LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085900.D
Acq On : 30 Mar 2016 21:46
Operator : UM/SJ
Sample : H2023-06
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6

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-BF032416.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	4.984	234	236	250	rVB	78211	122388	3.58%	0.458%
2	5.396	269	272	275	rBV	2476497	2638825	77.18%	9.871%
3	6.436	360	363	366	rBV	2122467	2824374	82.61%	10.565%
4	6.562	372	374	377	rBV	2271747	2951973	86.34%	11.042%
5	6.802	393	395	397	rBV	483805	648916	18.98%	2.427%
6	6.950	406	408	411	rBV	2199504	2223798	65.04%	8.318%
7	7.362	441	444	447	rBV	1491094	1894541	55.41%	7.087%
8	8.082	505	507	510	rBV	1029820	888209	25.98%	3.322%
9	9.168	599	602	604	rBV	2813821	3418919	100.00%	12.789%
10	9.556	634	636	638	rBV	620492	507794	14.85%	1.899%
11	9.773	653	655	657	rBV	129014	109392	3.20%	0.409%
12	9.842	658	661	663	rVB	774004	899687	26.31%	3.365%
13	10.002	672	675	679	rBV2	24143	53077	1.55%	0.199%
14	10.276	697	699	700	rVB	95654	123893	3.62%	0.463%
15	10.493	715	718	721	rBV	44975	79073	2.31%	0.296%
16	10.631	727	730	732	rBV	1711504	1834056	53.64%	6.861%
17	10.745	738	740	744	rBV	135035	166702	4.88%	0.624%
18	10.939	755	757	761	rVB2	16407	35398	1.04%	0.132%
19	11.191	777	779	780	rBV	64713	55808	1.63%	0.209%
20	11.316	788	790	793	rBV	831478	807543	23.62%	3.021%
21	11.853	834	837	847	rBV	45902	66625	1.95%	0.249%
22	12.905	926	929	931	rBV	2602919	2360618	69.05%	8.830%
23	13.808	1005	1008	1016	rBV	50852	97688	2.86%	0.365%
24	13.957	1018	1021	1023	rBV	671633	614626	17.98%	2.299%
25	14.699	1084	1086	1090	rBV	161183	183188	5.36%	0.685%
26	15.374	1142	1145	1150	rBV	455862	616537	18.03%	2.306%
27	16.837	1271	1273	1279	rVB2	21880	41059	1.20%	0.154%
28	17.283	1308	1312	1320	rVB8	15651	48434	1.42%	0.181%
29	18.208	1389	1393	1398	rVB2	19263	53827	1.57%	0.201%
30	19.020	1459	1464	1469	rBV4	32588	138137	4.04%	0.517%
31	19.180	1473	1478	1484	rVB3	72611	228156	6.67%	0.853%

Sum of corrected areas: 26733261

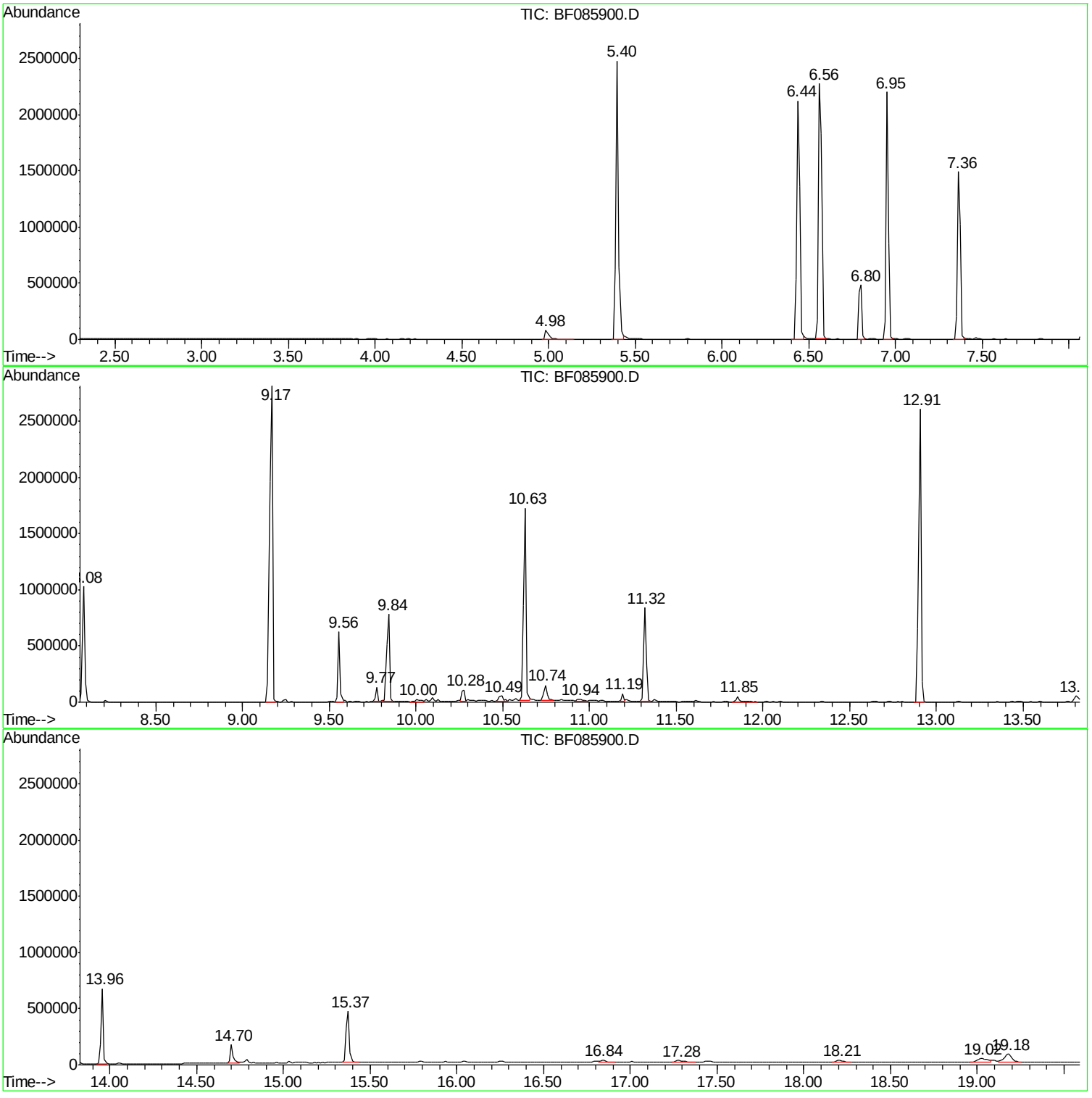
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085900.D
Acq On : 30 Mar 2016 21:46
Operator : UM/SJ
Sample : H2023-06
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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\BF033016\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

