LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FLATBUSHFB-2-10317

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	2.035	9	13	32	rVB4	23345	184263	2.67%	0.363%
2	4.093	191	193	197	rBV	61088	95424	1.38%	0.188%
3	4.801	253	255	264	rBV	815051	1065764	15.47%	2.100%
4	5.258	293	295	298	rBV	2665687	3200293	46.45%	6.307%
5	6.321	385	388	390	rBV	2288818	2189785	31.78%	4.315%
6	6.436	395	398	400	rBV	5896119	5945681	86.29%	11.717%
7	6.653	415	417	420	rBV	1048993	1372001	19.91%	2.704%
8	6.813	428	431	434	rBV	4773355	5490175	79.68%	10.820%
9	7.236	464	468	470	rBV	4090495	5314848	77.14%	10.474%
10	7.944	527	530	533	rBV	2252564	2059628	29.89%	4.059%
11	9.030	621	625	627	rBV	6099556	6890198	100.00%	13.579%
12	9.693	680	683	686	rBV	1810904	1602299	23.25%	3.158%
13	10.482	749	752	755	rBV	3167840	3669822	53.26%	7.232%
14	11.168	810	812	815	rBV	1426311	1514844	21.99%	2.985%
15	12.768	948	952	954	rBV	4874325	6364623	92.37%	12.543%
16	13.796	1040	1042	1045	rBV	1258175	1330113	19.30%	2.621%
17	14.882	1135	1137	1140	rBV	75114	76064	1.10%	0.150%
18	15.168	1159	1162	1165	rBV	809515	1138509	16.52%	2.244%
19	15.214	1165	1166	1169	rVB	126728	131671	1.91%	0.259%
20	15.591	1196	1199	1204	rBV	143162	197733	2.87%	0.390%
21	16.025	1234	1237	1243	rVB	140515	263899	3.83%	0.520%
22	16.540	1278	1282	1286	rBV	98760	209881	3.05%	0.414%
23	17.134	1330	1334	1340	rVB	80336	196621	2.85%	0.387%
24	17.831	1391	1395	1400	rVB	45513	128789	1.87%	0.254%
25	18.677	1464	1469	1474	rBV2	32985	109546	1.59%	0.216%

