LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086332.D
Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

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-BF042016.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	2.304	17	19	21	rVB2	357042	425676	13.05%	1.161%
2	5.047	256	259	265	rBV	713596	910699	27.91%	2.484%
3	5.470	293	296	298	rBV	2799210	3239823	99.29%	8.838%
4	5.870	329	331	334	rBV	92464	82972	2.54%	0.226%
5	6.499	383	386	396	rBV	2605401	3248480	99.56%	8.861%
6	6.636	396	398	400	rBV	3395299	3262988	100.00%	8.901%
7	6.865	416	418	421	rBV	1212573	1240996	38.03%	3.385%
8	7.025	430	432	434	rBV	2829184	2613195	80.09%	7.128%
9	7.287	452	455	459	rVB2	25447	38318	1.17%	0.105%
10	7.425	465	467	470	rBV	1226045	1715040	52.56%	4.678%
11	7.527	474	476	484	rVB2	39259	91361	2.80%	0.249%
12	7.893	504	508	512	rBV5	10738	36036	1.10%	0.098%
13	8.156	528	531	533	rBV	1422282	1474039	45.17%	4.021%
14	9.173	616	620	622	rBV2	21536	35272	1.08%	0.096%
15	9.230	622	625	627	rBV	3336261	2990839	91.66%	8.159%
16	9.311	631	632	637	rVB2	25804	45425	1.39%	0.124%
17	9.562	652	654	658	rBV3	20712	38920	1.19%	0.106%
18	9.619	658	659	662	rBV	219954	239177	7.33%	0.652%
19	9.768	670	672	674	rBV	54118	66083	2.03%	0.180%
20	9.848	676	679	681	rVB	38436	54509	1.67%	0.149%
21	9.905	682	684	687	rBV	1365315	1329349	40.74%	3.626%
22	10.339	721	722	724	rBV	74103	61707	1.89%	0.168%
23	10.556	738	741	745	rVB2	30890	52477	1.61%	0.143%
24	10.694	750	753	760	rBV	1433682	1587214	48.64%	4.330%
25	10.819	762	764	768	rVB	75872	129254	3.96%	0.353%
26	10.945	770	775	777	rVB6	27876	64509	1.98%	0.176%
27	11.265	800	803	804	rBV	41967	43634	1.34%	0.119%
28	11.391	812	814	818	rBV2	1321235	1509387	46.26%	4.117%
29	11.448	818	819	822	rVB2	47104	92533	2.84%	0.252%
30	11.619	831	834	835	rBV2	37214	72789	2.23%	0.199%
31	11.722	841	843	845	rVB3	27420	32967	1.01%	0.090%
32	11.894	855	858	859	rBV	42899	57584	1.76%	0.157%
33	11.916	859	860	862	rVV	89236	104879	3.21%	0.286%
34	12.008	866	868	872	rVB2	44347	86511	2.65%	0.236%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086332.D
Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

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-BF042016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.065	872	873	875	rBV2	28465	50007	1.53%	0.136%
36	12.191	882	884	889	rVB4	29055	61547	1.89%	0.168%
37	12.374	898	900	902	rBV2	28818	48897	1.50%	0.133%
38	12.477	907	909	912	rVV4	33490	75981	2.33%	0.207%
39	12.602	917	920	922	rBV	347520	346599	10.62%	0.945%
40	12.797	936	937	938	rBV	100210	121339	3.72%	0.331%
41	12.831	938	940	941	rVB	278659	267599	8.20%	0.730%
42	12.979	950	953	955	rBV	1967501	2400943	73.58%	6.549%
43	13.162	967	969	971	rBV	66586	103803	3.18%	0.283%
44	13.208	971	973	976	rVB2	107458	150709	4.62%	0.411%
45	13.505	997	999	1001	rBV	98569	118474	3.63%	0.323%
46	13.551	1001	1003	1004	rBV	152824	144738	4.44%	0.395%
47	13.894	1030	1033	1037	rBV3	329017	696455	21.34%	1.900%
48	14.031	1042	1045	1049	rVV2	810912	1361924	41.74%	3.715%
49	14.191	1057	1059	1062	rBV	210509	320258	9.81%	0.874%
50	14.500	1084	1086	1088	rBV	409695	395530	12.12%	1.079%
51	15.128	1139	1141	1144	rBV	431385	465350	14.26%	1.269%
52	15.254	1148	1152	1153	rBV4	275076	695516	21.32%	1.897%
53	15.403	1163	1165	1168	rBV	202210	276174	8.46%	0.753%
54	15.460	1168	1170	1181	rVB2	488790	1172495	35.93%	3.198%
55	15.917	1208	1210	1213	rVB	212080	309888	9.50%	0.845%