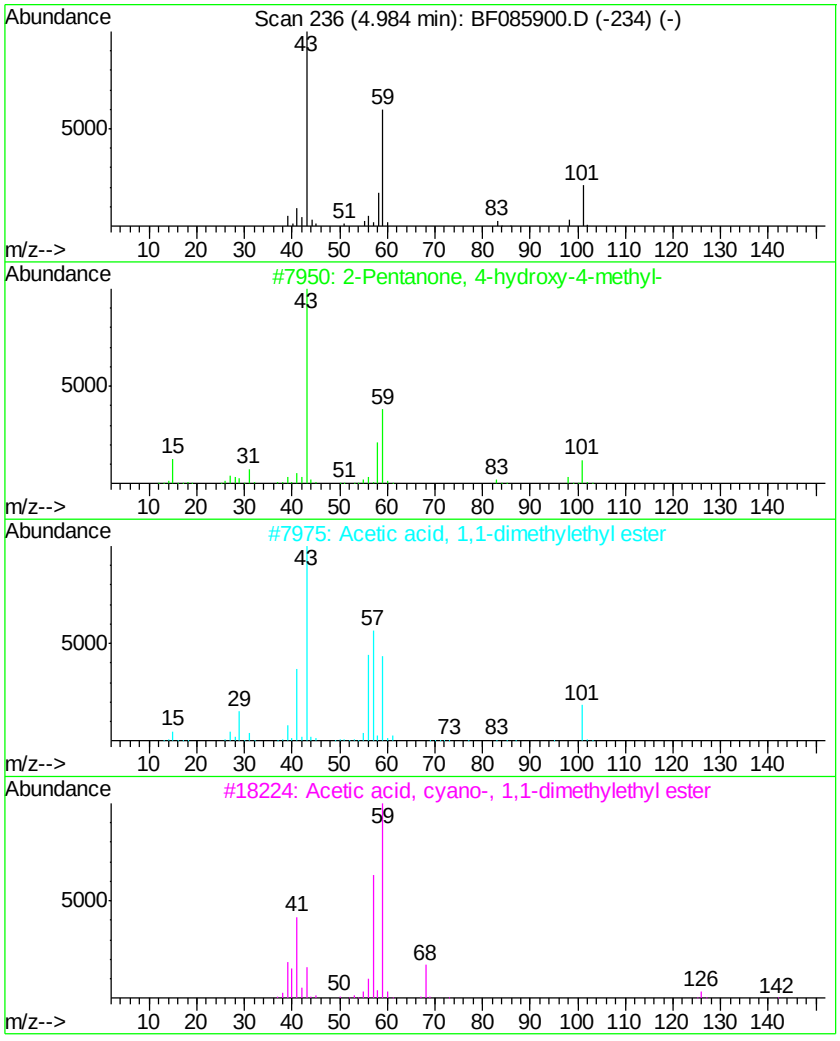
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

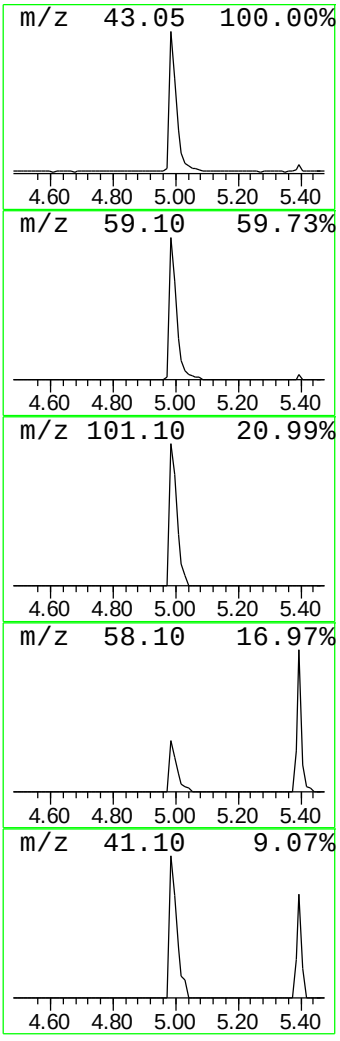
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	3.77 ng	122388	1,4-Dichlorobenzene-d4	6.80

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	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085900.D
Acq On : 30 Mar 2016 21:46
Operator : UM/SJ
Sample : H2023-06
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

