	rBV	56275	120200	1.85%	0.319%
24	17.157	1329	1336	1343	rBV7	15861	70488	1.09%	0.187%
25	17.534	1365	1369	1377	rVB	38278	102233	1.58%	0.271%

Sum of corrected areas: 37723475

LSC Report - Integrated Chromatogram

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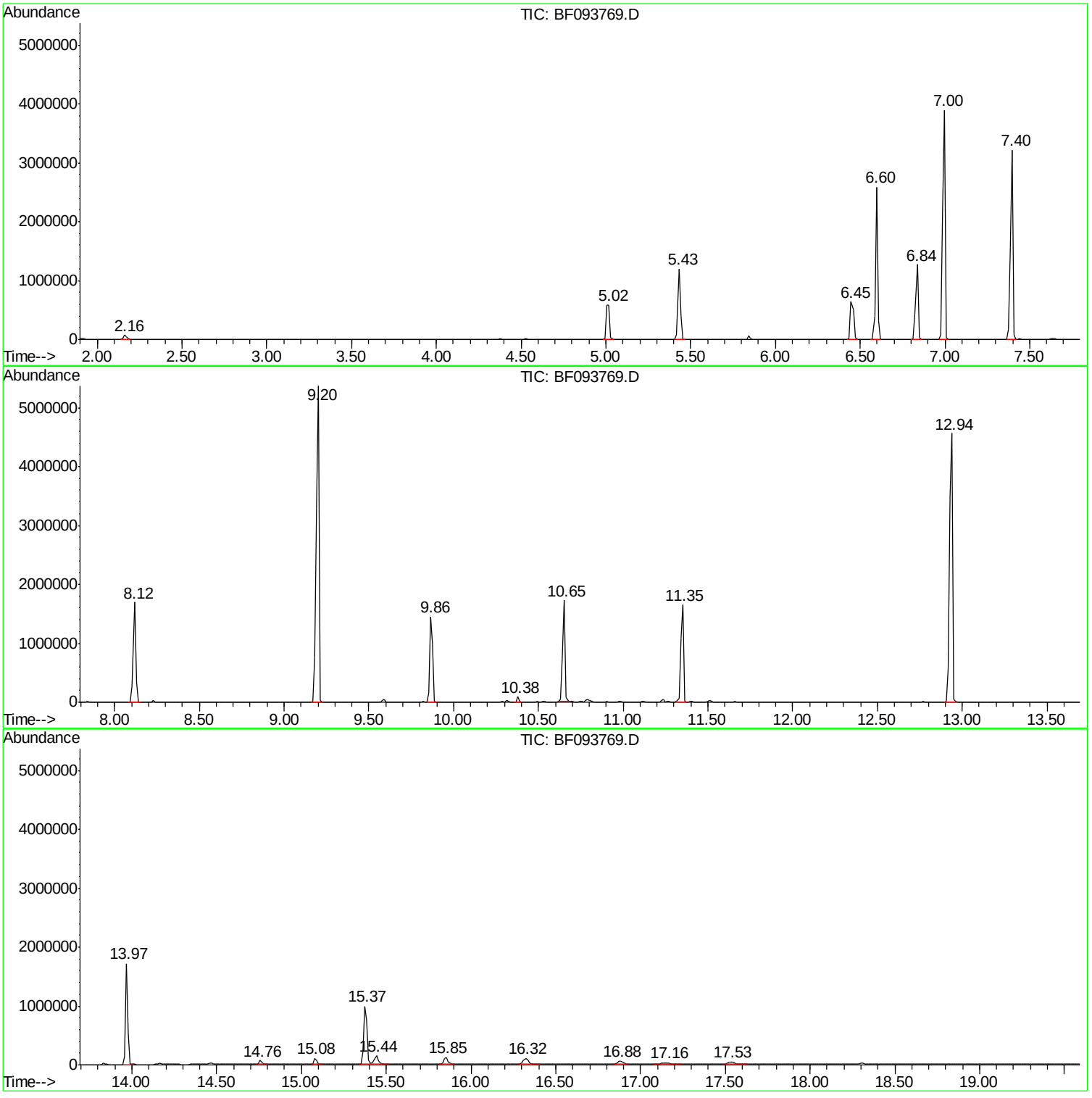
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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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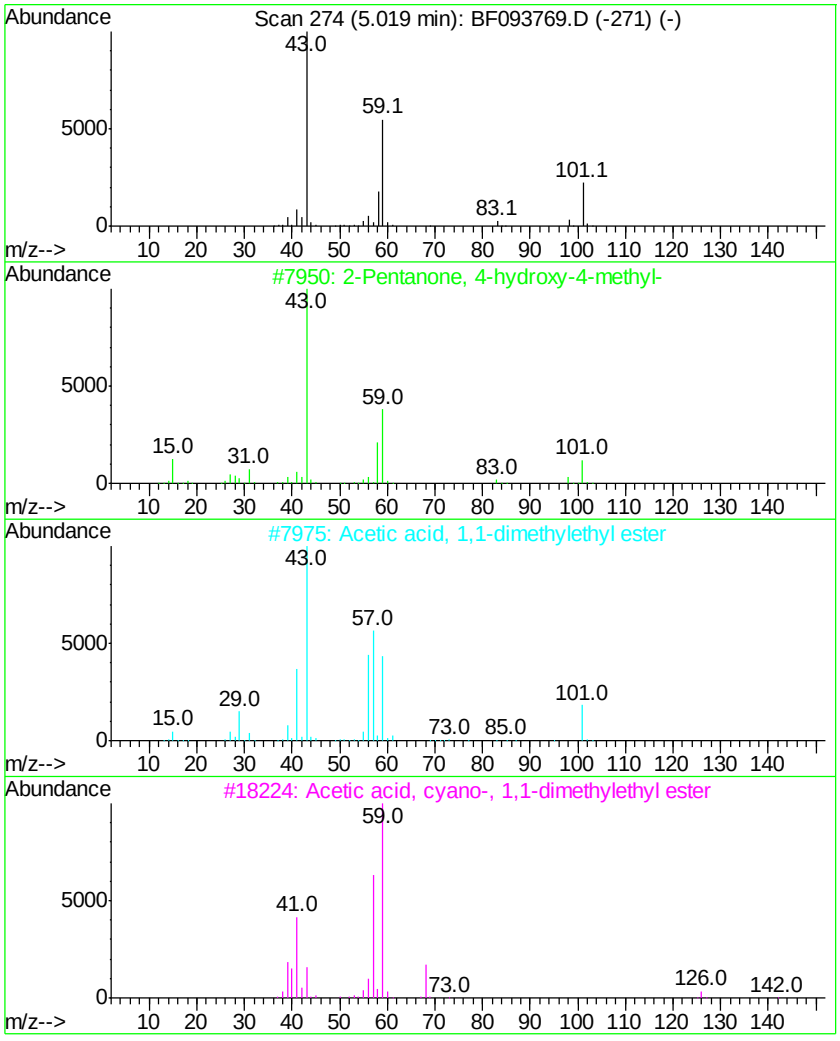
