LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087265.D
Acq On : 21 May 2016 11:33
Operator : UM/SJ
Sample : H3154-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-01-0-2

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-BF051716.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	1.701	8	10	50	rVB	2380902	4744129	100.00%	10.958%
2	4.684	270	271	287	rBV	217275	546939	11.53%	1.263%
3	5.141	309	311	334	rBV	3475955	4035669	85.07%	9.322%
4	6.227	403	406	413	rBV	3809687	4256104	89.71%	9.831%
5	6.330	413	415	417	rBV	4564606	4454965	93.90%	10.290%
6	6.559	433	435	443	rVB	678405	860218	18.13%	1.987%
7	6.707	446	448	451	rBV	3087035	2921231	61.58%	6.747%
8	7.130	483	485	488	rBV	2311816	2605602	54.92%	6.018%
9	7.839	545	547	550	rBV	985187	1138849	24.01%	2.631%
10	8.925	639	642	644	rBV	4461114	4525444	95.39%	10.453%
11	9.027	648	651	657	rVB3	44560	69914	1.47%	0.161%
12	9.325	675	677	681	rBV	709906	620684	13.08%	1.434%
13	9.530	694	695	697	rBV	57041	56612	1.19%	0.131%
14	9.588	697	700	704	rBV	1459558	1411323	29.75%	3.260%
15	10.033	737	739	740	rVB	117845	98198	2.07%	0.227%
16	10.250	755	758	761	rBV	37211	58280	1.23%	0.135%
17	10.376	767	769	772	rBV	2548477	2667791	56.23%	6.162%
18	10.502	778	780	787	rVB	139564	179601	3.79%	0.415%
19	10.948	817	819	820	rBV	66084	60679	1.28%	0.140%
20	11.062	827	829	833	rVB	1306423	1237408	26.08%	2.858%
21	11.439	860	862	864	rVB	139302	112940	2.38%	0.261%
22	11.588	873	875	881	rVB2	56566	138001	2.91%	0.319%
23	11.793	891	893	895	rVB	55918	48326	1.02%	0.112%
24	11.988	909	910	913	rVB	97694	110181	2.32%	0.254%
25	12.479	951	953	956	rBV	284040	245841	5.18%	0.568%
26	12.559	958	960	962	rVB	60474	52118	1.10%	0.120%
27	12.651	965	968	970	rBV	3822859	4023633	84.81%	9.294%
28	13.176	1012	1014	1016	rBV	111955	132658	2.80%	0.306%
29	13.497	1040	1042	1045	rVB	70792	71558	1.51%	0.165%
30	13.691	1056	1059	1066	rBV	957998	961444	20.27%	2.221%
31	15.040	1175	1177	1190	rVB	545444	731601	15.42%	1.690%
32	16.731	1321	1325	1331	rBV5	26428	63391	1.34%	0.146%
33	18.308	1460	1463	1470	rVB8	16927	52600	1.11%	0.121%

LSC Area Percent Report

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Misc :
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ClientSampleId :
SED-01-0-2

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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-BF051716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