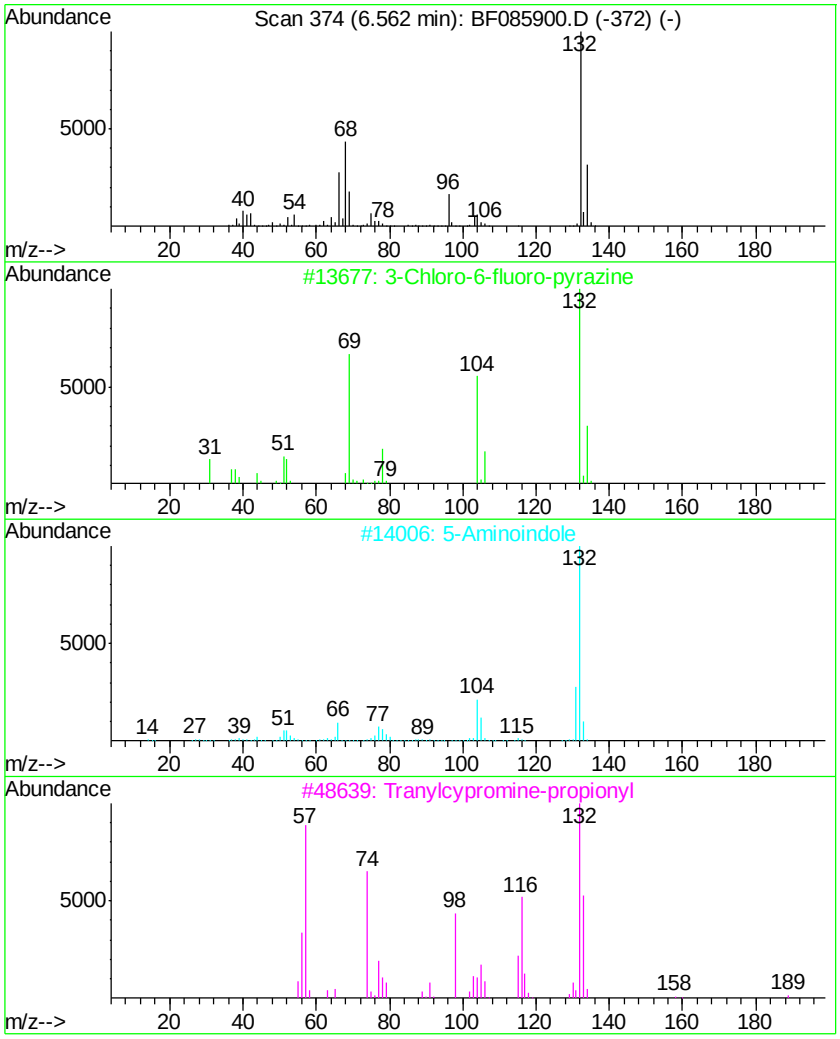
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

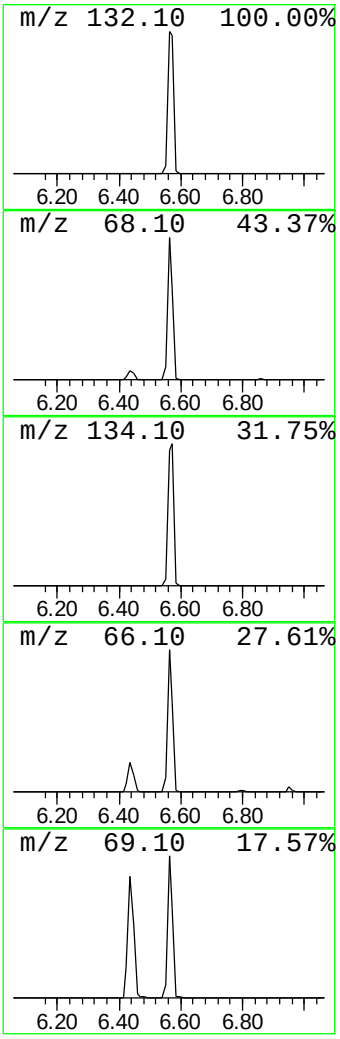
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	90.98 ng	2951970	1,4-Dichlorobenzene-d4	6.80

