LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

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-BF101015.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	5.017	249	252	263	rVB	678336	950253	51.14%	5.220%
2	5.440	286	289	291	rBV	1526707	1641816	88.36%	9.020%
3	6.469	377	379	382	rBV	1057500	1565124	84.23%	8.598%
4	6.606	388	391	393	rBV	1845131	1734388	93.34%	9.528%
5	6.834	409	411	414	rBV	510352	480756	25.87%	2.641%
6	6.994	422	425	427	rBV	1540363	1412845	76.04%	7.762%
7	7.406	458	461	467	rBV	981072	1003427	54.00%	5.512%
8	7.497	467	469	475	rVB2	11865	25918	1.39%	0.142%
9	8.126	521	524	526	rBV	706824	640266	34.46%	3.517%
10	9.200	616	618	621	rBV	1816124	1858060	100.00%	10.208%
11	9.600	650	653	655	rBV	441464	362469	19.51%	1.991%
12	9.875	675	677	680	rBV	497947	694290	37.37%	3.814%
13	10.309	711	715	716	rBV	35679	45239	2.43%	0.249%
14	10.675	744	747	749	rBV	883527	1093706	58.86%	6.008%
15	10.778	754	756	761	rVB	51041	58404	3.14%	0.321%
16	11.223	794	795	797	rBV	29145	32102	1.73%	0.176%
17	11.360	805	807	810	rBV	471194	612754	32.98%	3.366%
18	11.658	831	833	834	rBV	20635	20499	1.10%	0.113%
19	11.898	852	854	856	rBV	80013	90100	4.85%	0.495%
20	12.092	870	871	874	rBV3	18351	19240	1.04%	0.106%
21	12.561	910	912	917	rVB	19568	38974	2.10%	0.214%
22	12.641	917	919	920	rBV2	26504	21558	1.16%	0.118%
23	12.663	920	921	924	rVB3	103994	100719	5.42%	0.553%
24	12.766	928	930	933	rBV2	163737	236283	12.72%	1.298%
25	12.892	939	941	944	rBV2	22473	24548	1.32%	0.135%
26	12.949	944	946	949	rBV	1408249	1547392	83.28%	8.501%