Sum of corrected areas: 36658868

LSC Report - Integrated Chromatogram

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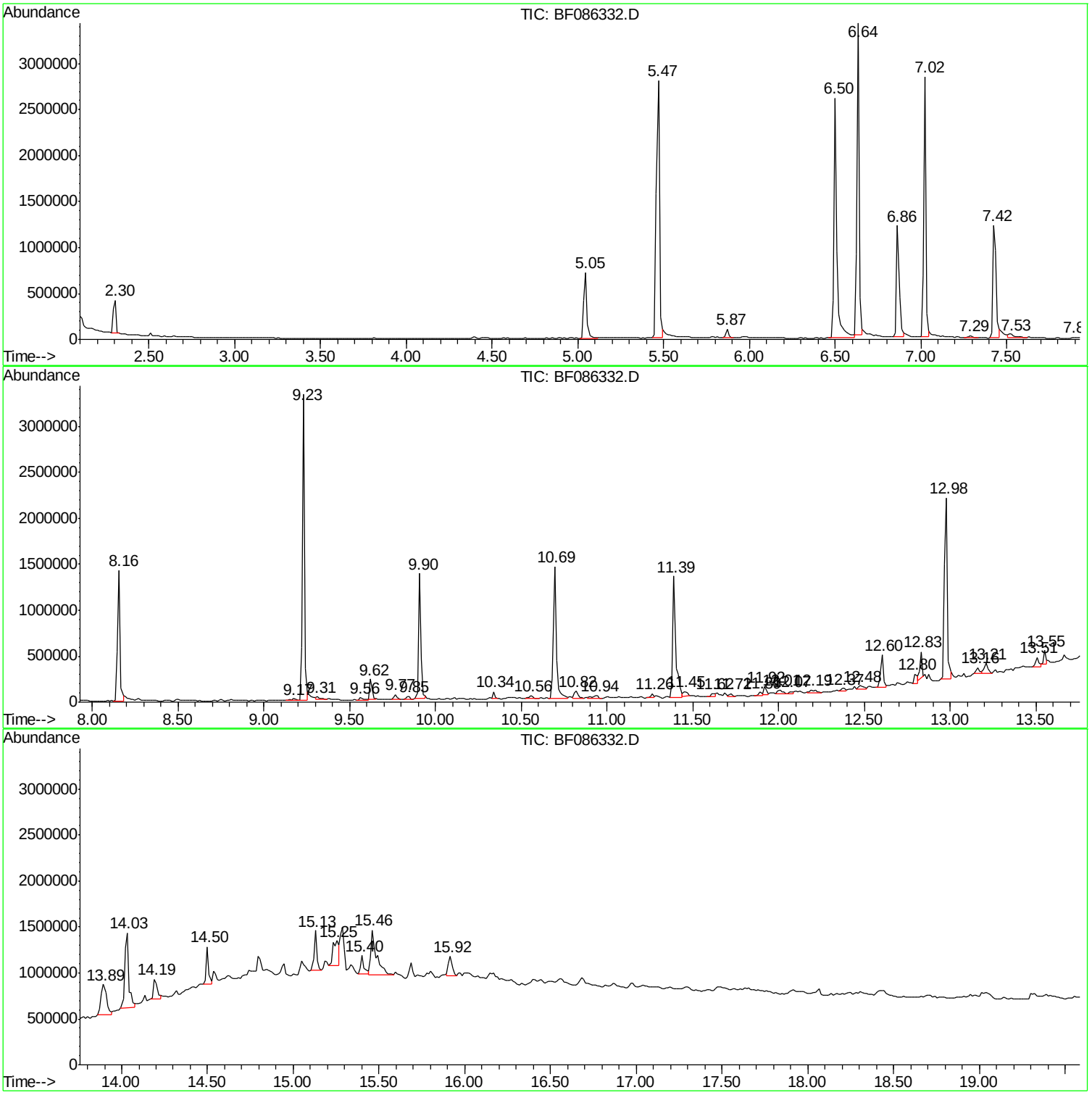
Data File : BF086332.D
Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.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\BF042016\
Data File : BF086332.D
Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

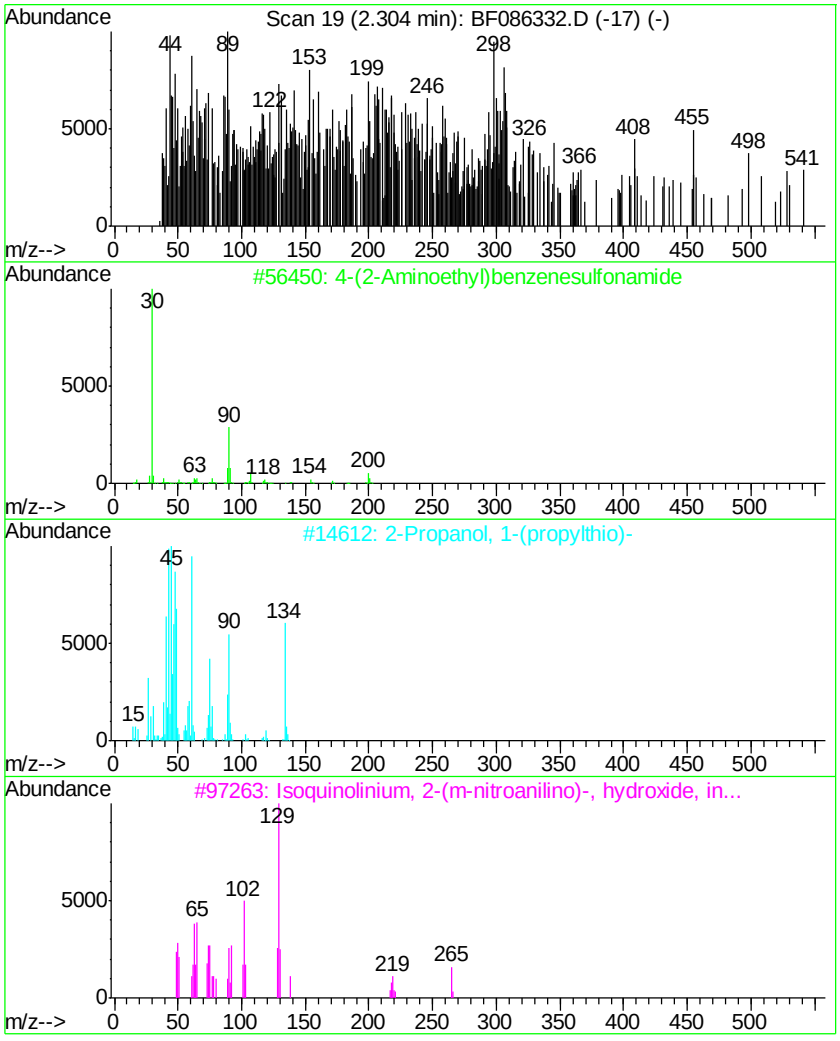
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

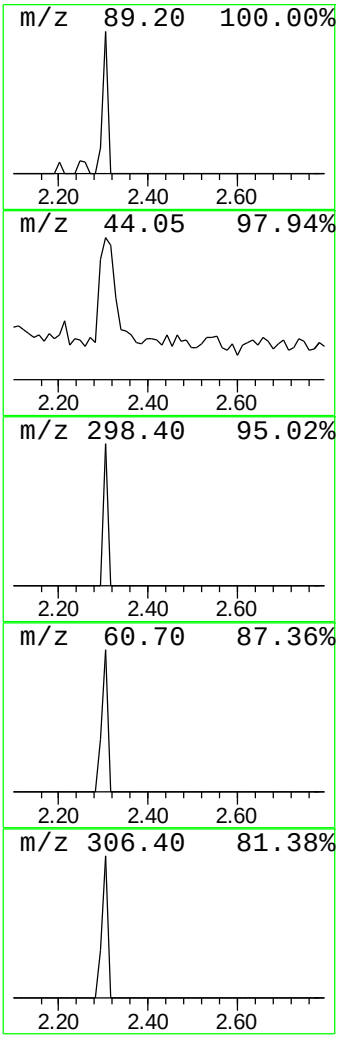
****

Peak Number 1 unknown2.30 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	6.86 ng	425676	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	22
2	2-Propanol, 1-(propylthio)-	134	C6H14OS	053957-22-5	18
3	Isoquinolinium, 2-(m-nitroanilin...	265	C15H11N3O2	031383-03-6	15
4	Dihydroepinatalensine	303	C17H21NO4	098843-28-8	15
5	Thiazole-4-carboxylic acid, 2-ch...	262	C9H11ClN2O3S	084345-00-6	15