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Data File : BF085900.D
Acq On : 30 Mar 2016 21:46
Operator : UM/SJ
Sample : H2023-06
Misc :
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Instrument : BNA_F
ClientSampleId : B-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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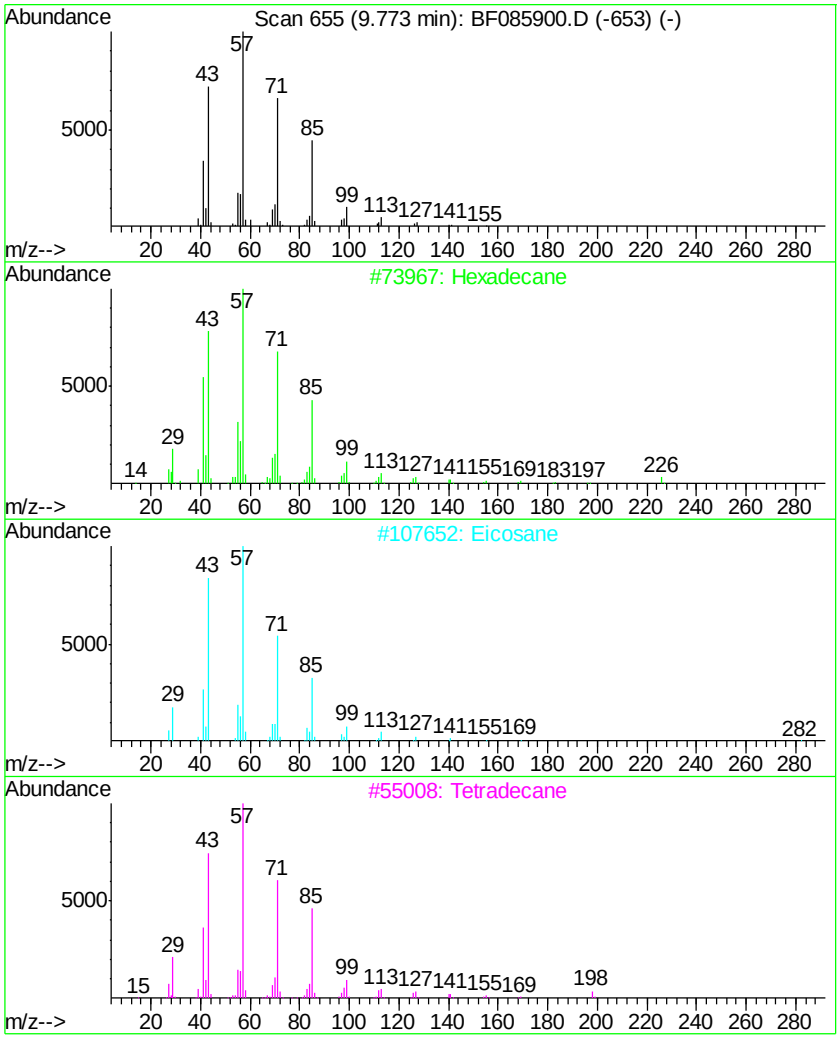
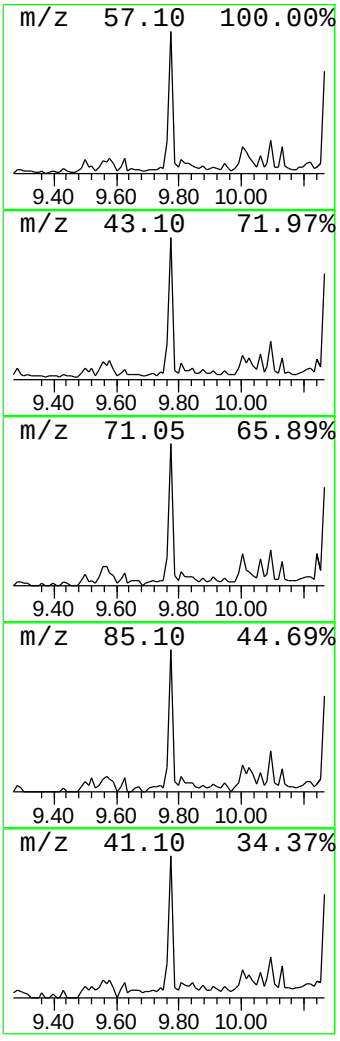
Peak Number 4 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.77	2.43 ng	109392	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tetradecane	198	C14H30	000629-59-4	87
4	Pentadecane	212	C15H32	000629-62-9	86
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085900.D
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Operator : UM/SJ
Sample : H2023-06
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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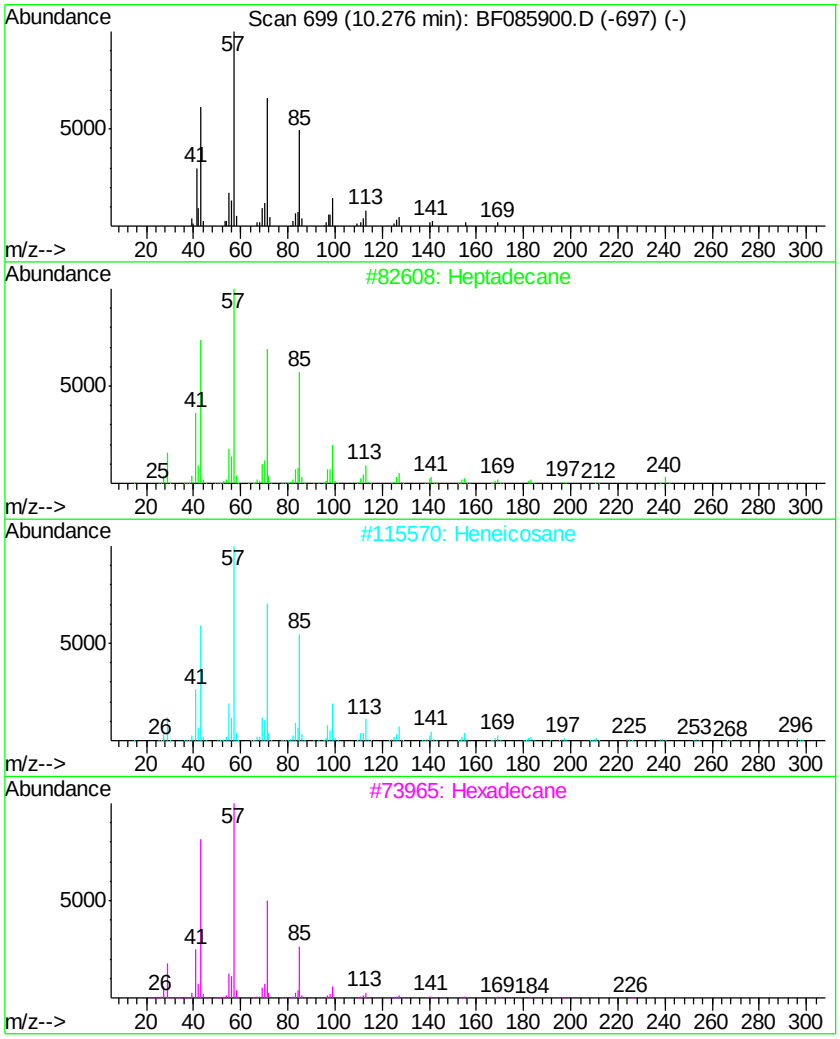
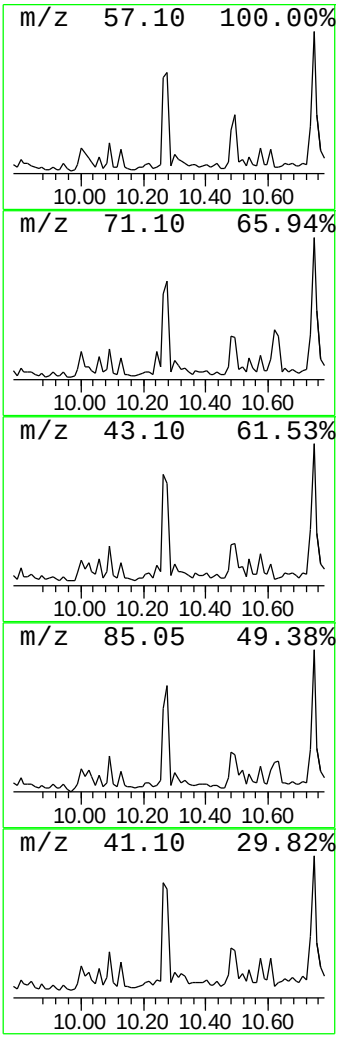
Peak Number 5 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	2.75 ng	123893	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tetradecane	198	C14H30	000629-59-4	87
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