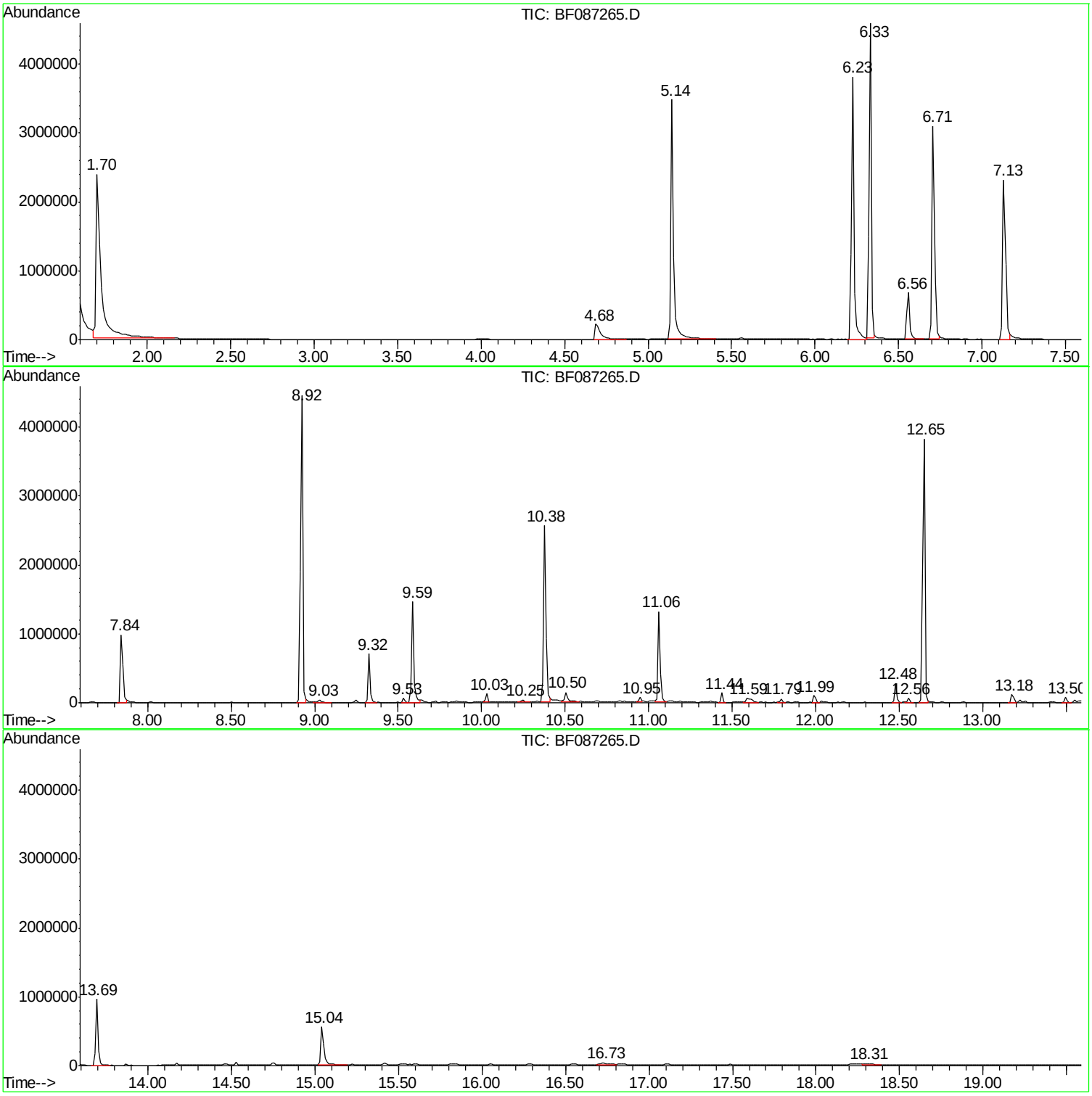
Sum of corrected areas: 43293932

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087265.D
Acq On : 21 May 2016 11:33
Operator : UM/SJ
Sample : H3154-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-01-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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