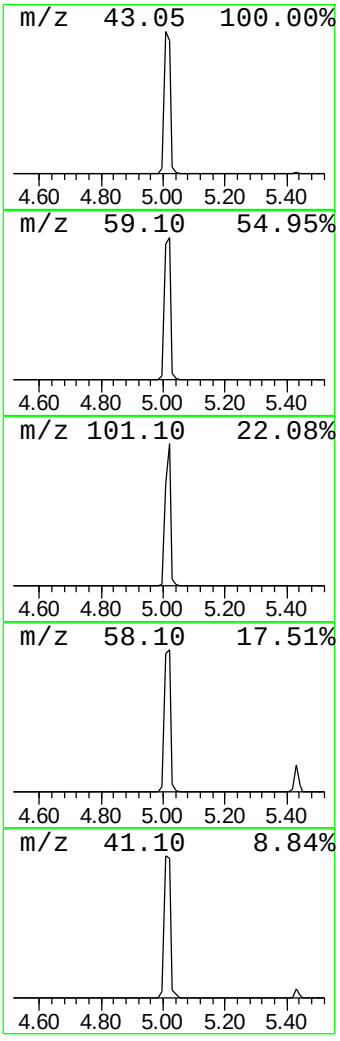
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	14.20 ng	834373	1,4-Dichlorobenzene-d4	6.84

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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
Data File : BF093769.D
Acq On : 20 Mar 2017 17:35
Operator : SJ/MA
Sample : I2263-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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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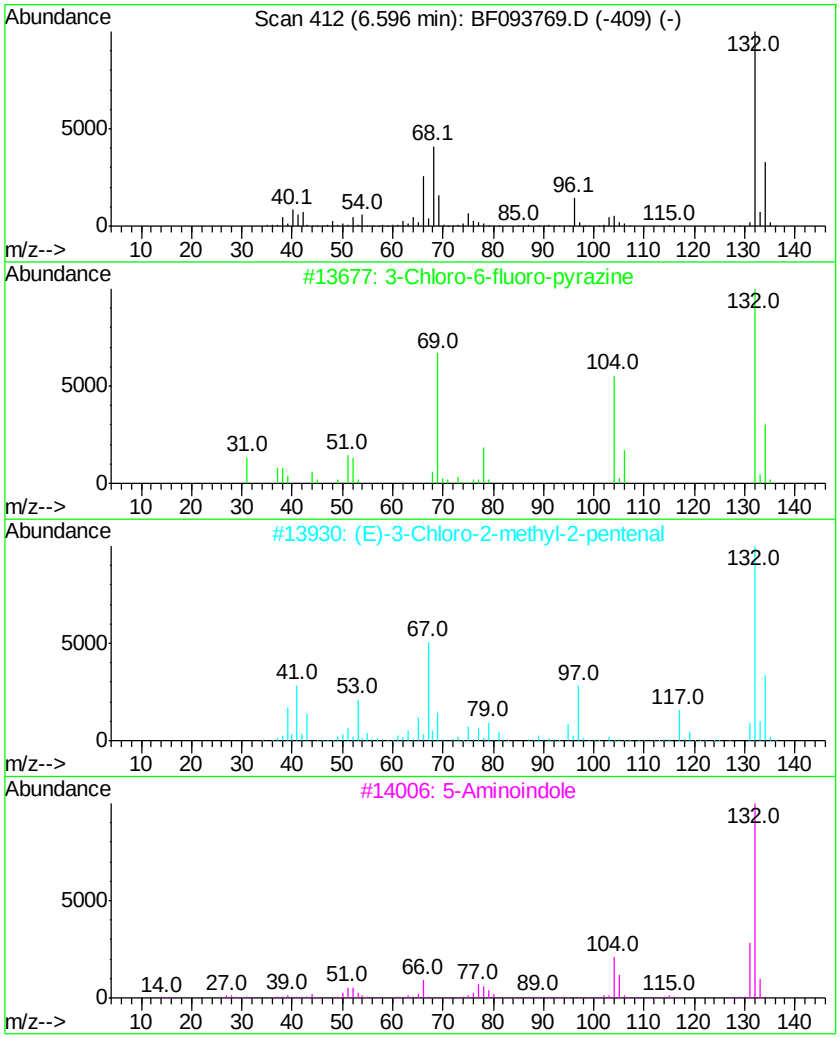