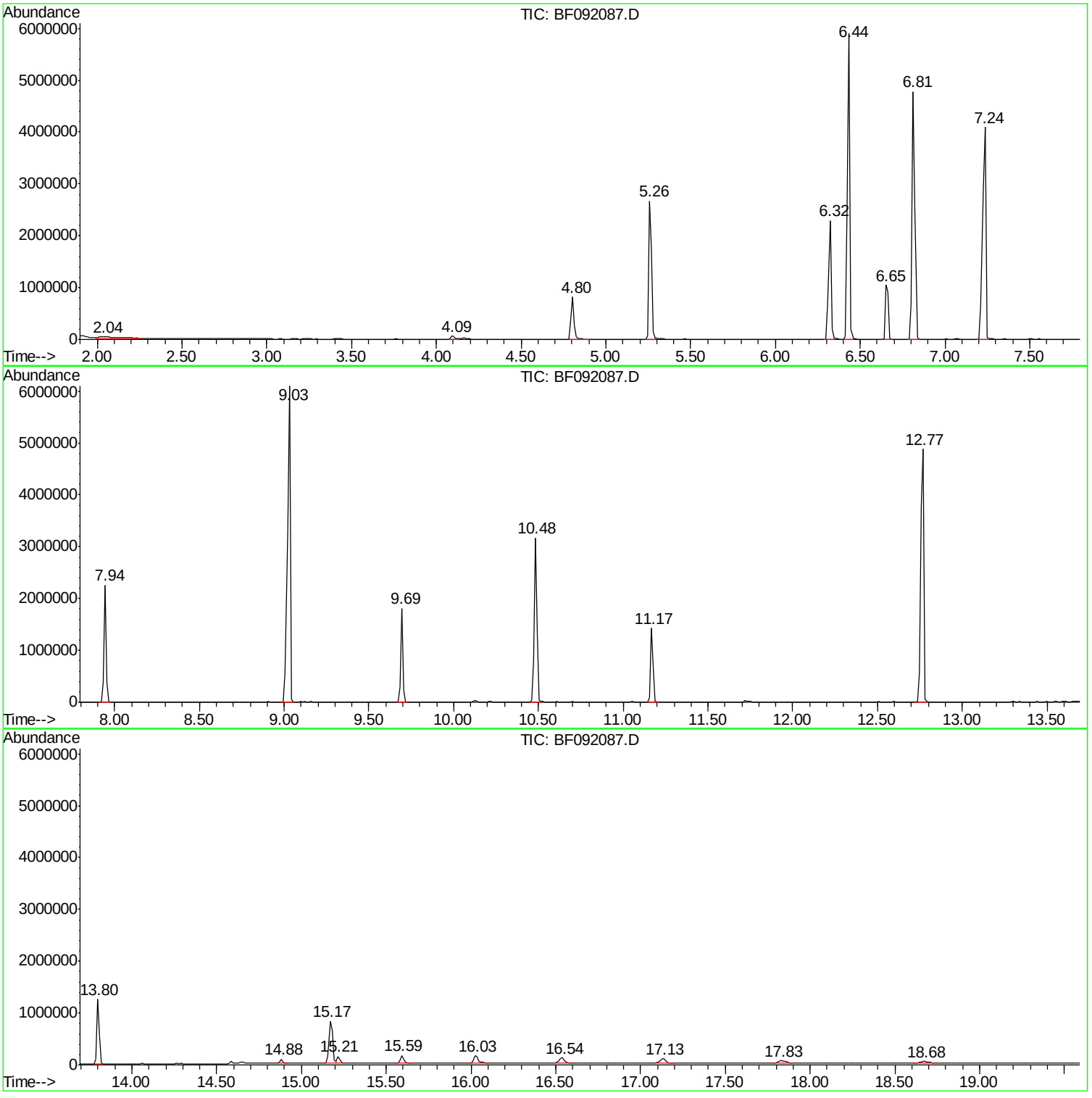
Sum of corrected areas: 50742474

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FLATBUSHFB-2-10317

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FLATBUSHFB-2-10317

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

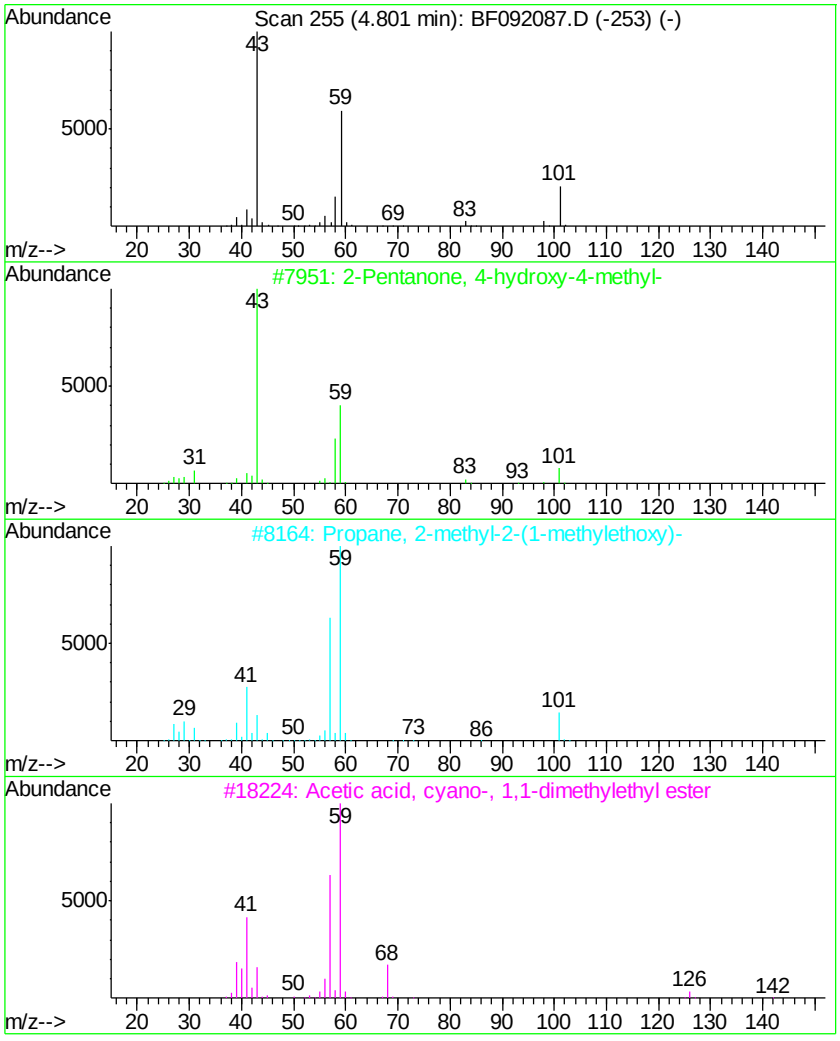
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