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086332.D
Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

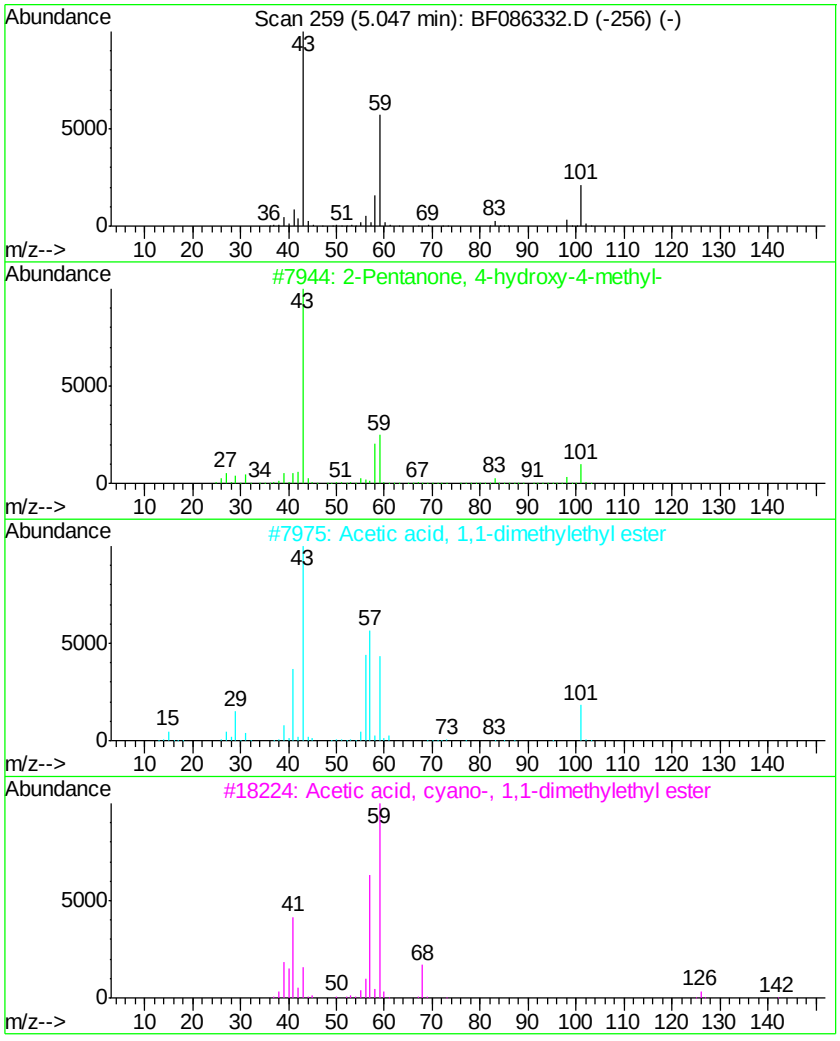
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

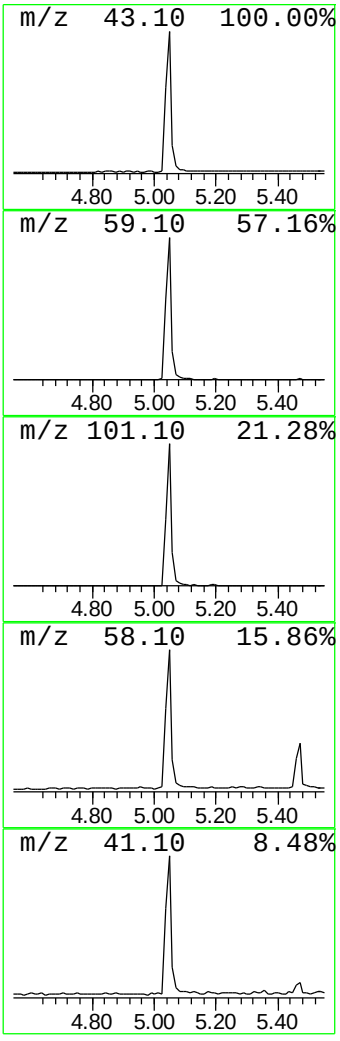
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	14.68 ng	910699	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086332.D
Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

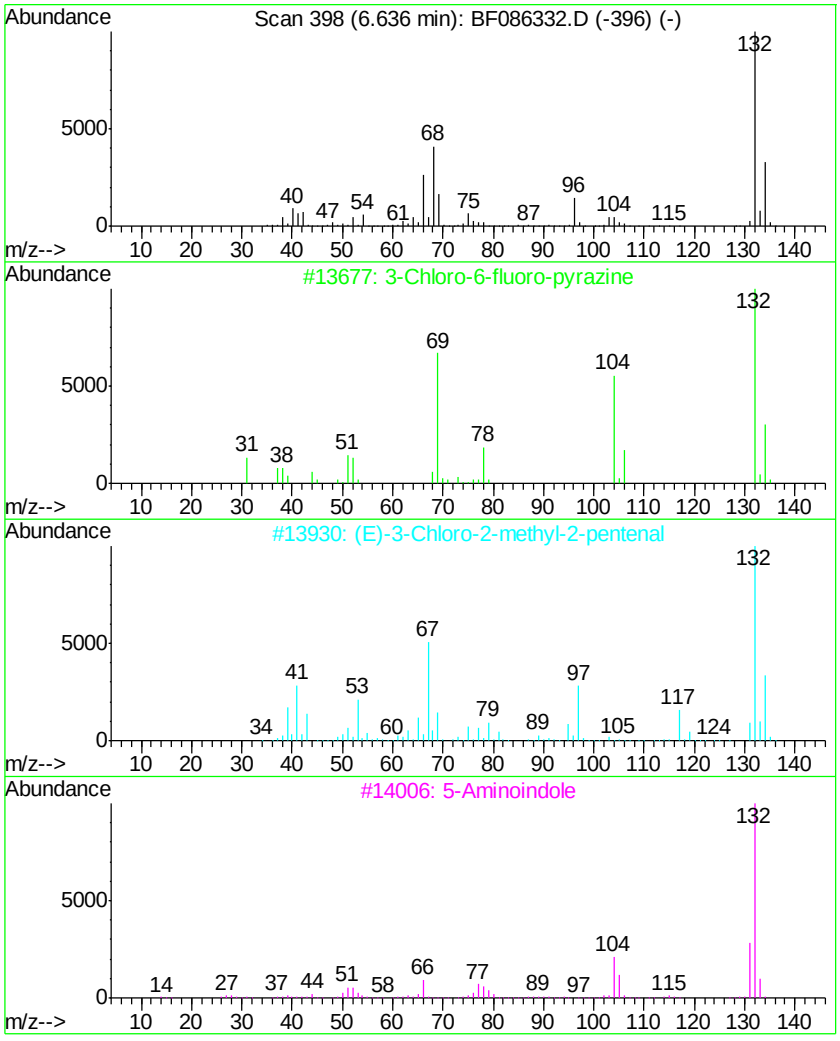
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