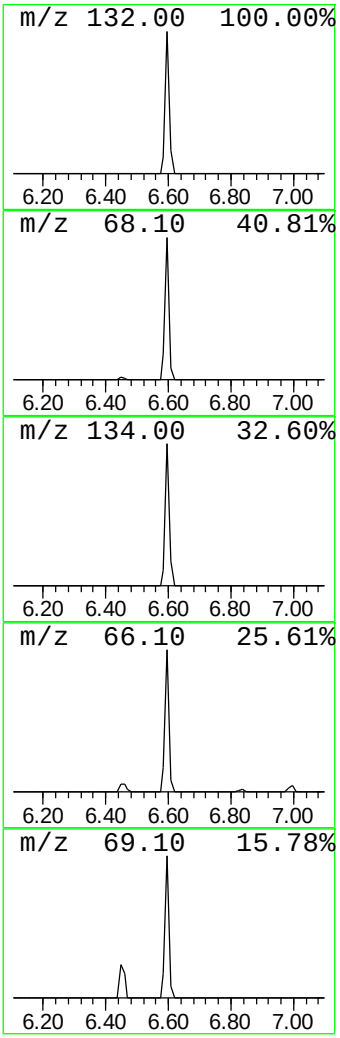
Peak Number 2 unknown6.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	38.46 ng	2260910	1,4-Dichlorobenzene-d4	6.84

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : I2263-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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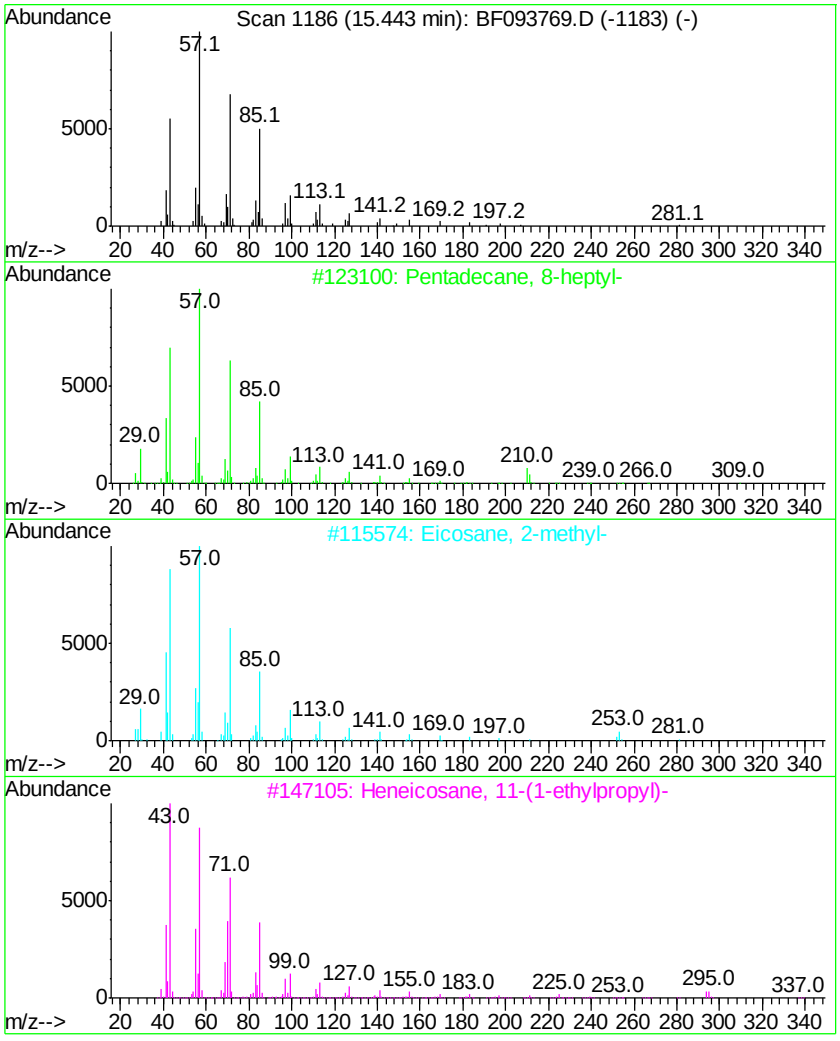
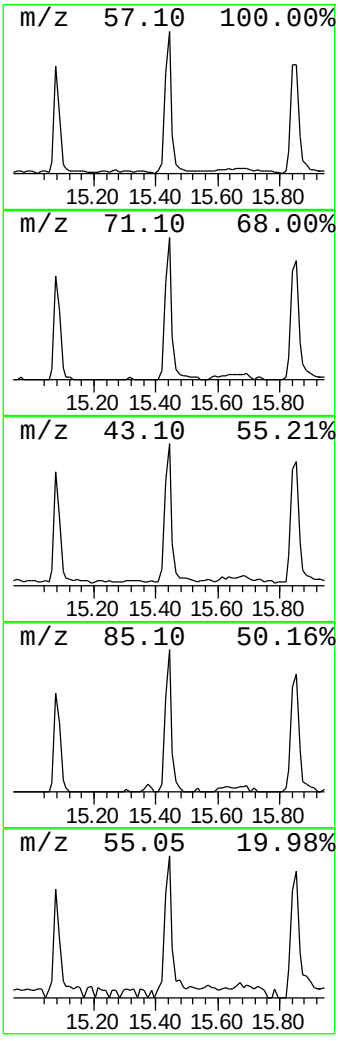