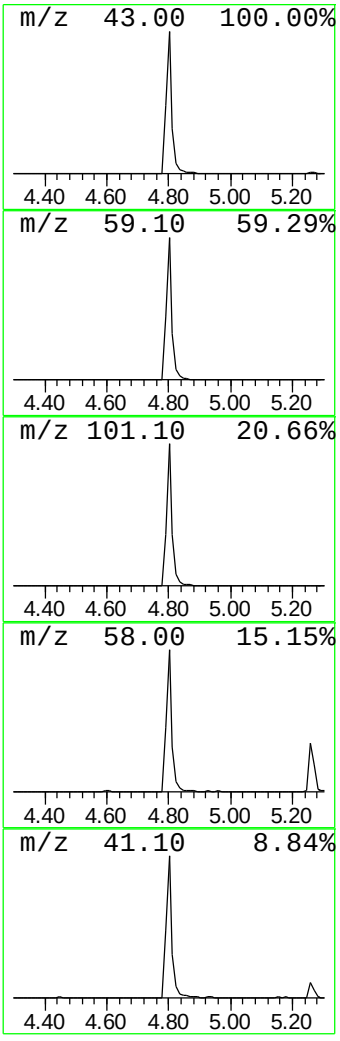
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	15.54 ng	1065760	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FLATBUSHFB-2-10317

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

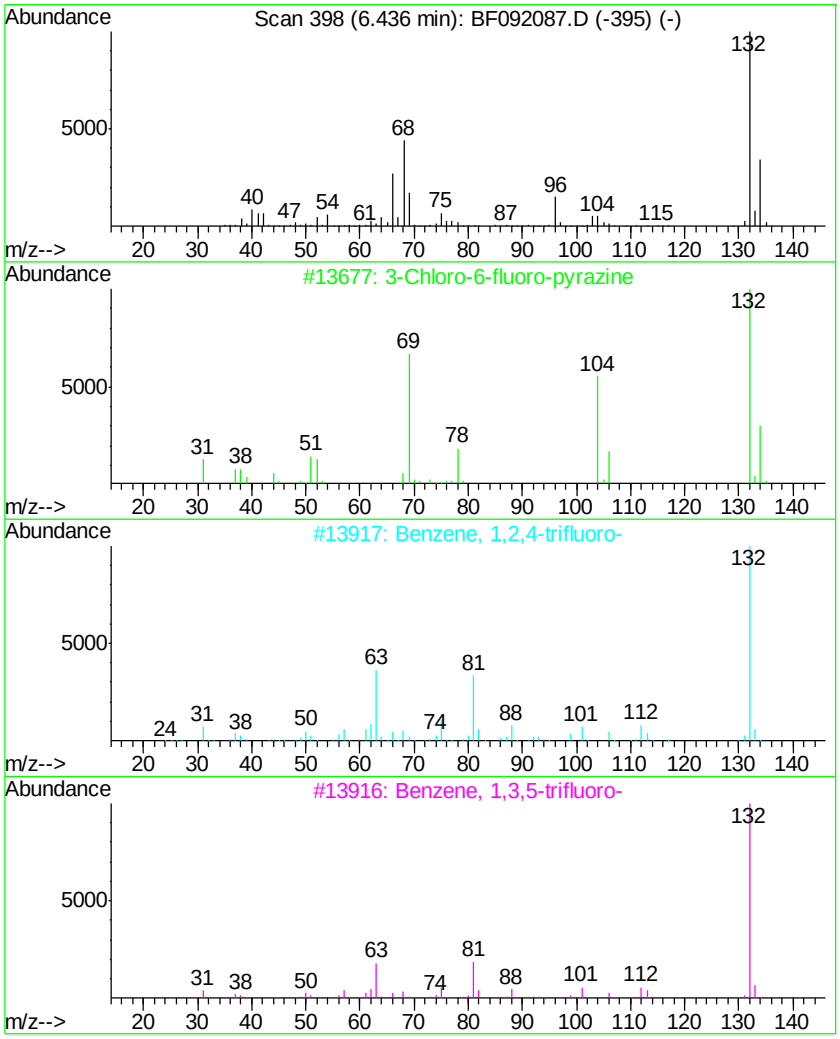
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