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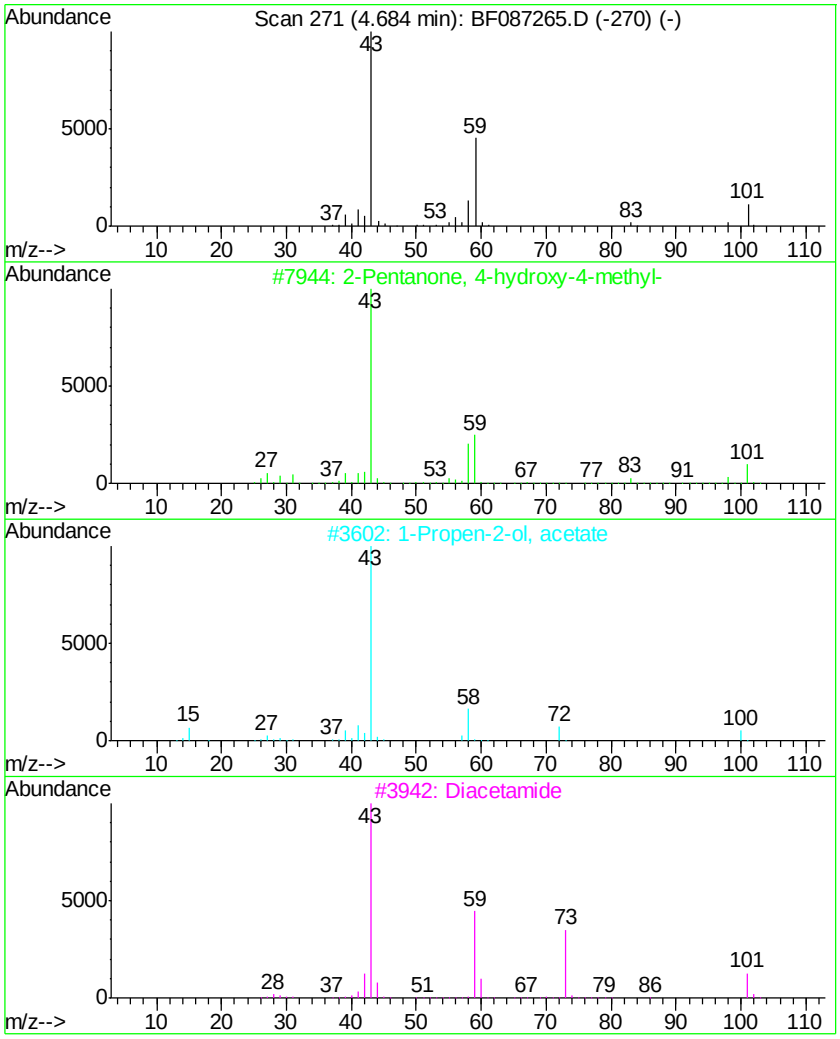
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	12.72 ng	546939	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9
5	dl-4-Amino-3-hydroxybutyric acid	119	C4H9NO3	000352-21-6	9



Library Search Compound Report

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Data File : BF087265.D
Acq On : 21 May 2016 11:33
Operator : UM/SJ
Sample : H3154-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SED-01-0-2

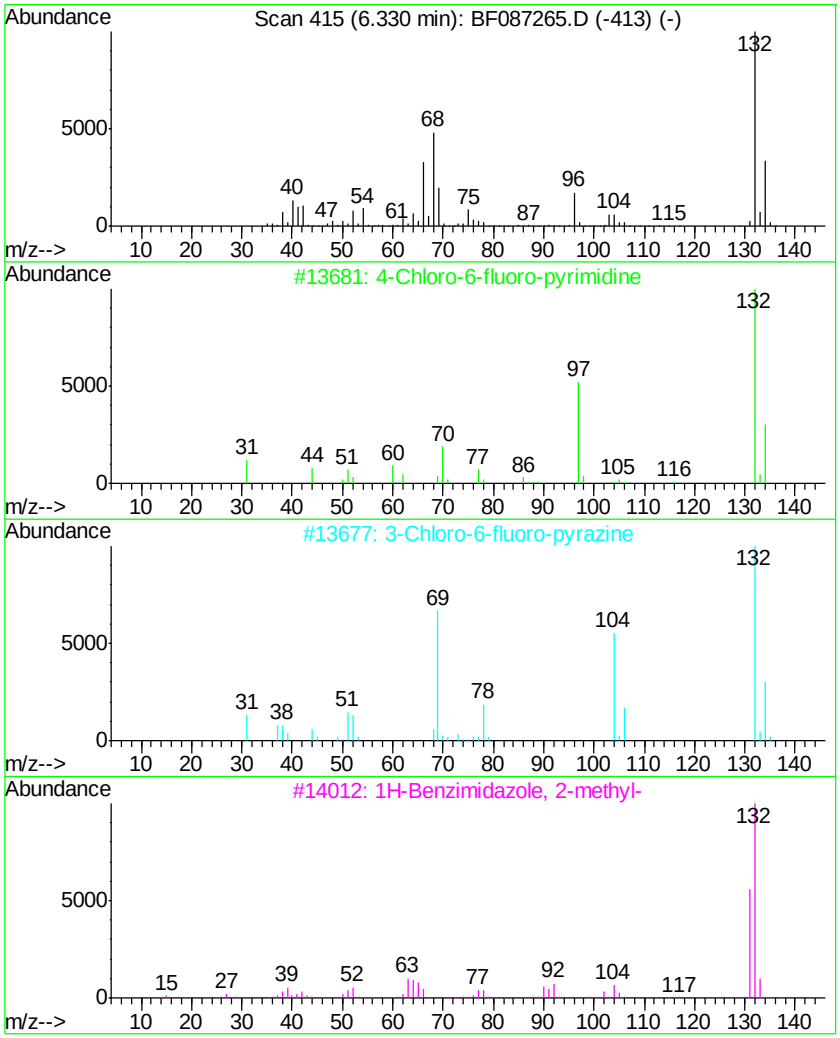
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