27	13.429	986	988	990	rVV	87518	78112	4.20%	0.429%
28	13.475	990	992	994	rVB	41016	34363	1.85%	0.189%
29	13.841	1022	1024	1033	rVB	139647	230143	12.39%	1.264%
30	14.001	1036	1038	1041	rVV	424440	480171	25.84%	2.638%
31	14.161	1050	1052	1056	rBV2	14525	27022	1.45%	0.148%
32	14.469	1076	1079	1086	rBV2	31503	80285	4.32%	0.441%
33	14.767	1102	1105	1107	rBV	16754	23655	1.27%	0.130%
34	14.835	1109	1111	1114	rVV	18373	25226	1.36%	0.139%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.915	1116	1118	1120	rBV2	15400	19421	1.05%	0.107%
36	15.098	1131	1134	1135	rBV	28479	43380	2.33%	0.238%
37	15.441	1161	1164	1169	rBV	377981	501950	27.01%	2.758%
38	15.875	1199	1202	1205	rBV	79964	126813	6.83%	0.697%
39	15.932	1205	1207	1211	rBV3	24158	50754	2.73%	0.279%
40	16.355	1240	1244	1245	rBV3	10826	21661	1.17%	0.119%
41	16.915	1291	1293	1296	rVB2	10860	19355	1.04%	0.106%
42	17.007	1298	1301	1306	rVB6	6192	19130	1.03%	0.105%
43	17.384	1329	1334	1339	rBV6	15242	51273	2.76%	0.282%
44	18.355	1415	1419	1424	rVB5	10635	34064	1.83%	0.187%
45	19.350	1504	1506	1511	rVB6	8831	24921	1.34%	0.137%

Sum of corrected areas: 18202829

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
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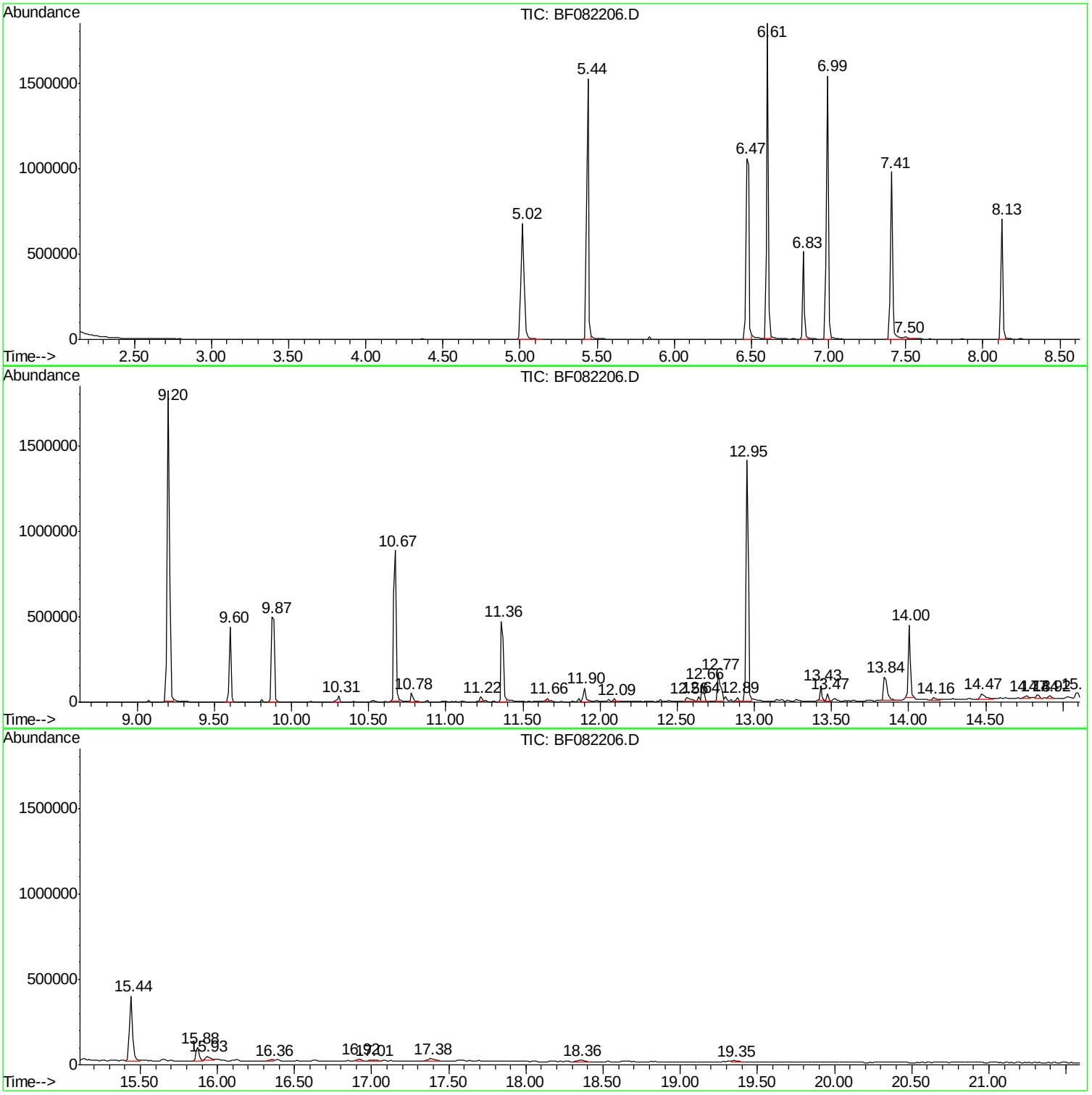
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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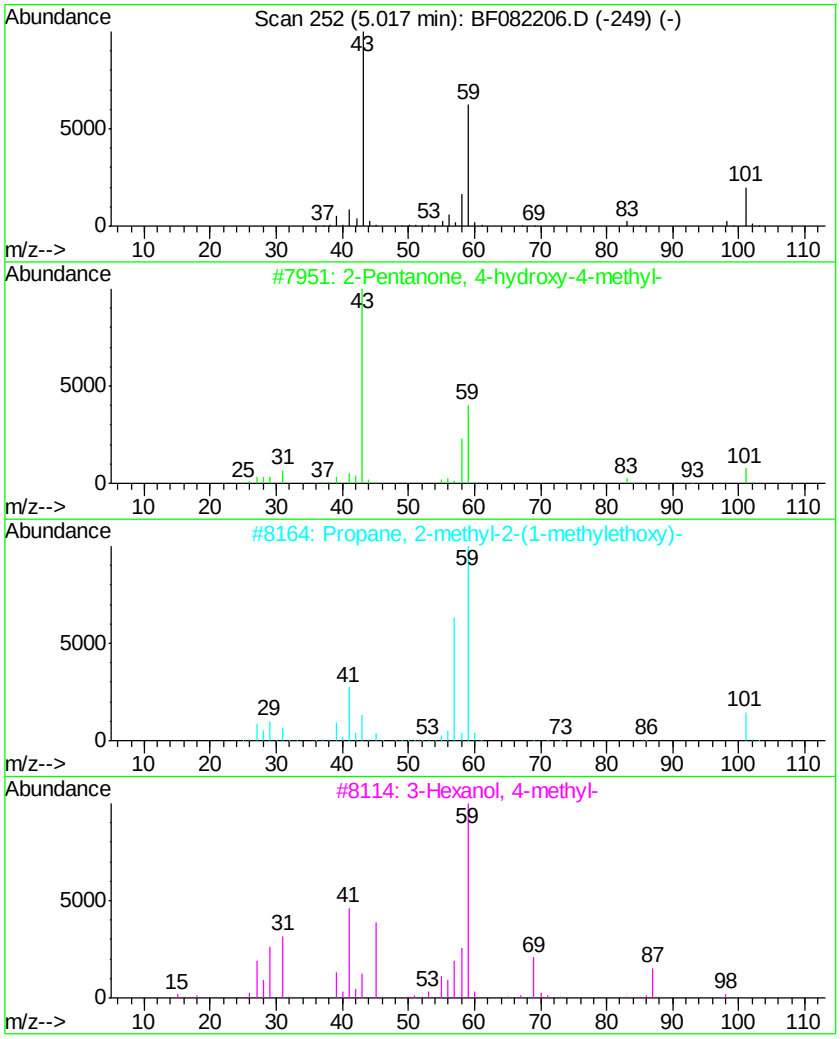
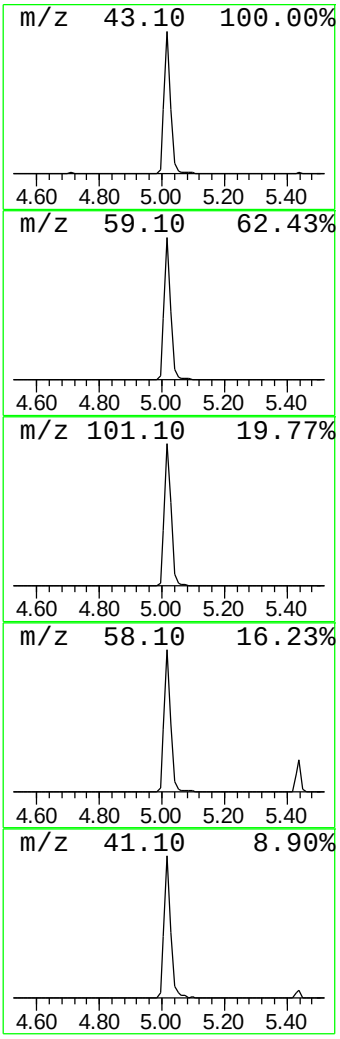
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	39.53 ng	950253	1,4-Dichlorobenzene-d4	6.83