Peak Number 4 Pentadecane, 8-heptyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	3.05 ng	209703	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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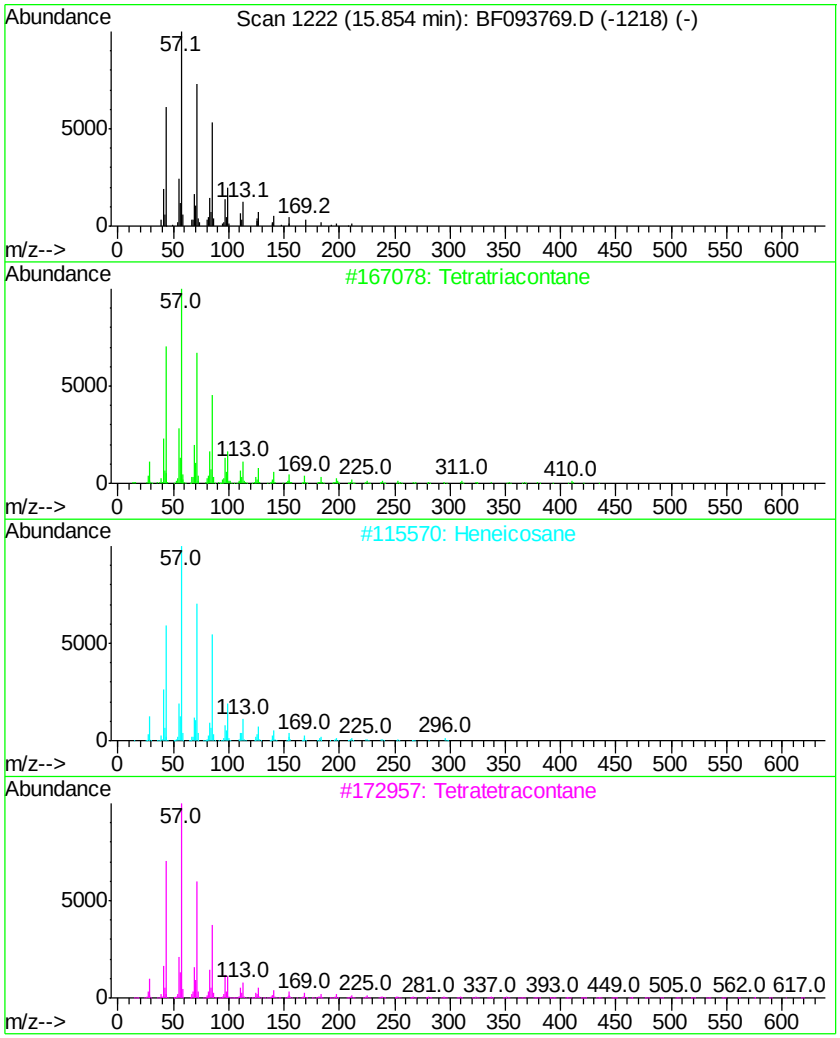
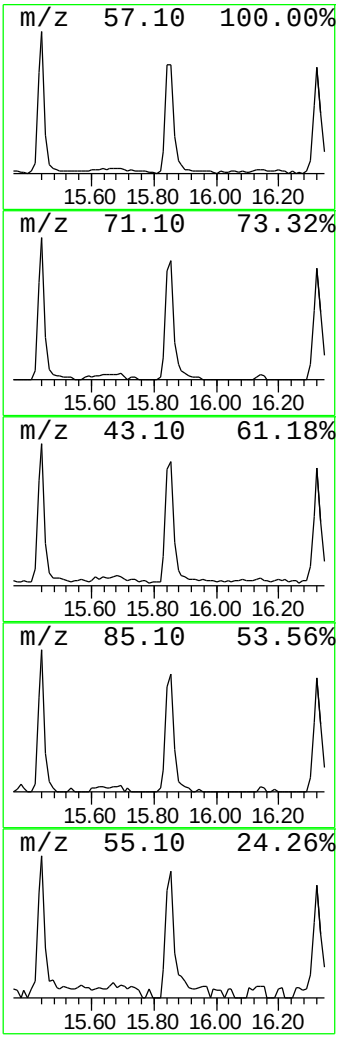
Peak Number 5 Tetratriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	3.00 ng	206087	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Octacosane	394	C28H58	000630-02-4	91