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Data File : BF085900.D
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Operator : UM/SJ
Sample : H2023-06
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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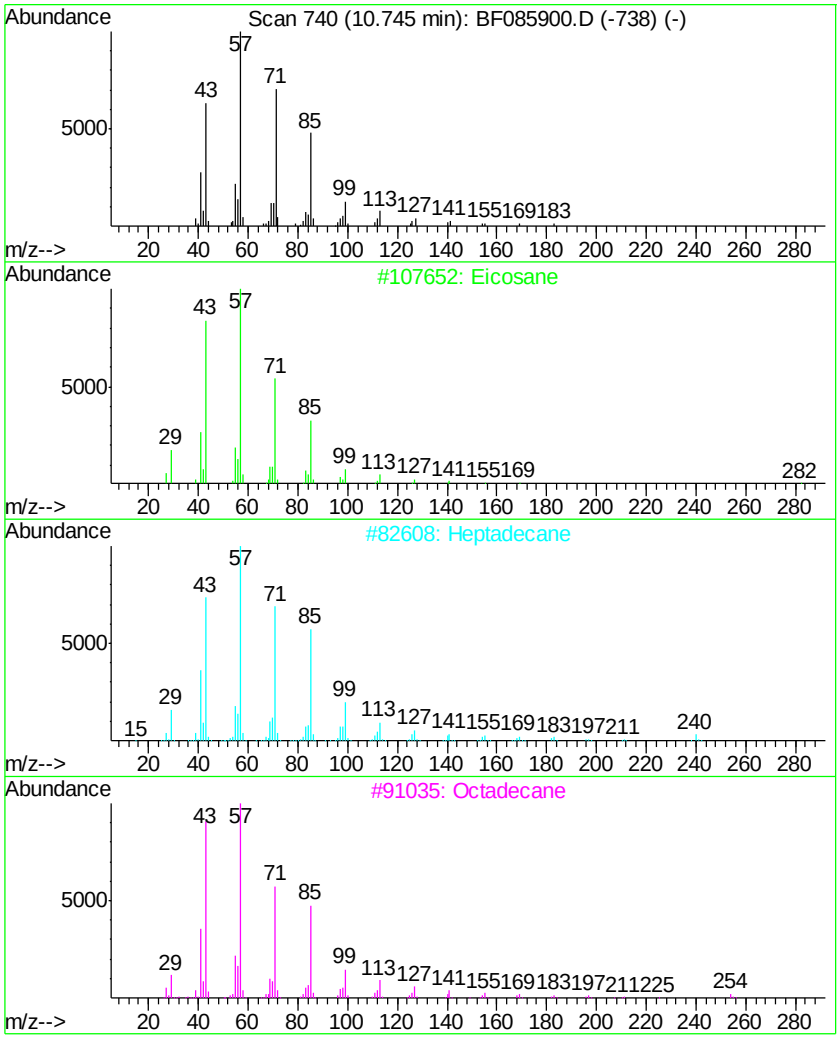
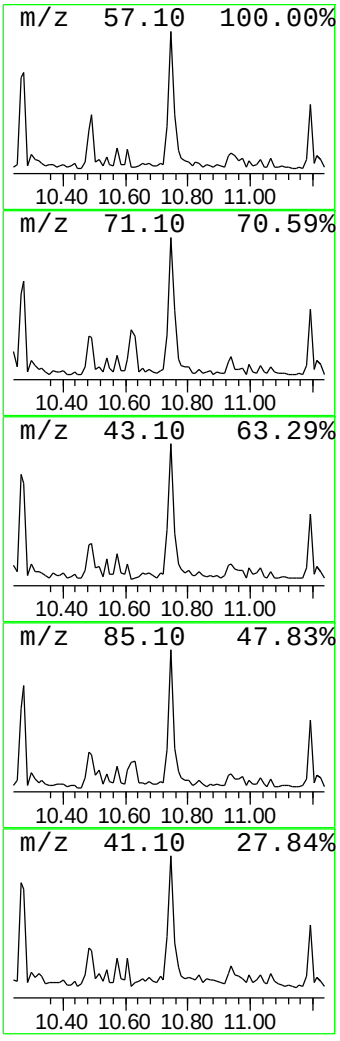
Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	4.13 ng	166702	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Nonadecane	268	C19H40	000629-92-5	87





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Operator : UM/SJ
Sample : H2023-06
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