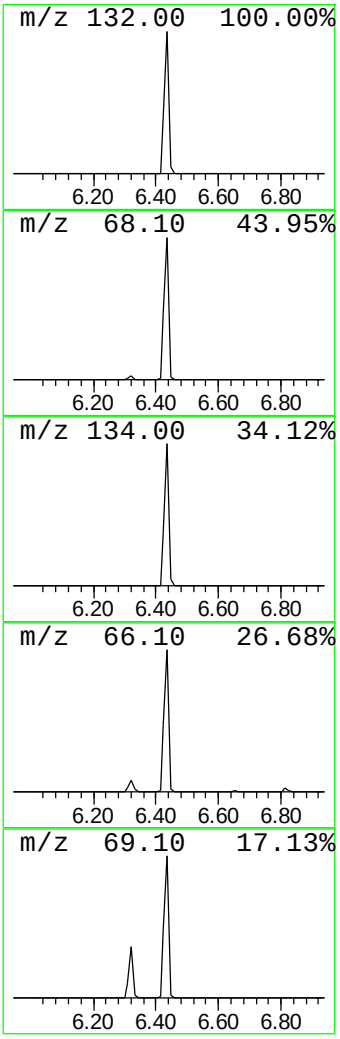
****

Peak Number 3 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	86.67 ng	5945680	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FLATBUSHFB-2-10317

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

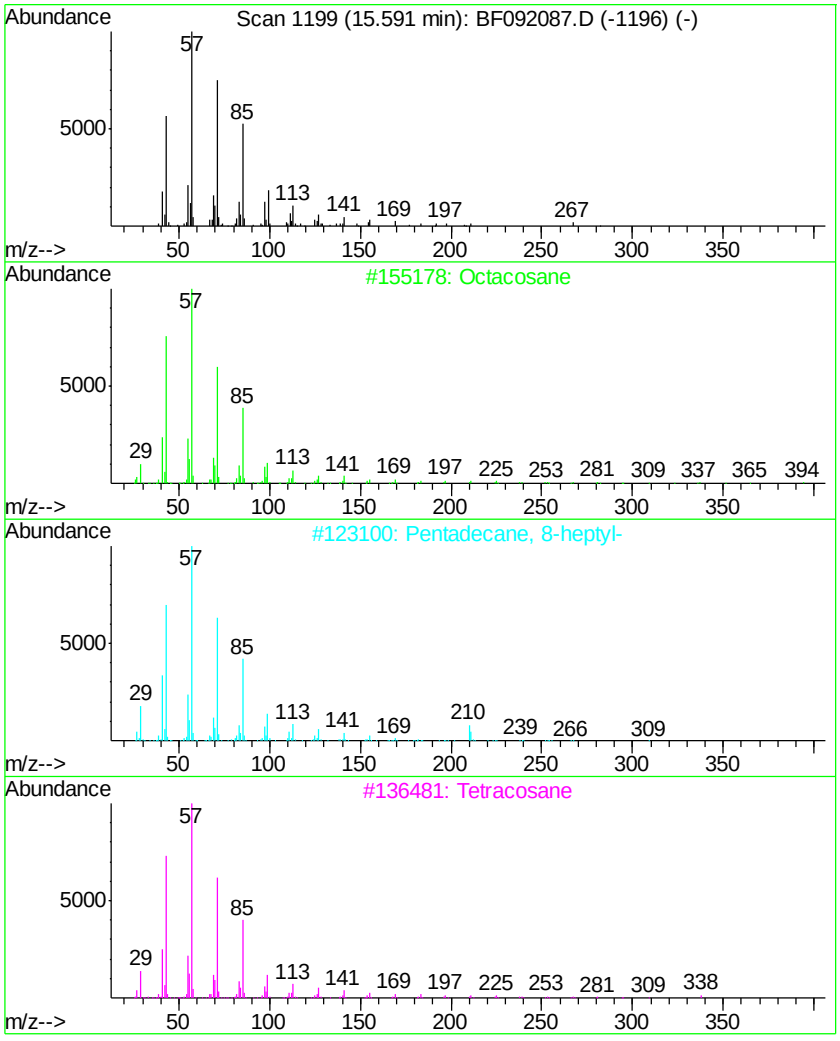
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