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	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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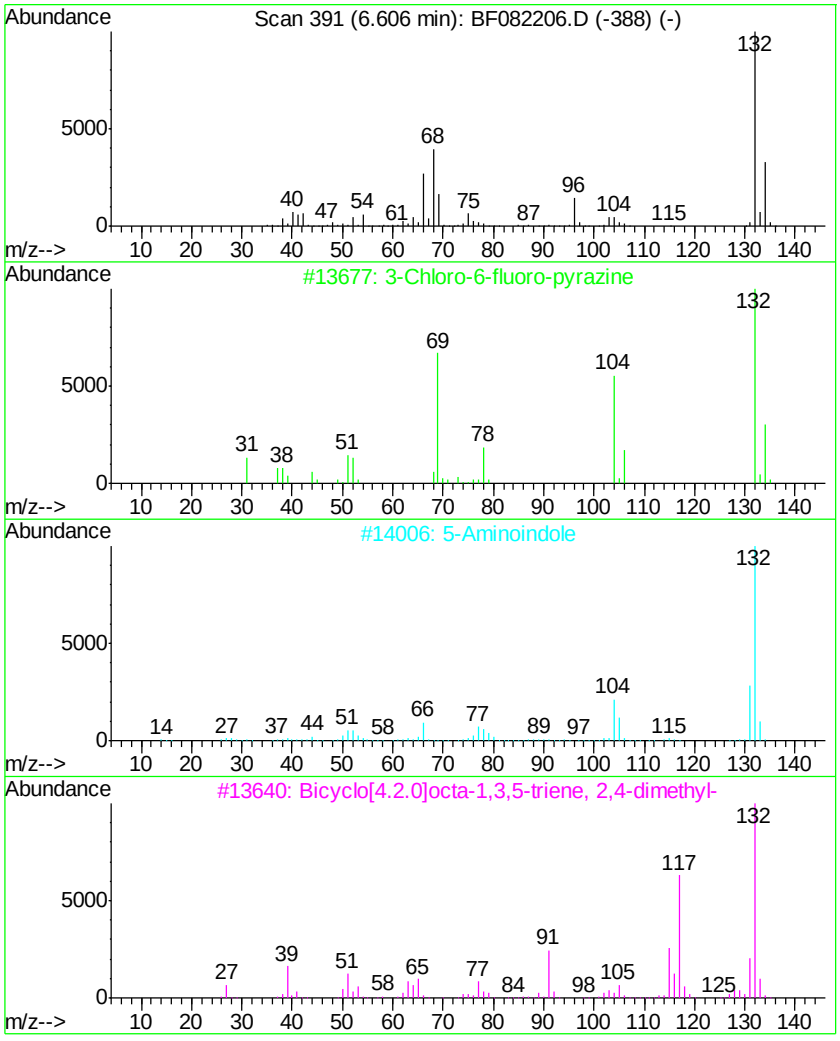
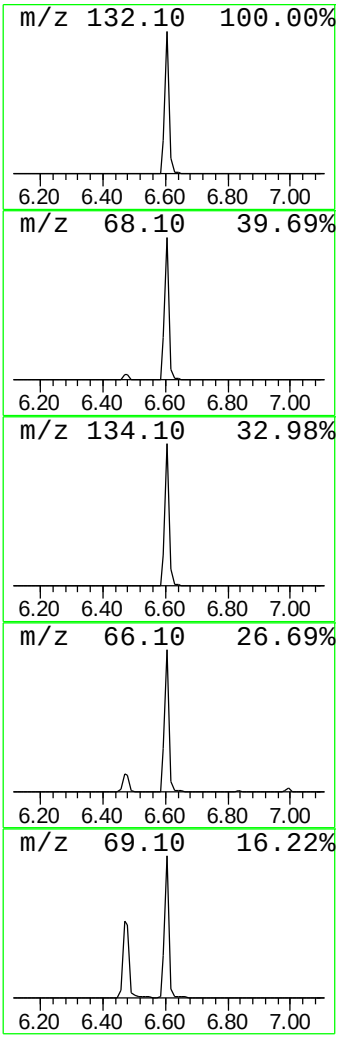
Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	72.15 ng	1734390	1,4-Dichlorobenzene-d4	6.83

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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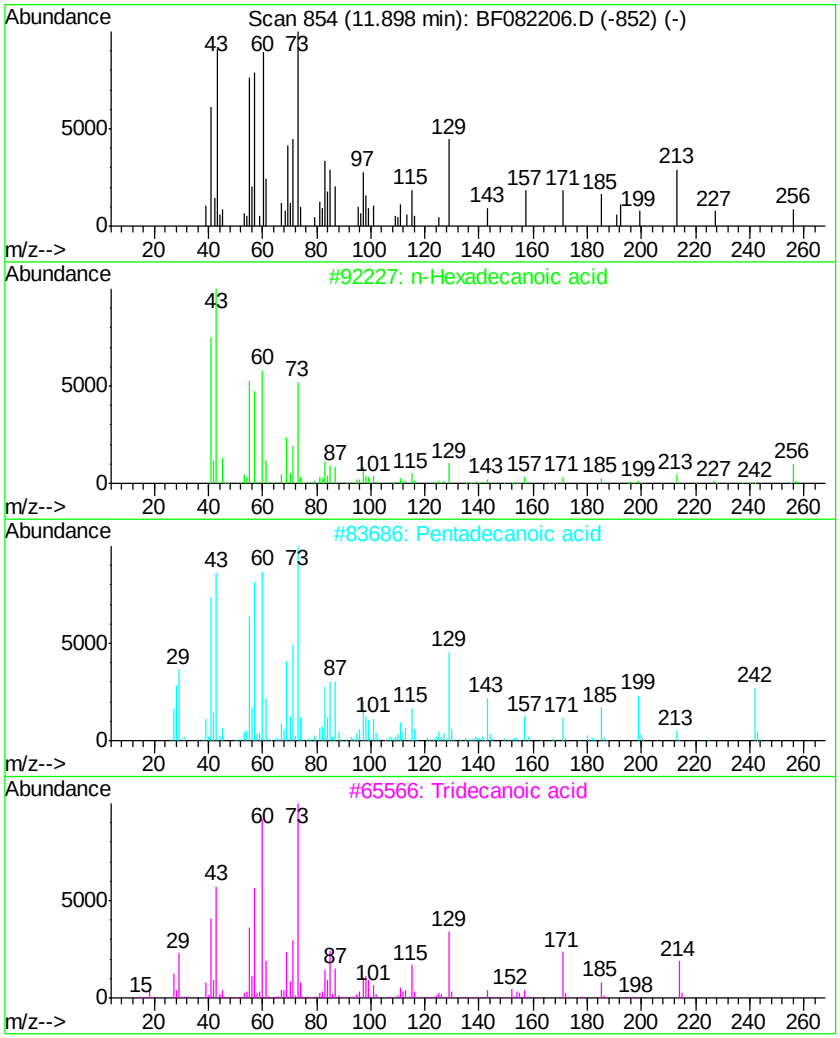
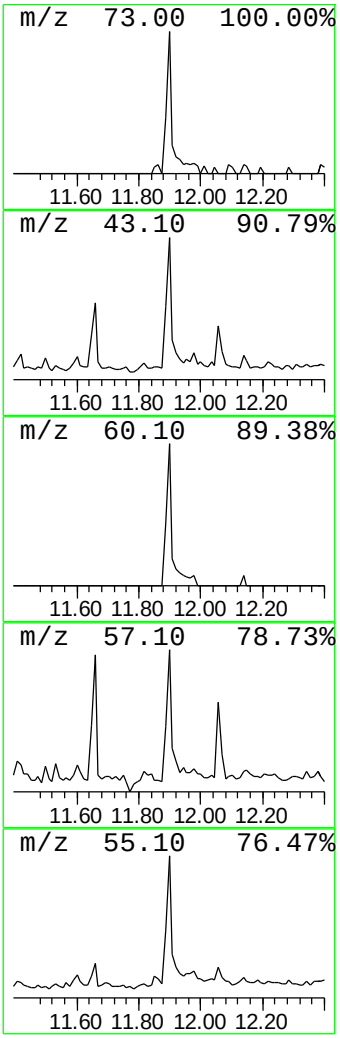
Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.94 ng	90100	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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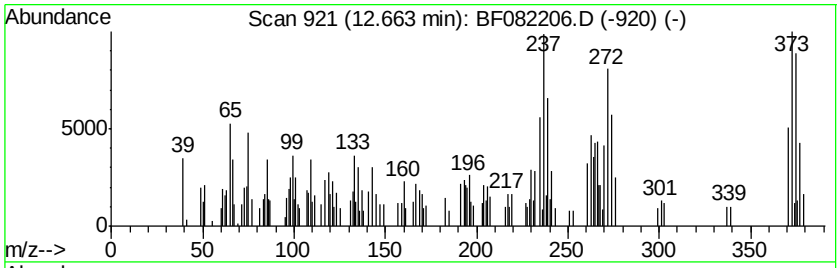