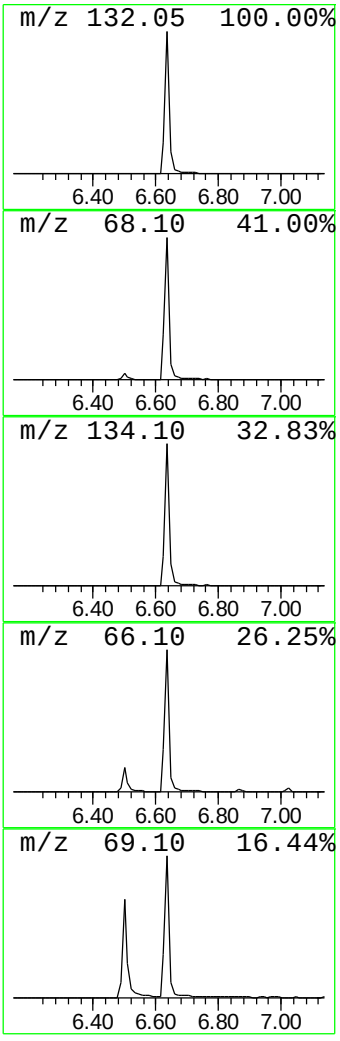
****

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	52.59 ng	3262990	1,4-Dichlorobenzene-d4	6.86

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
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Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

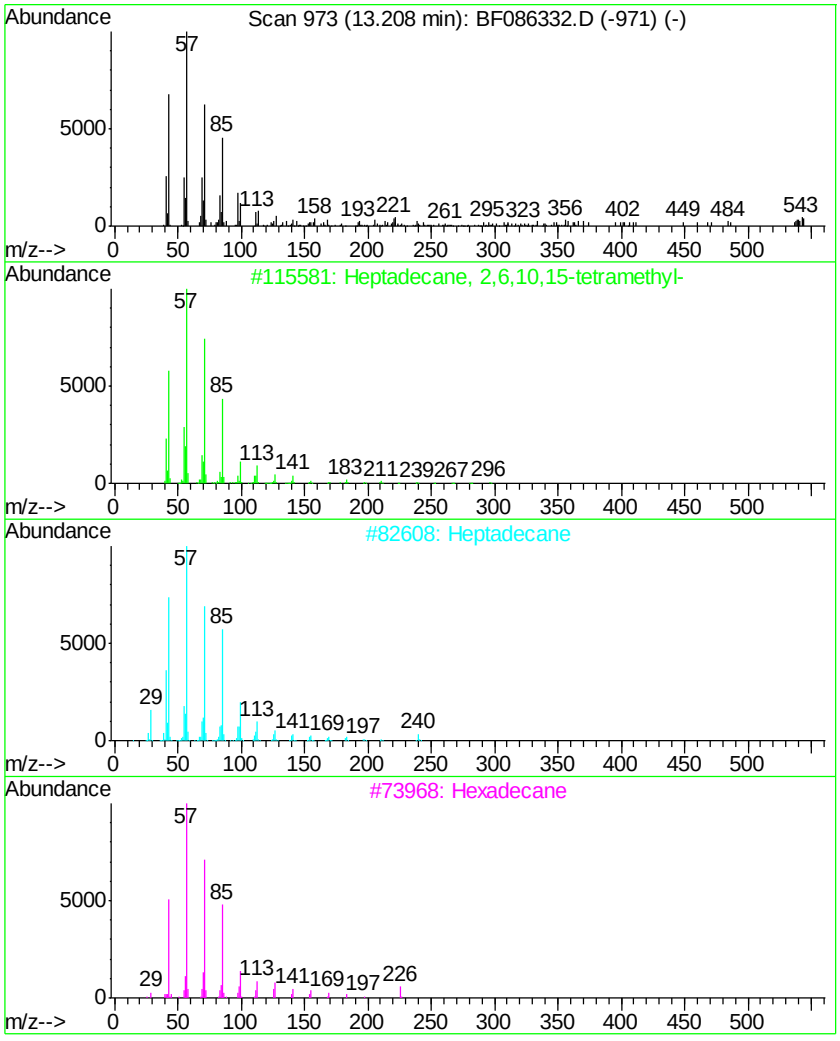
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

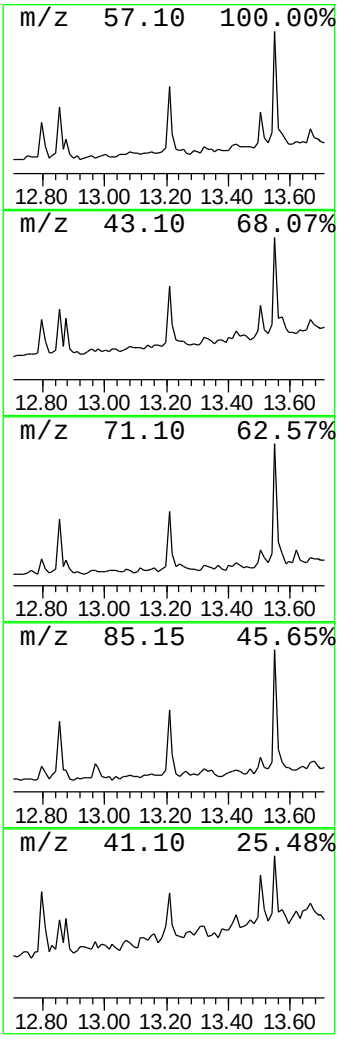
****

Peak Number 5 Heptadecane, 2,6,10,15-tetr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	2.21 ng	150709	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2	Heptadecane	240	C17H36	000629-78-7	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Heneicosane	296	C21H44	000629-94-7	70
5	Docosane	310	C22H46	000629-97-0	62