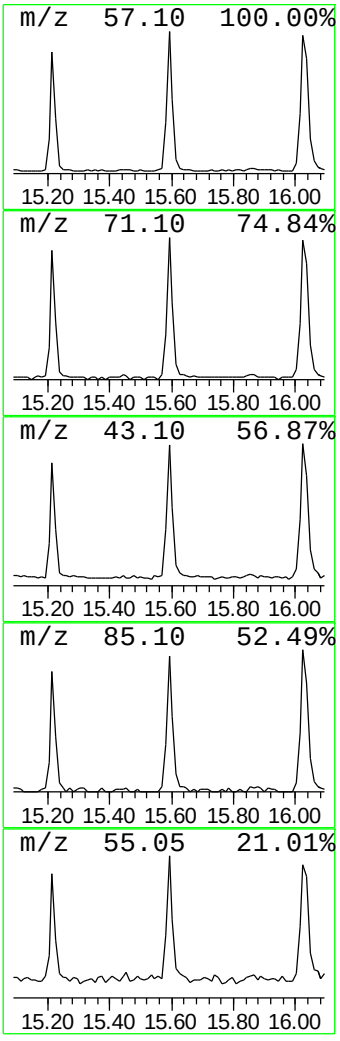
****

Peak Number 5 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	3.47 ng	197733	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FLATBUSHFB-2-10317

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

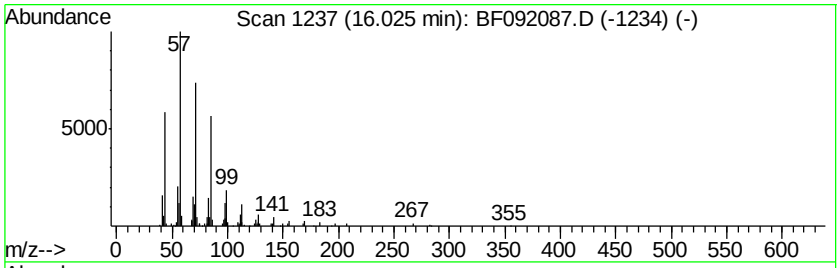
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

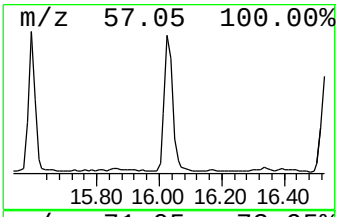
****

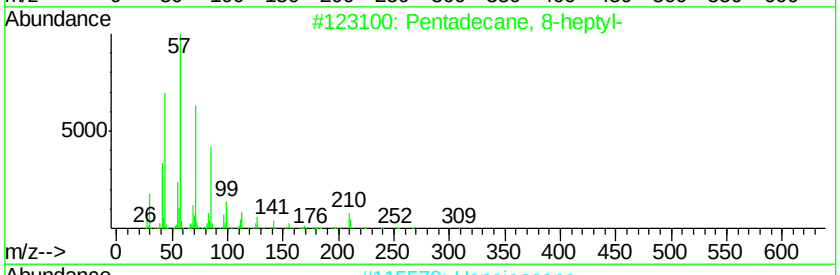
Peak Number 6 Pentadecane, 8-heptyl- Concentration Rank 4