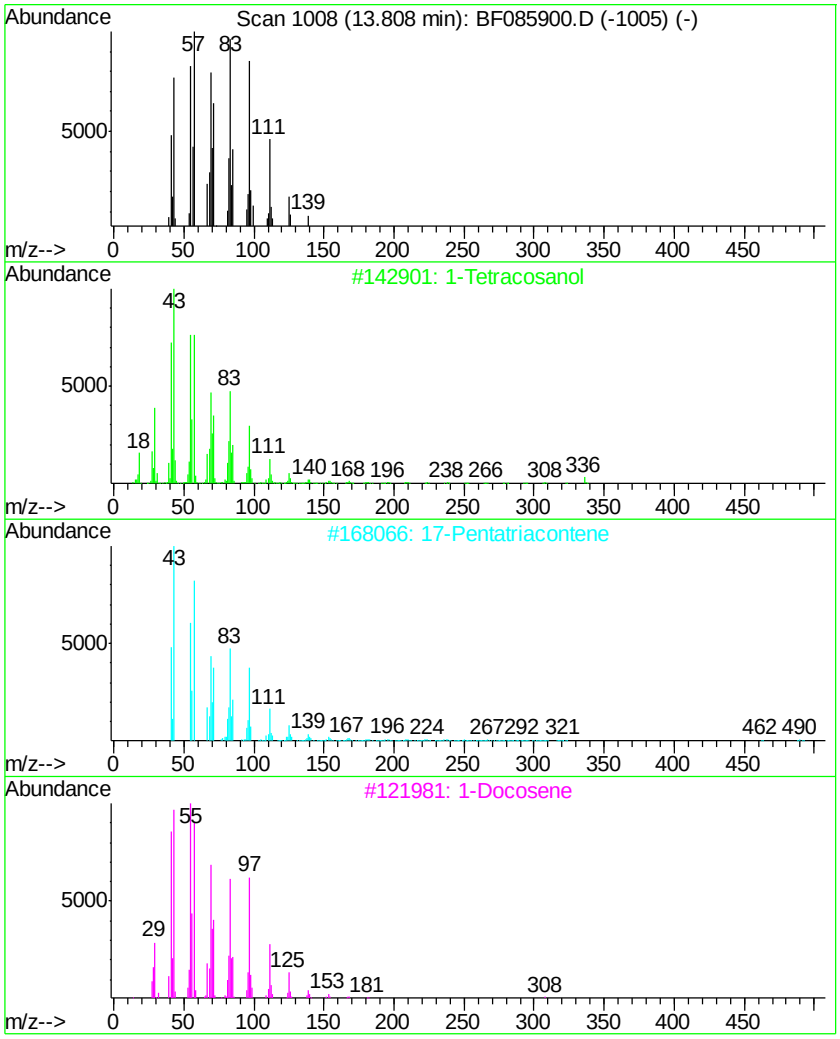
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

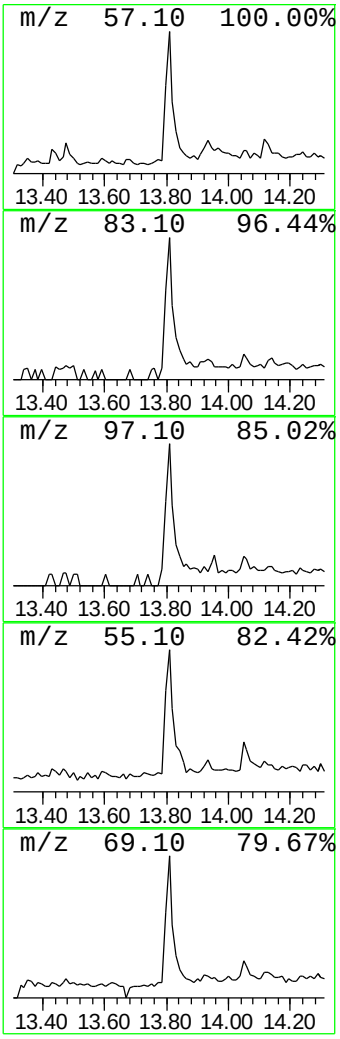
****

Peak Number 7 1-Tetracosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.18 ng	97688	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosanol	354	C24H50O	000506-51-4	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	86
3	1-Docosene	308	C22H44	001599-67-3	81
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	78
5	1-Hexacosanol	382	C26H54O	000506-52-5	72





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Sample : H2023-06
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Instrument : BNA_F
ClientSampleId : B-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

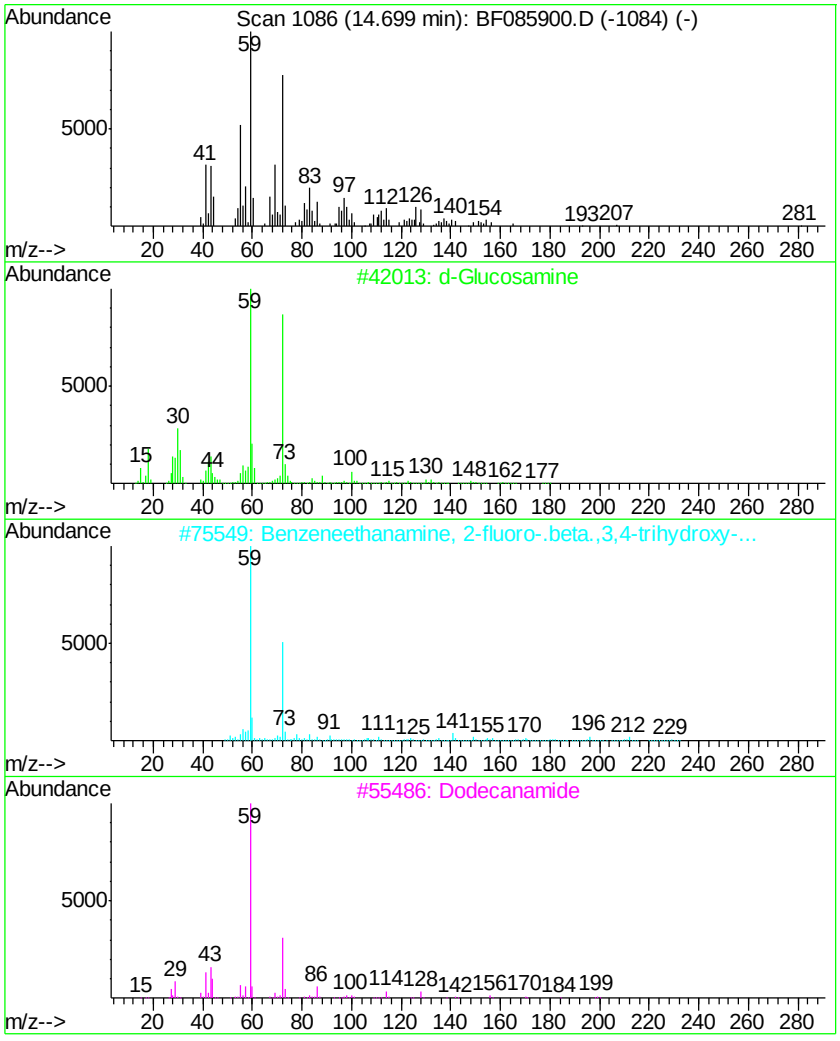
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