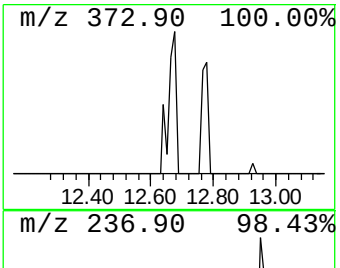
Peak Number 5 unknown12.66 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	3.29 ng	100719	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8-Dichloro-2-oxa-6-selenaadama...	272	C8H10Cl2OSe	1000189-96-4	35
2	1,4-Dibromo-2,5-difluorobenzene	270	C6H2Br2F2	000327-51-5	25
3	1,2-Dibromo-4,5-difluorobenzene	270	C6H2Br2F2	064695-78-9	25
4	1,2-Dichloro-3-iodobenzene	272	C6H3Cl2I	002401-21-0	15
5	2,4-Dichloroiodobenzene	272	C6H3Cl2I	029898-32-6	15





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
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Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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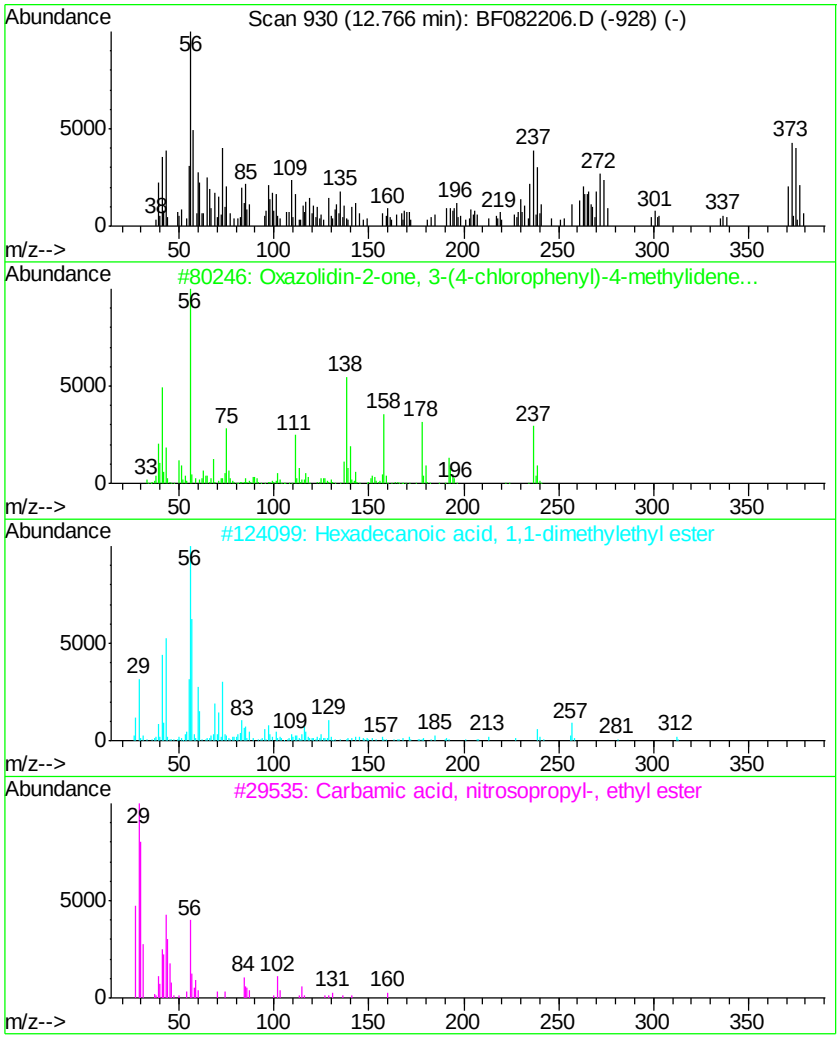