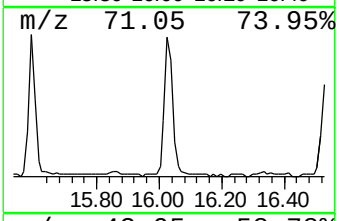
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	4.64 ng	263899	Perylene-d12	15.17

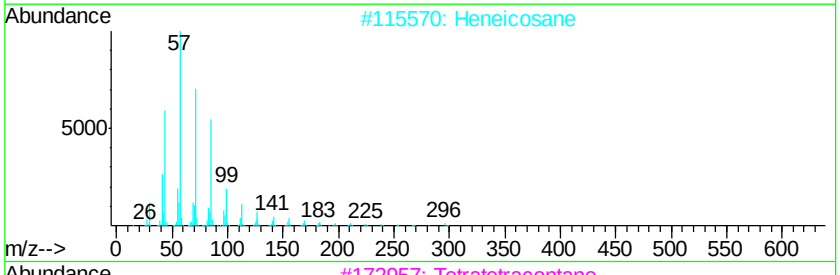
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5	Hexatriacontane	507	C36H74	000630-06-8	86

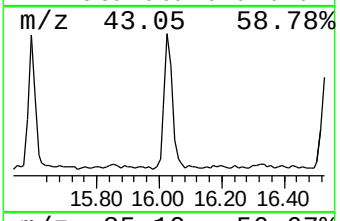


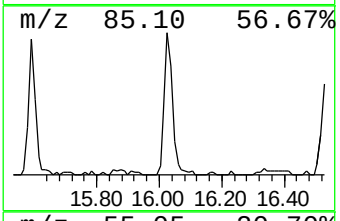


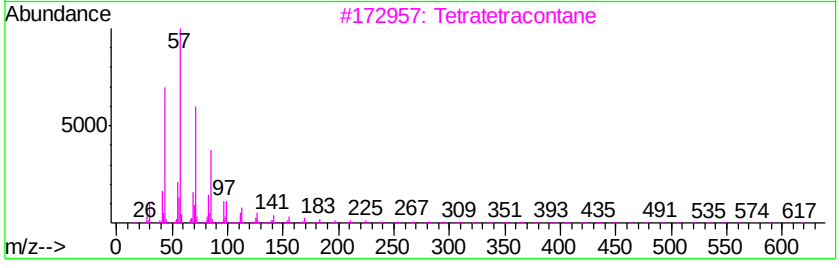


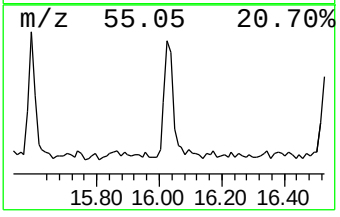












Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FLATBUSHFB-2-10317

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

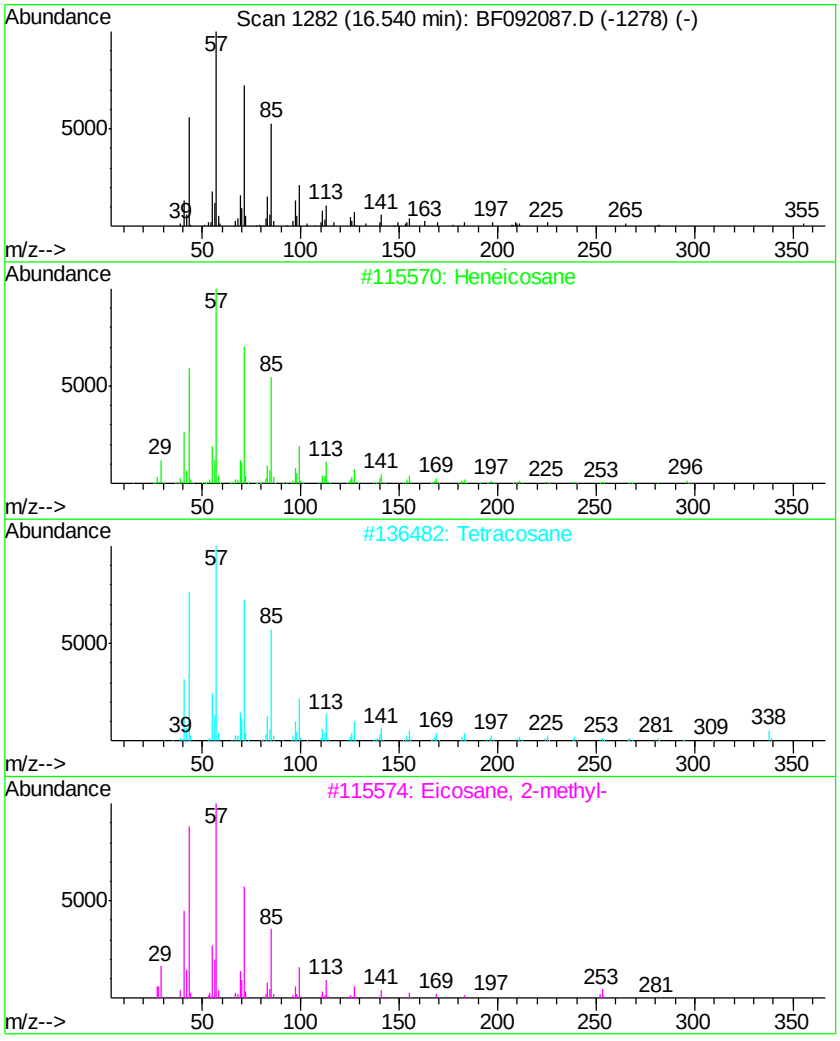
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

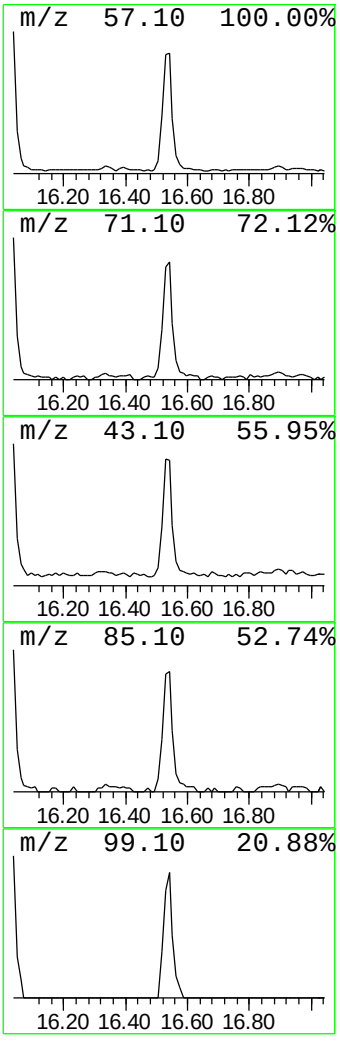
****

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	3.69 ng	209881	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FLATBUSHFB-2-10317