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.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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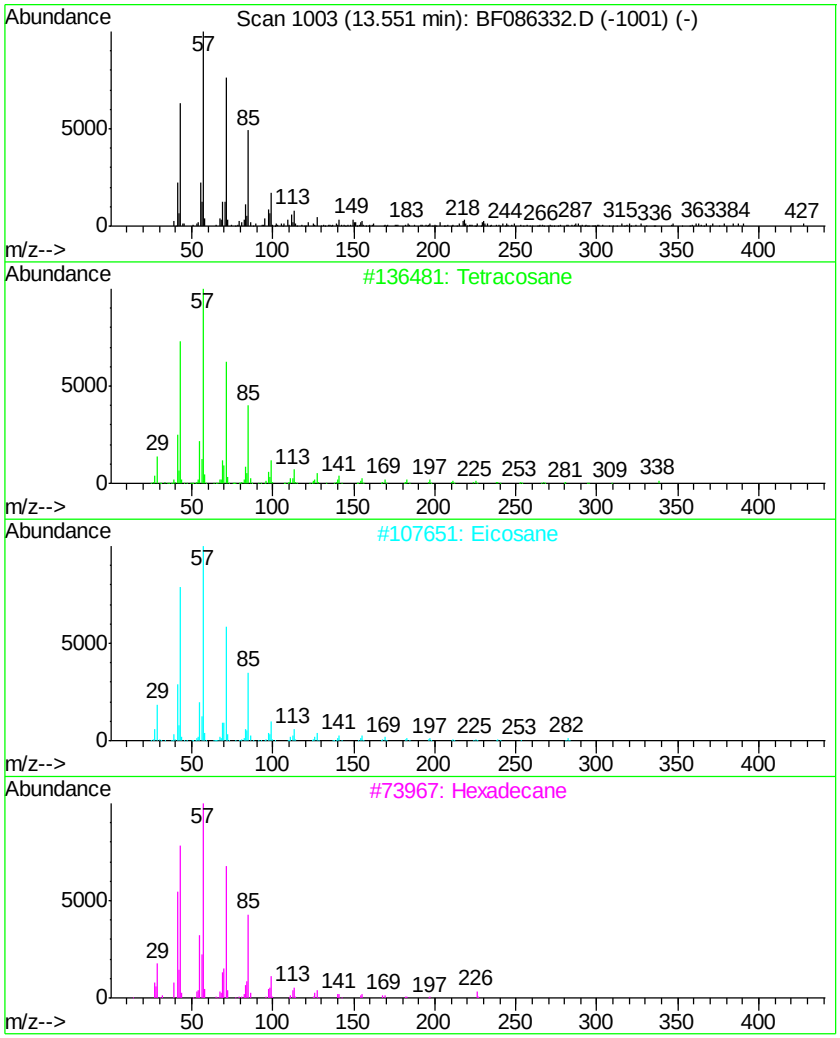
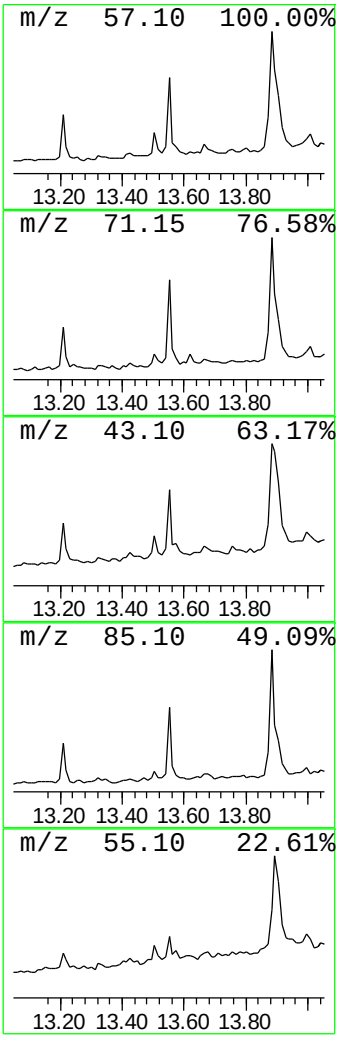
Peak Number 6 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.13 ng	144738	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Eicosane	282	C20H42	000112-95-8	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Pentacosane	352	C25H52	000629-99-2	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	70





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Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.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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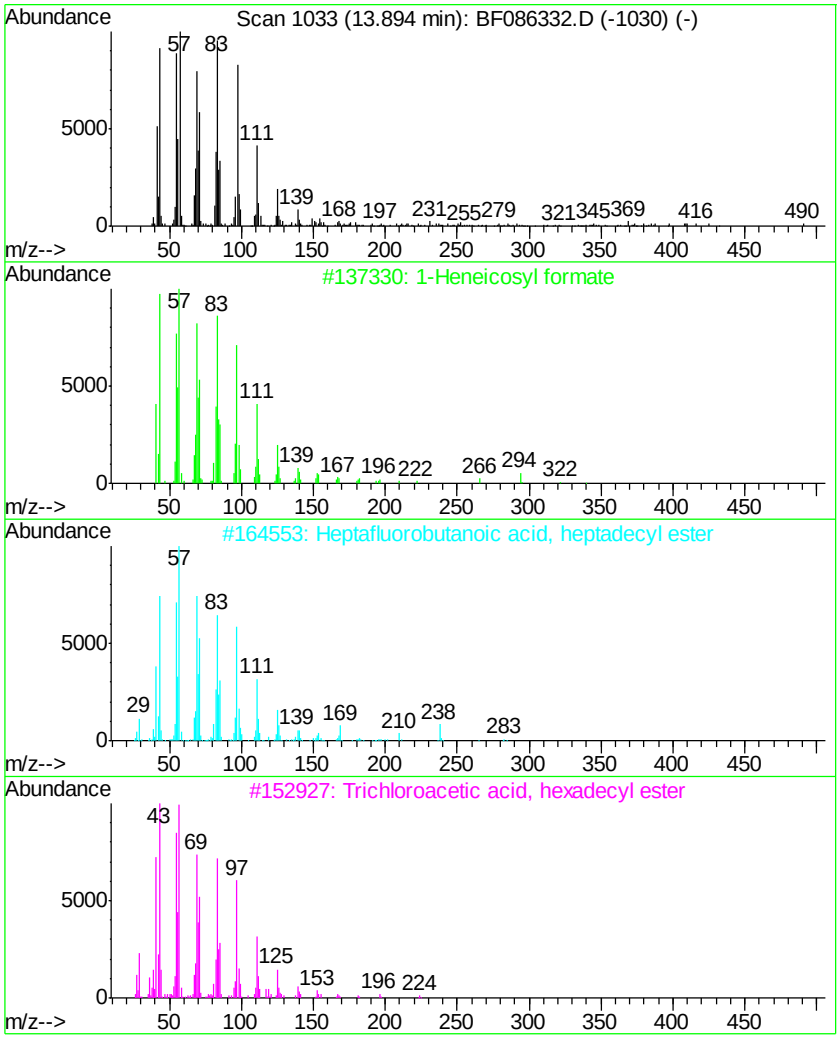
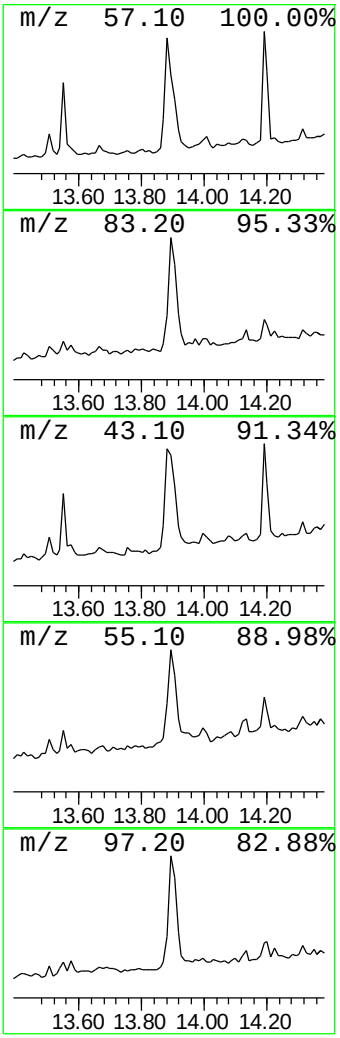
Peak Number 7 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	10.23 ng	696455	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