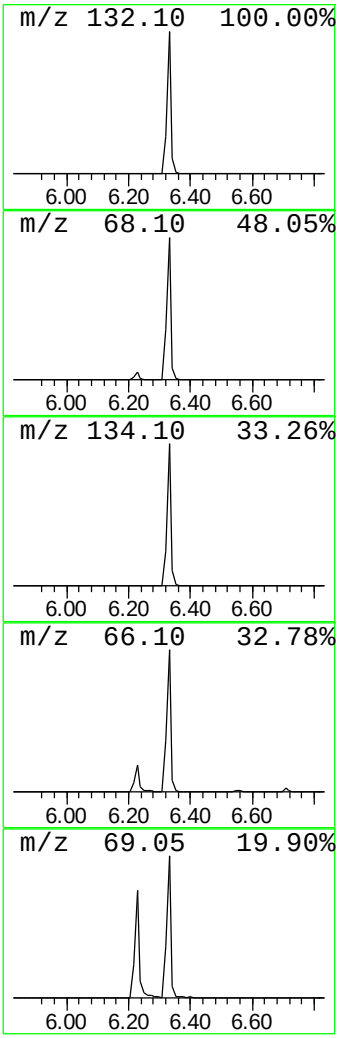
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	103.58 ng	4454970	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
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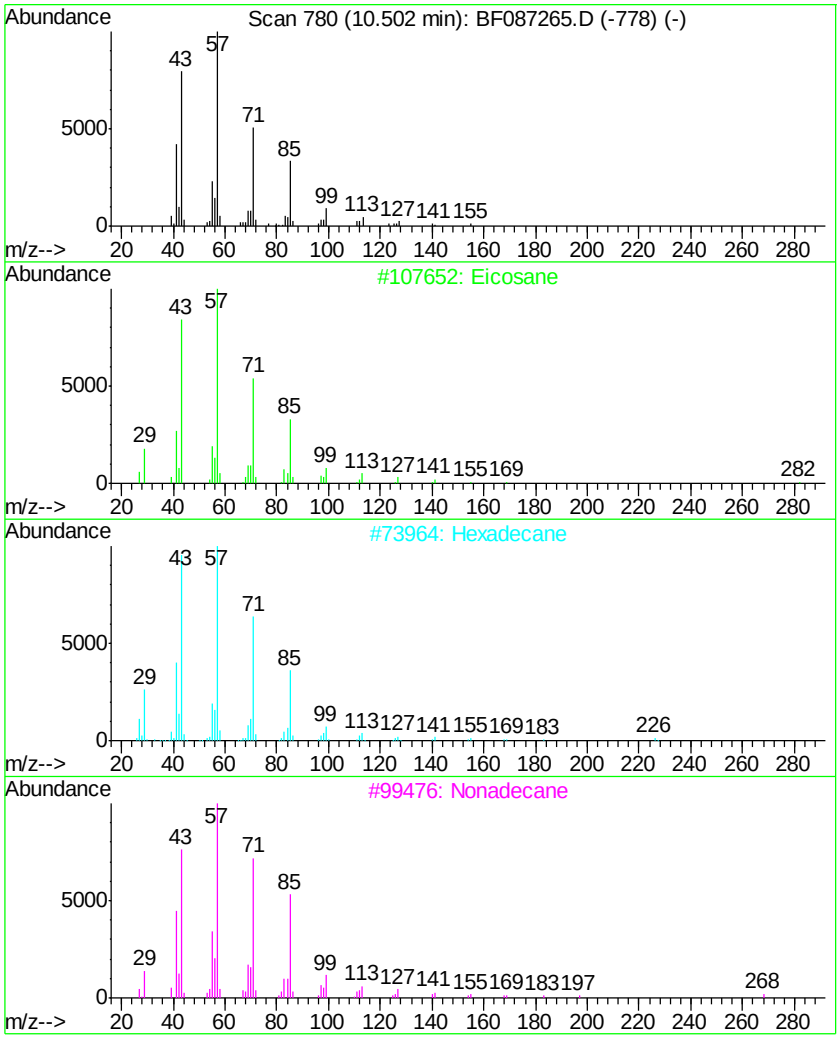
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