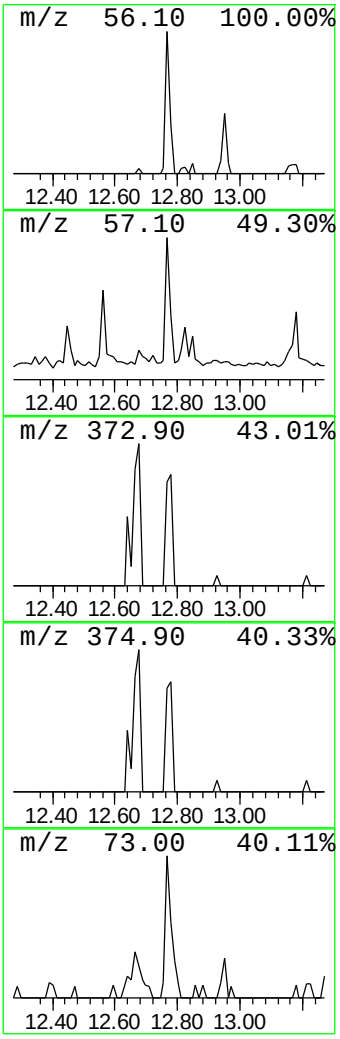
Peak Number 6 unknown12.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	9.84 ng	236283	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one, 3-(4-chlorophe...	237	C12H12ClNO2	055476-05-6	22
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	10
3	Carbamic acid, nitrosopropyl-, e...	160	C6H12N2O3	019935-86-5	9
4	1,5-Pentanediamine	102	C5H14N2	000462-94-2	9
5	3,4,4,6-Tetramethyl-2-(m-chlorop...	266	C14H19ClN2O	053004-31-2	9





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ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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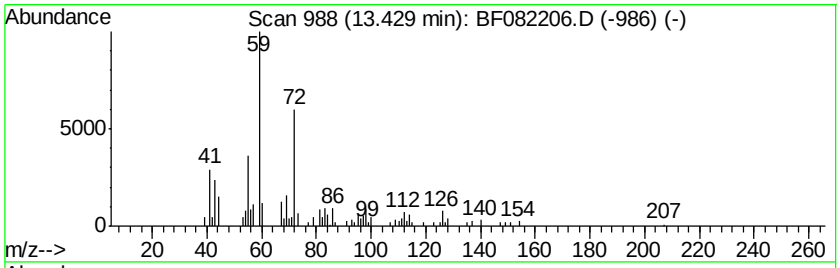
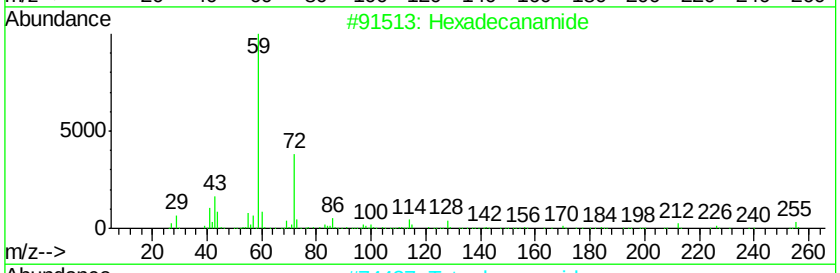
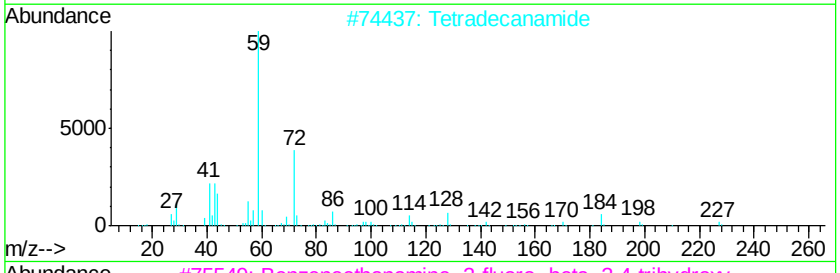