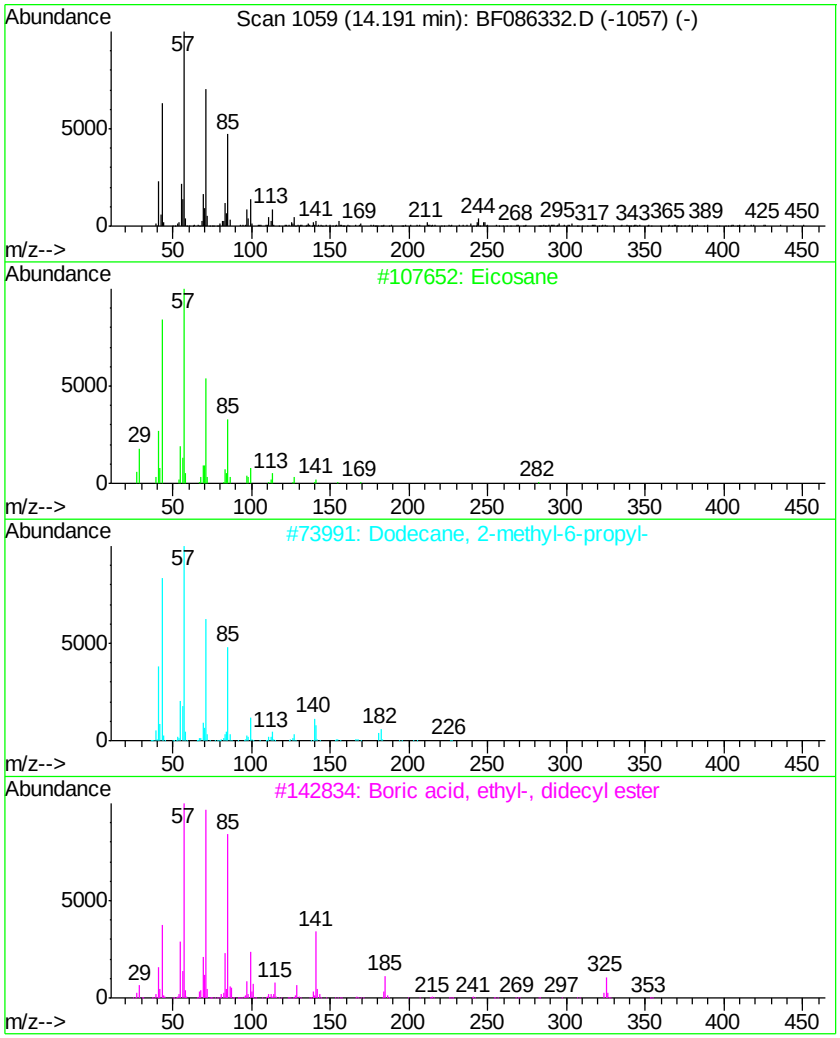
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