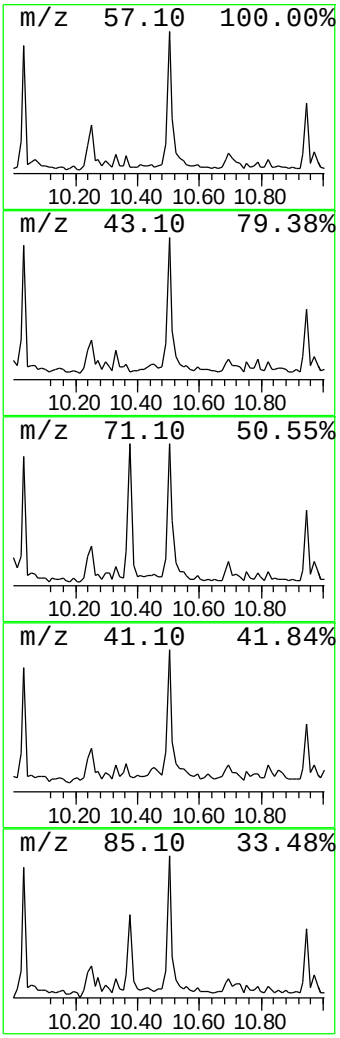
****

Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	2.90 ng	179601	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Nonadecane	268	C19H40	000629-92-5	86
4	Tridecane	184	C13H28	000629-50-5	86
5	Tetradecane	198	C14H30	000629-59-4	80





Library Search Compound Report

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SED-01-0-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