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

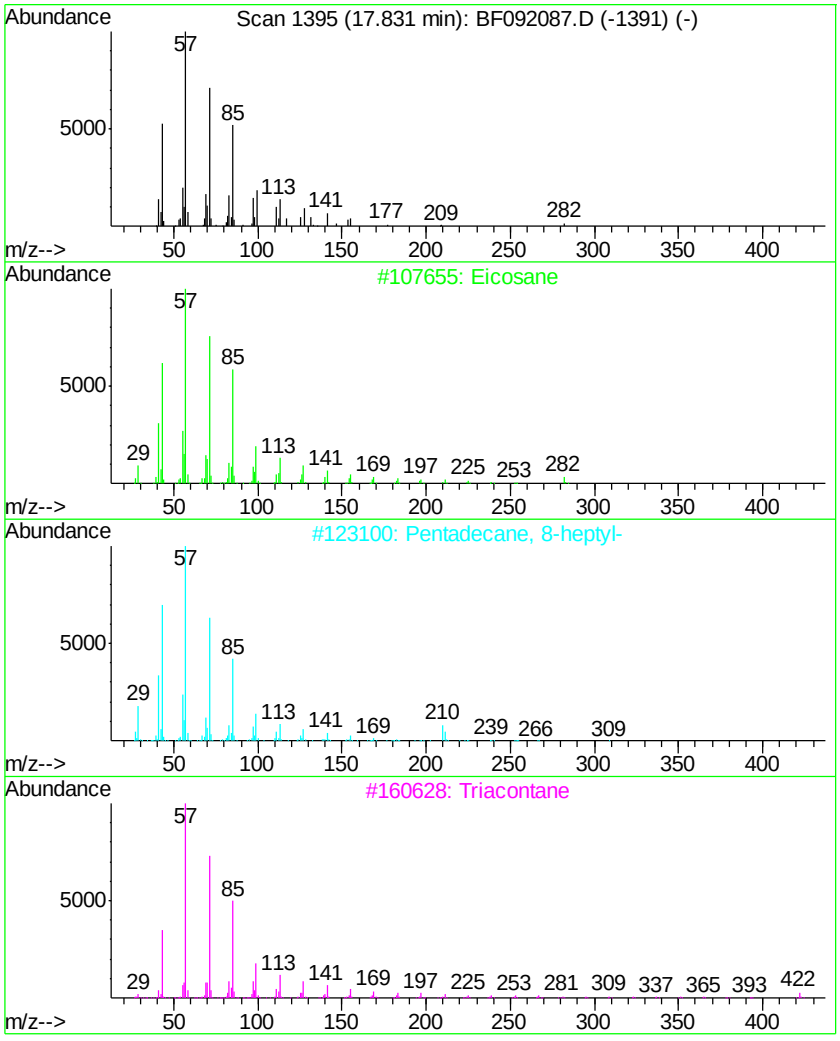
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

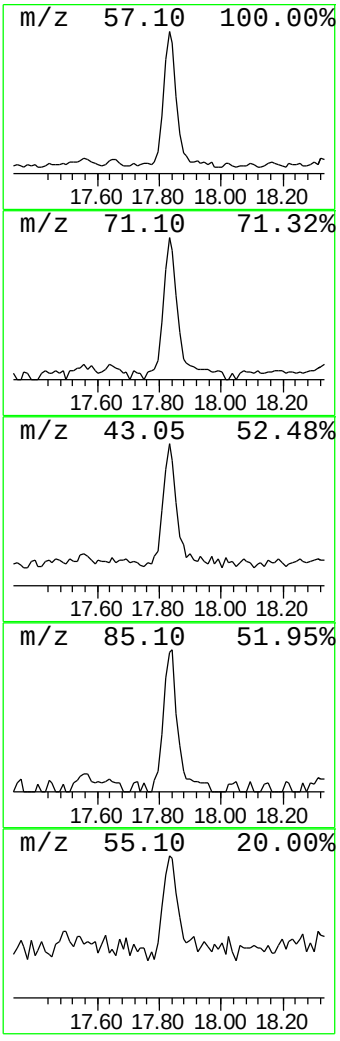
****

Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	2.26 ng	128789	Perylene-d12	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
3	Triacontane	422	C30H62	000638-68-6	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	Hexatriacontane	507	C36H74	000630-06-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010417\
Data File : BF092087.D
Acq On : 5 Jan 2017 00:09
Operator : UM/SJ
Sample : I1004-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FLATBUSHFB-2-10317

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...	4.80	15.5	ng	1065760	1	6.66	1372000	20.0
unknown6.44	6.44	86.7	ng	5945680	1	6.66	1372000	20.0
Octacosane	15.59	3.5	ng	197733	6	15.17	1138510	20.0
Pentadecane, 8-he...	16.03	4.6	ng	263899	6	15.17	1138510	20.0
Heneicosane	16.54	3.7	ng	209881	6	15.17	1138510	20.0
Eicosane	17.83	2.3	ng	128789	6	15.17	1138510	20.0