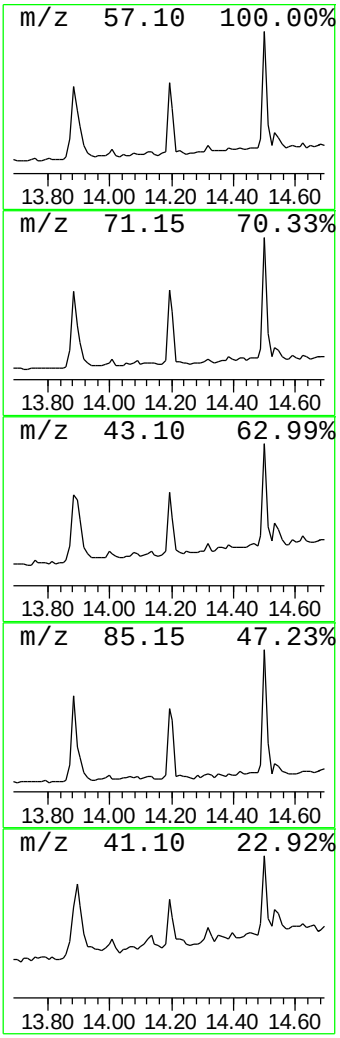
****

Peak Number 8 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	4.70 ng	320258	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	87
3	Boric acid, ethyl-, didecyl ester	354	C22H47BO2	1000152-34-4	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Heneicosane	296	C21H44	000629-94-7	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
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Operator : UM/SJ
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Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.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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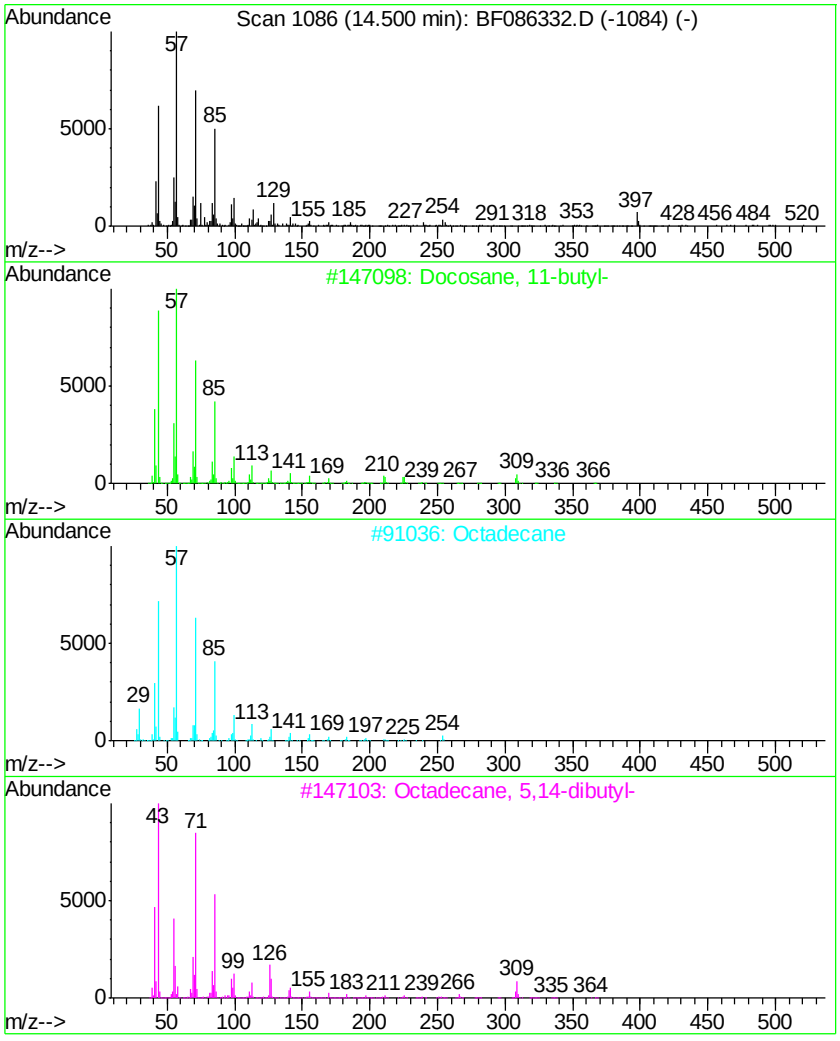
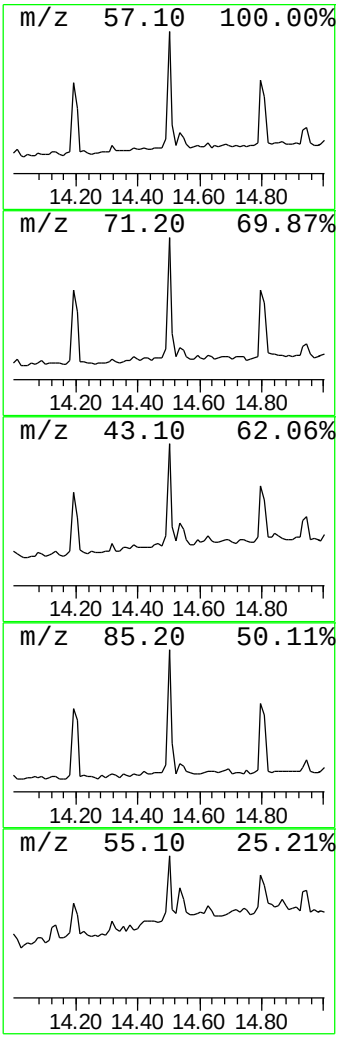
Peak Number 9 Docosane, 11-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	5.81 ng	395530	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2	Octadecane	254	C18H38	000593-45-3	93
3	Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	89
4	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	81
5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	78