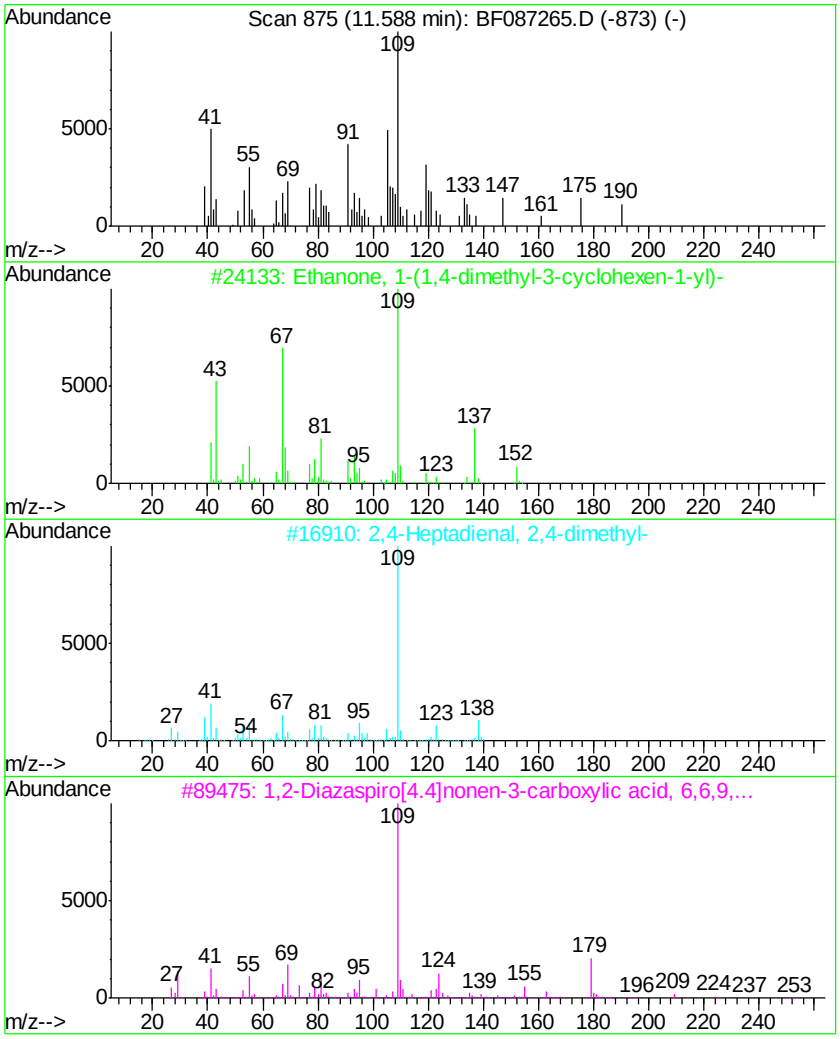
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

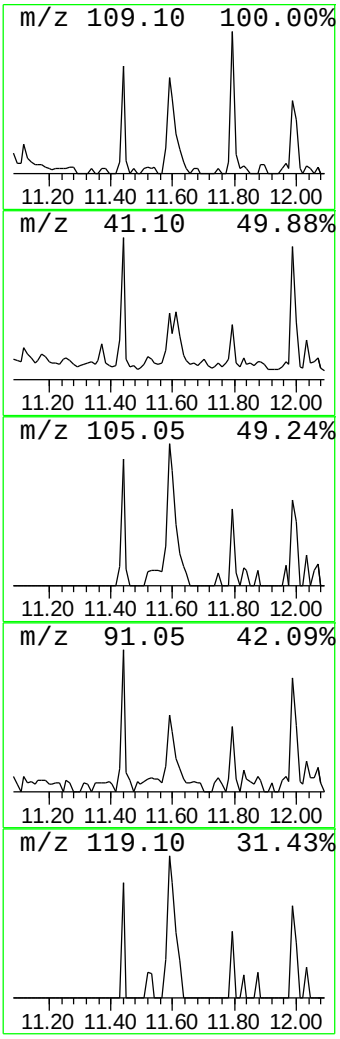
****

Peak Number 6 unknown11.59 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.23 ng	138001	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	35
2	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	27
3	1,2-Diazaspiro[4.4]nonen-3-carbo...	252	C14H24N2O2	1000164-25-9	27
4	3-Pyridinol, 6-methyl-	109	C6H7NO	001121-78-4	27
5	Pyridine, 4-methoxy-	109	C6H7NO	000620-08-6	27