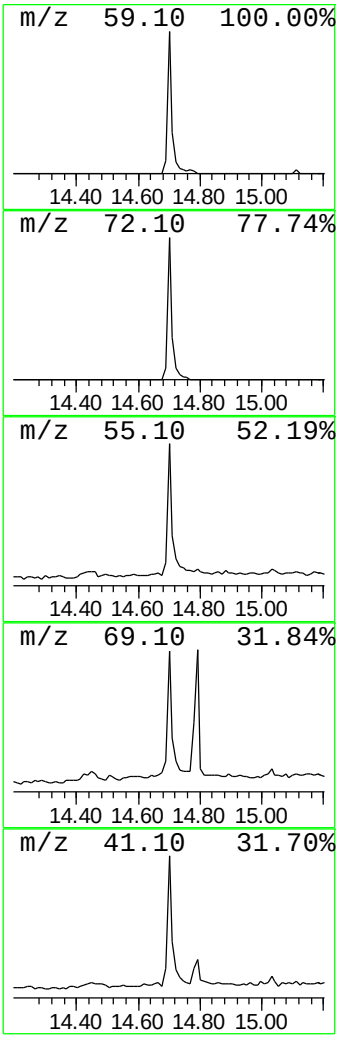
****

Peak Number 8 d-Glucosamine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	5.94 ng	183188	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	d-Glucosamine	179	C6H13NO5	000090-77-7	50
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50
3	Dodecanamide	199	C12H25NO	001120-16-7	47
4	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	47
5	Tetradecanamide	227	C14H29NO	000638-58-4	38





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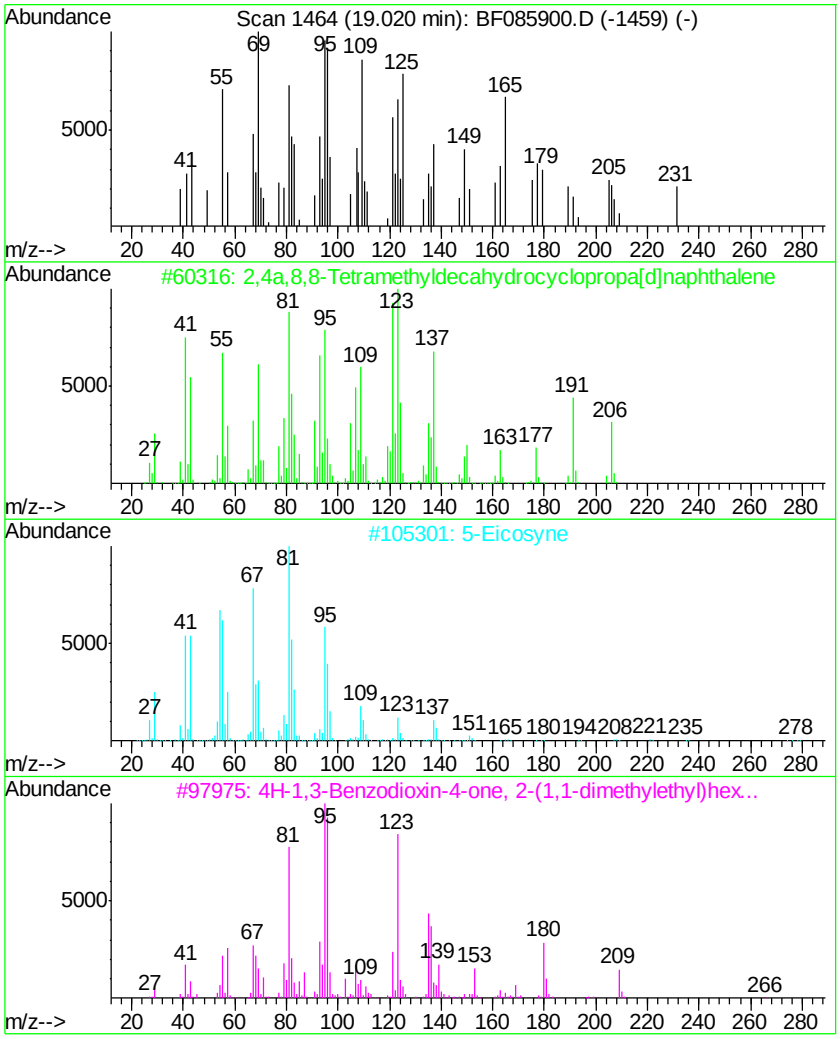
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

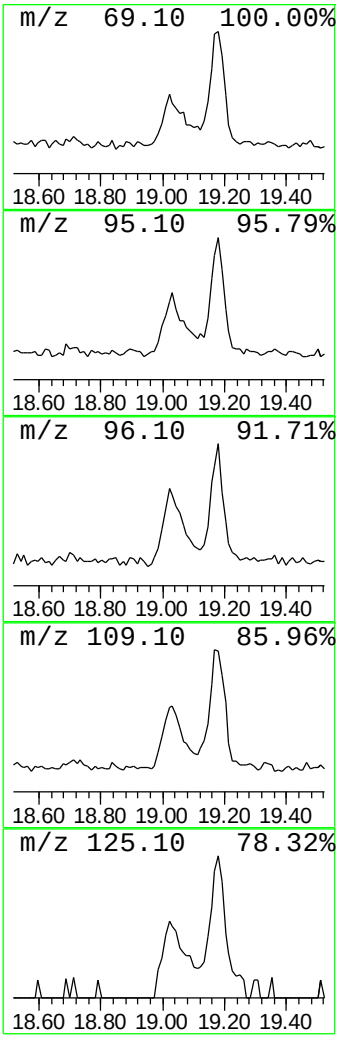
****

Peak Number 9 unknown19.02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	4.48 ng	138137	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	45
2	5-Eicosyne	278	C20H38	074685-31-7	22
3	4H-1,3-Benzodioxin-4-one, 2-(1,1...	266	C16H26O3	124899-18-9	22
4	2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	22
5	Naphthalene, decahydro-1,6-dimet...	208	C15H28	034315-85-0	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