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Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.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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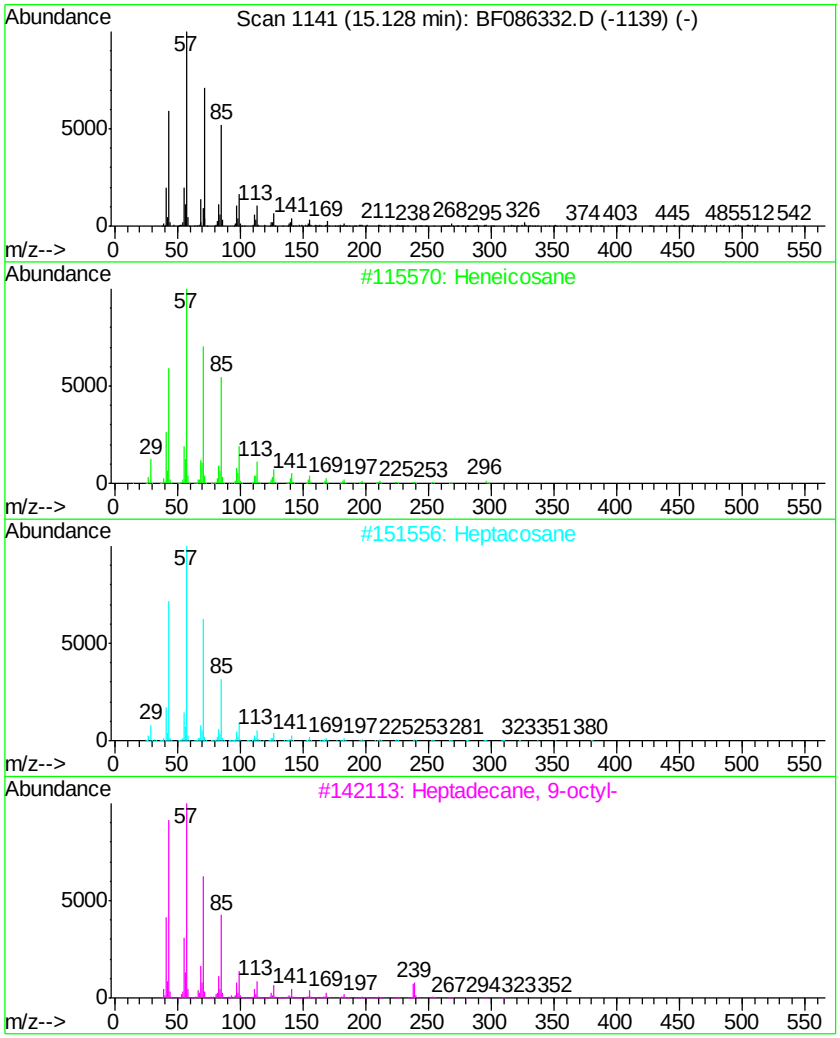
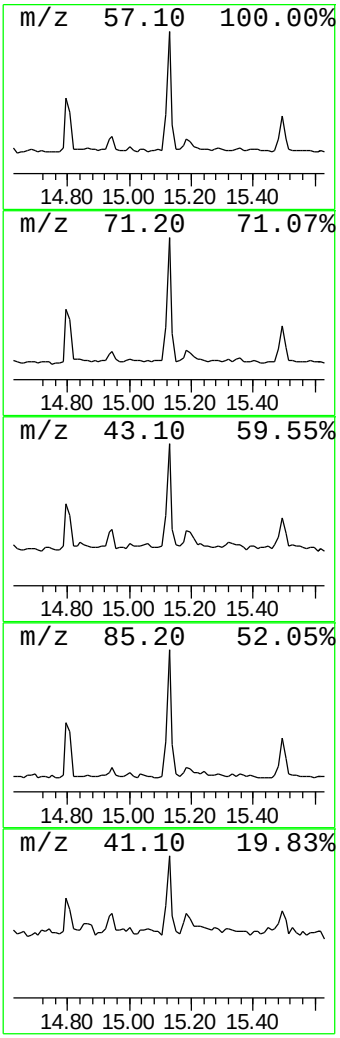
Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	7.94 ng	465350	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Heptacosane	380	C27H56	000593-49-7	96
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
4	Nonadecane	268	C19H40	000629-92-5	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042016\
Data File : BF086332.D
Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.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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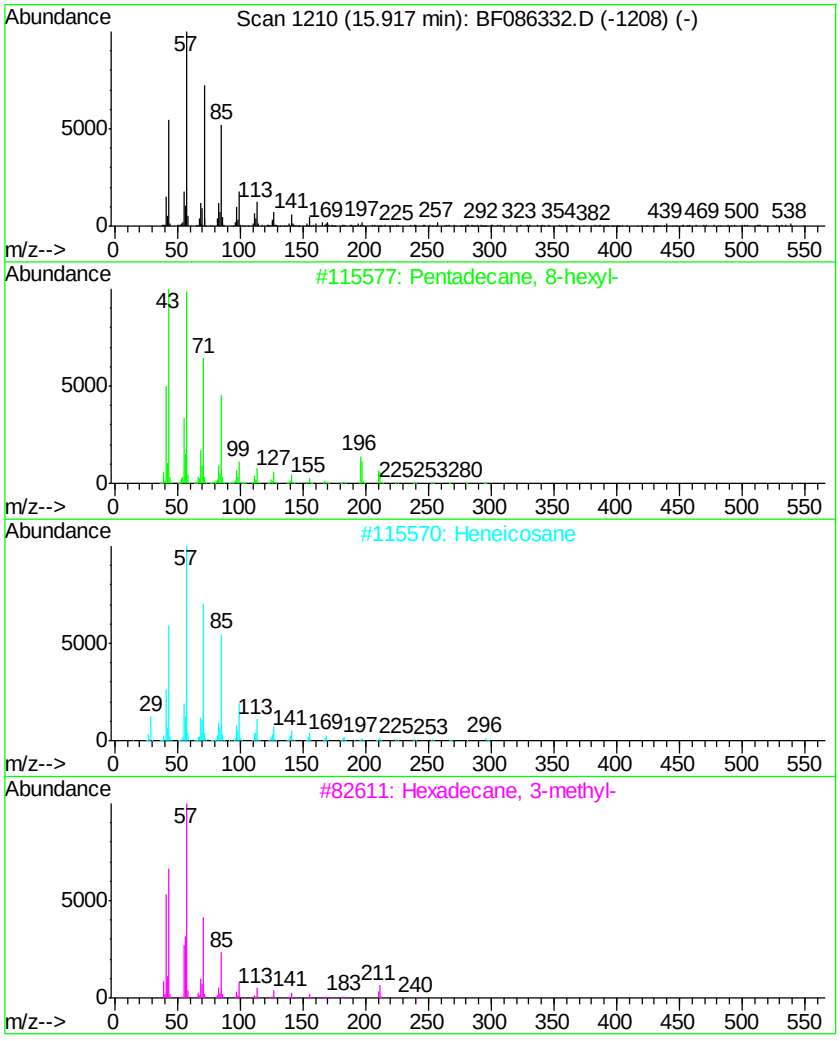
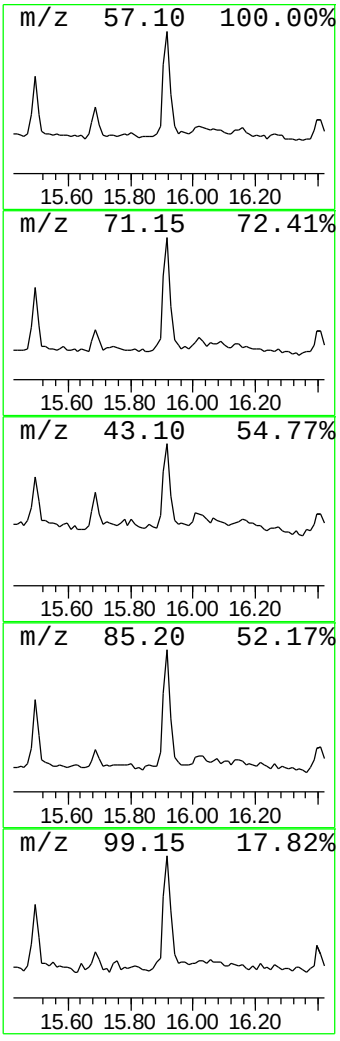
Peak Number 12 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	5.29 ng	309888	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
2	Heneicosane	296	C21H44	000629-94-7	81
3	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	81
4	Nonacosane	408	C29H60	000630-03-5	74
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042016\
Data File : BF086332.D
Acq On : 21 Apr 2016 2:27
Operator : UM/SJ
Sample : H2601-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RODNEY-AVE-PS(0-2)J

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042016.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
unknown2.30	2.30	6.9	ng	425676	1	6.86	1241000	20.0
2-Pentanone, 4-hy...	5.05	14.7	ng	910699	1	6.86	1241000	20.0
unknown6.64	6.64	52.6	ng	3262990	1	6.86	1241000	20.0
Heptadecane, 2,6,...	13.21	2.2	ng	150709	5	14.03	1361920	20.0
Tetracosane	13.55	2.1	ng	144738	5	14.03	1361920	20.0
1-Heneicosyl formate	13.89	10.2	ng	696455	5	14.03	1361920	20.0
Eicosane	14.19	4.7	ng	320258	5	14.03	1361920	20.0
Docosane, 11-butyl-	14.50	5.8	ng	395530	5	14.03	1361920	20.0
Heneicosane	15.13	7.9	ng	465350	6	15.46	1172500	20.0
Pentadecane, 8-he...	15.92	5.3	ng	309888	6	15.46	1172500	20.0