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Operator : SJ/MA
Sample : I2263-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105I

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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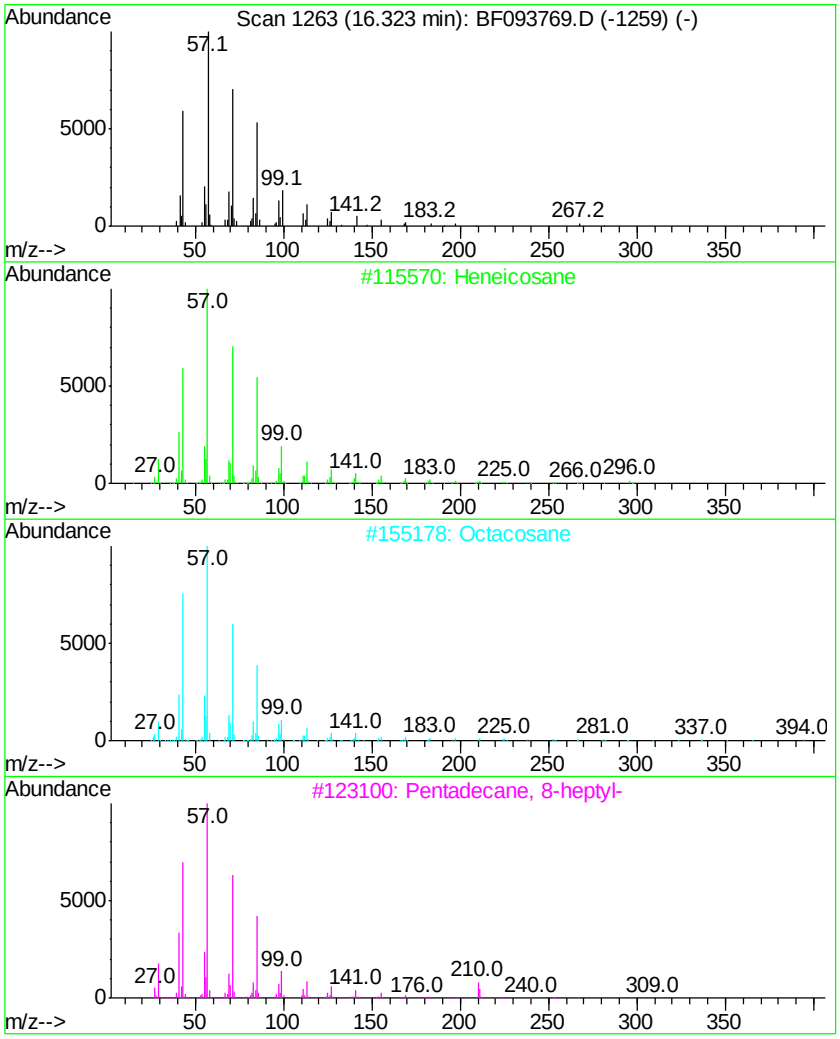
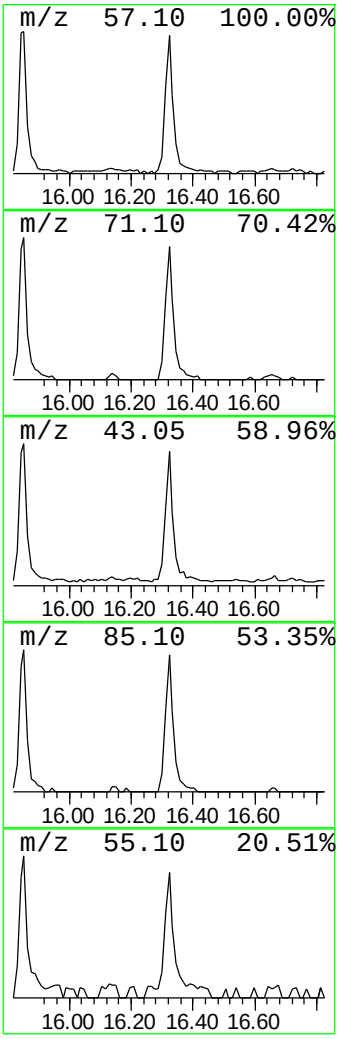
Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	2.97 ng	203760	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4	Hexadecane	226	C16H34	000544-76-3	87
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86





Tentatively Identified Compound (LSC) summary

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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...	5.02	14.2	ng	834373	1	6.84	1175590	20.0
unknown6.60	6.60	38.5	ng	2260910	1	6.84	1175590	20.0
Pentadecane, 8-he...	15.44	3.0	ng	209703	6	15.37	1372860	20.0
Tetratriacontane	15.85	3.0	ng	206087	6	15.37	1372860	20.0
Heneicosane	16.32	3.0	ng	203760	6	15.37	1372860	20.0