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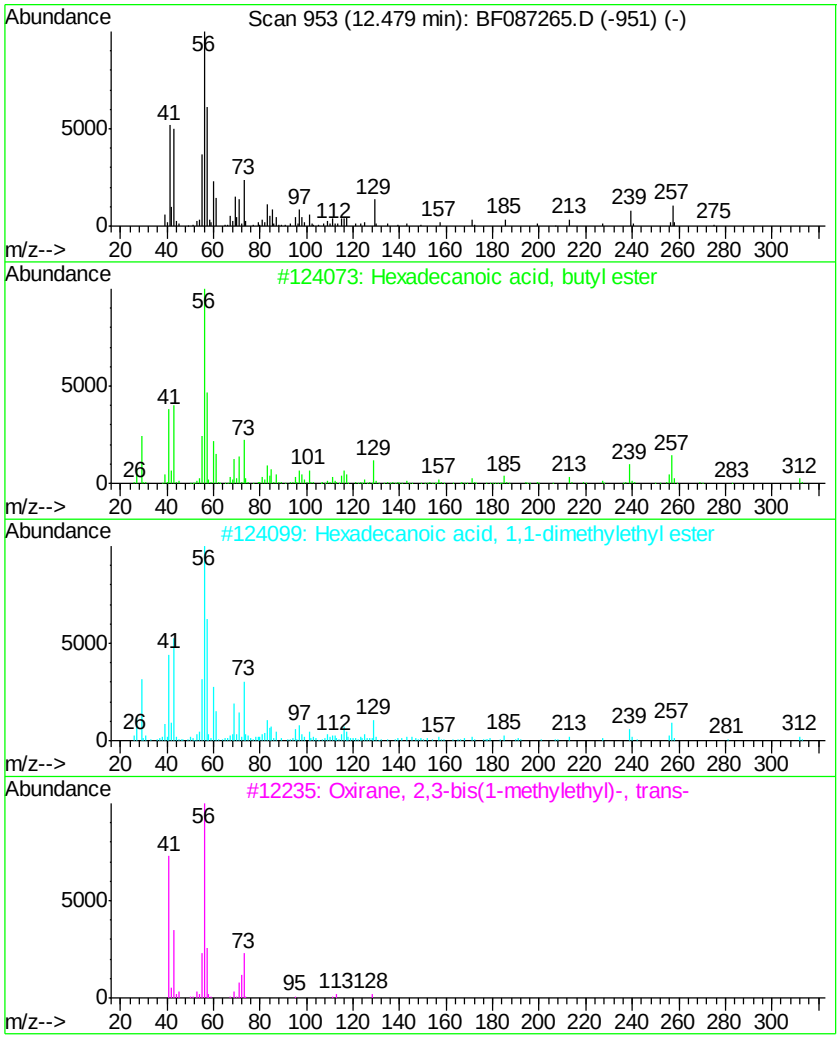
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

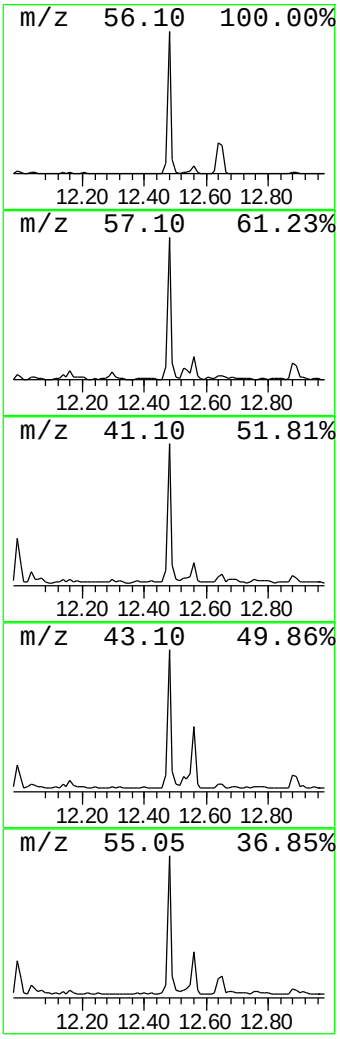
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	5.11 ng	245841	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	47
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35