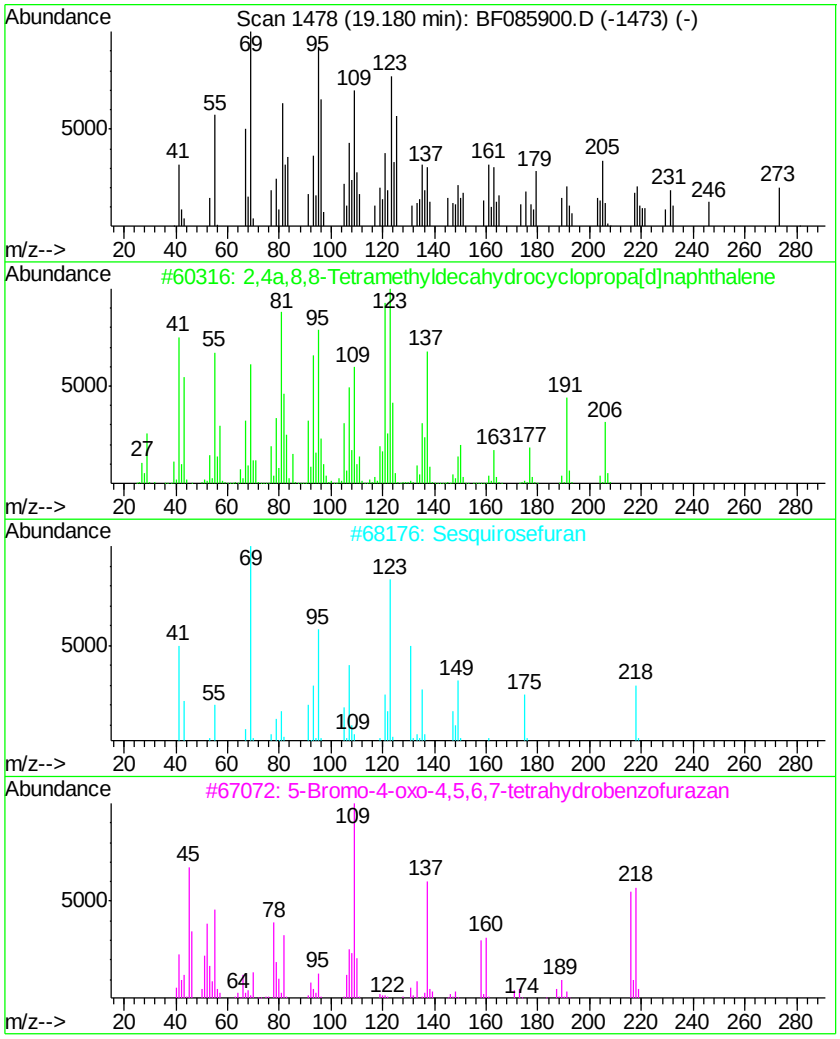
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

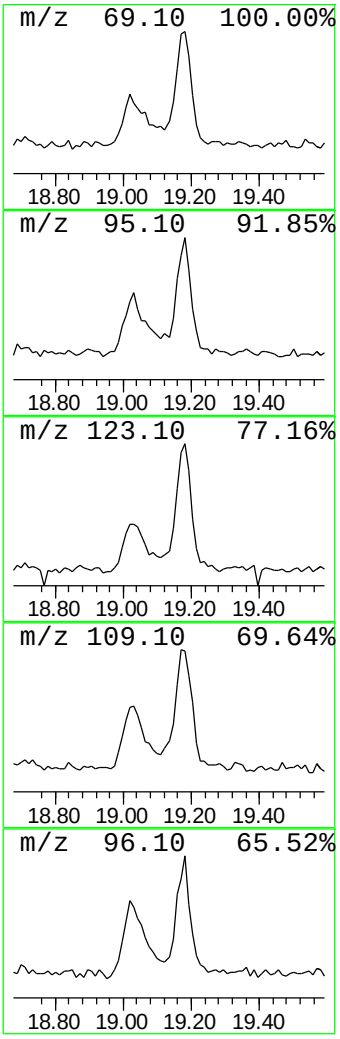
****

Peak Number 10 2,4a,8,8-Tetramethyldecahyd... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.18	7.40 ng	228156	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	53
2	Sesquirosefuran	218	C15H22O	039007-93-7	45
3	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	38
4	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	38
5	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085900.D
Acq On : 30 Mar 2016 21:46
Operator : UM/SJ
Sample : H2023-06
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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...	4.98	3.8	ng	122388	1	6.80	648916	20.0
unknown6.56	6.56	91.0	ng	2951970	1	6.80	648916	20.0
Hexadecane	9.77	2.4	ng	109392	3	9.84	899687	20.0
Heptadecane	10.28	2.8	ng	123893	3	9.84	899687	20.0
Eicosane	10.74	4.1	ng	166702	4	11.32	807543	20.0
1-Tetracosanol	13.81	3.2	ng	97688	5	13.96	614626	20.0
d-Glucosamine	14.70	5.9	ng	183188	6	15.37	616537	20.0
unknown19.02	19.02	4.5	ng	138137	6	15.37	616537	20.0
2,4a,8,8-Tetramet...	19.18	7.4	ng	228156	6	15.37	616537	20.0