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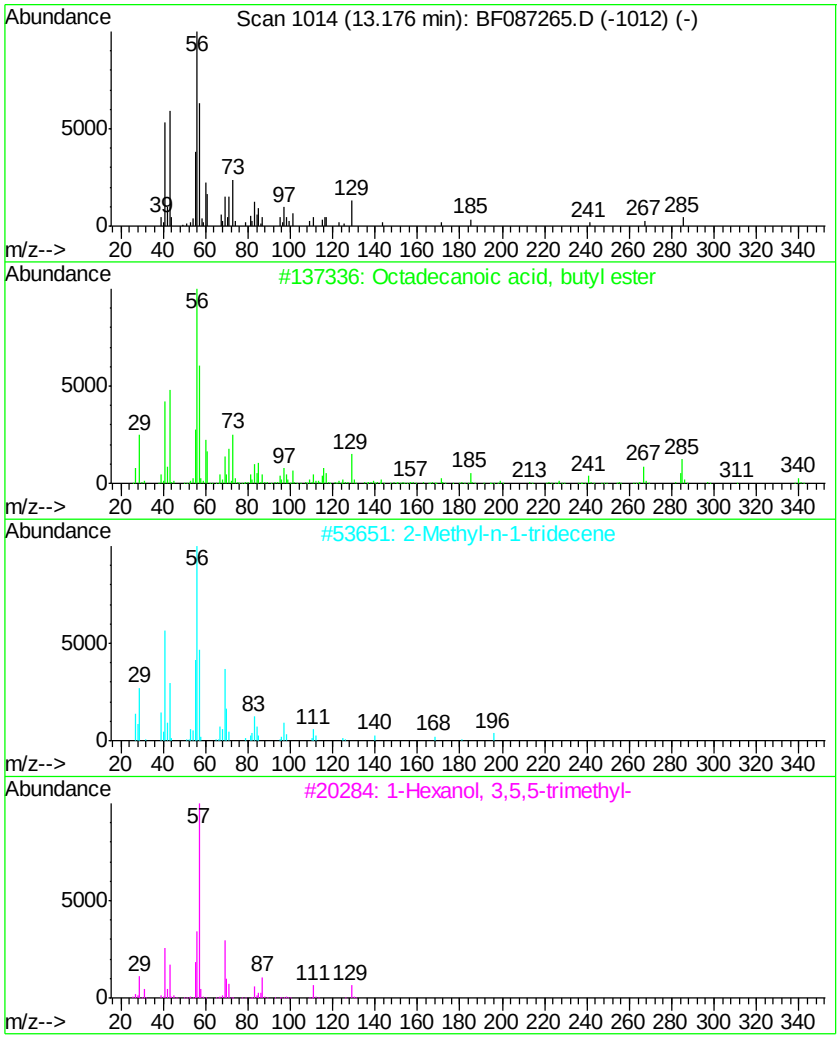
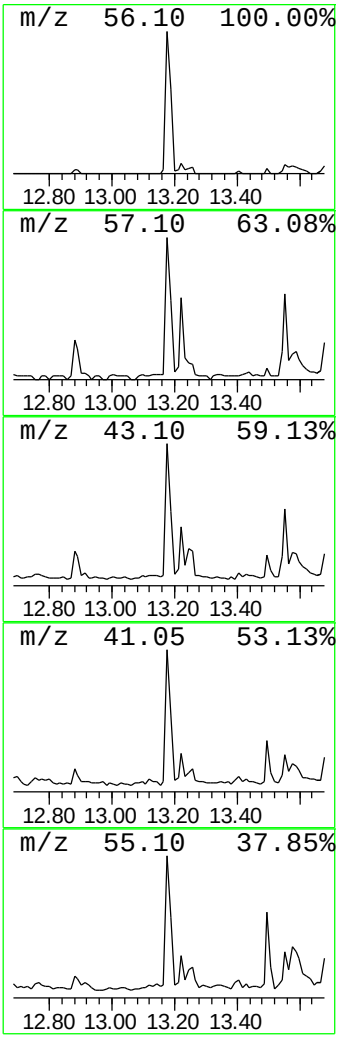
****

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	2.76 ng	132658	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
3	1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	37
4	Cyclopropane, propyl-	84	C6H12	002415-72-7	35
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	12.7	ng	546939	1	6.56	860218	20.0
unknown6.33	6.33	103.6	ng	4454970	1	6.56	860218	20.0
Eicosane	10.50	2.9	ng	179601	4	11.06	1237410	20.0
unknown11.59	11.59	2.2	ng	138001	4	11.06	1237410	20.0
Hexadecanoic acid...	12.48	5.1	ng	245841	5	13.69	961444	20.0
Octadecanoic acid...	13.18	2.8	ng	132658	5	13.69	961444	20.0