Peak Number 7 Hexadecanamide Concentration Rank 9

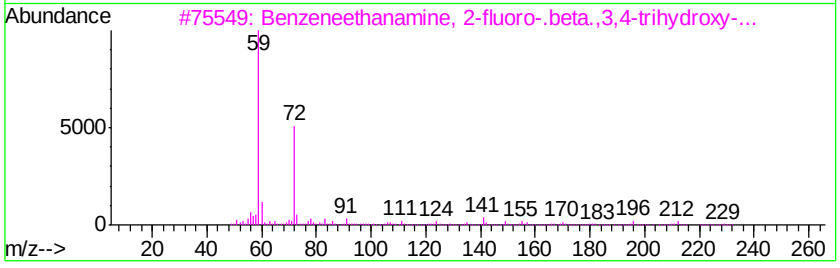
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	3.25 ng	78112	Chrysene-d12	14.00

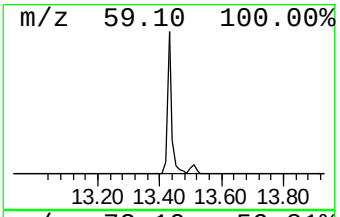
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	72
2	Tetradecanamide	227	C14H29NO	000638-58-4	64
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	Octanamide	143	C8H17NO	000629-01-6	53

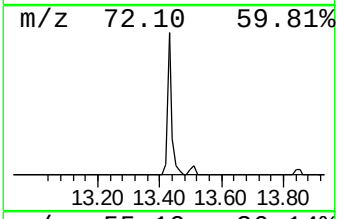


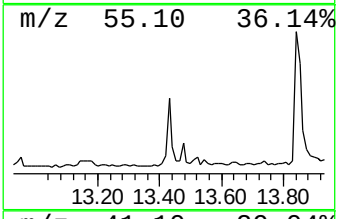


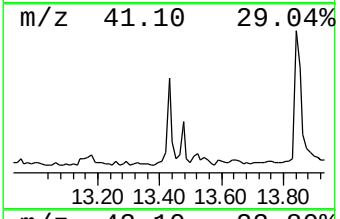


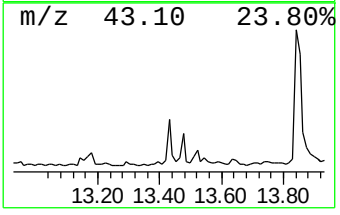












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Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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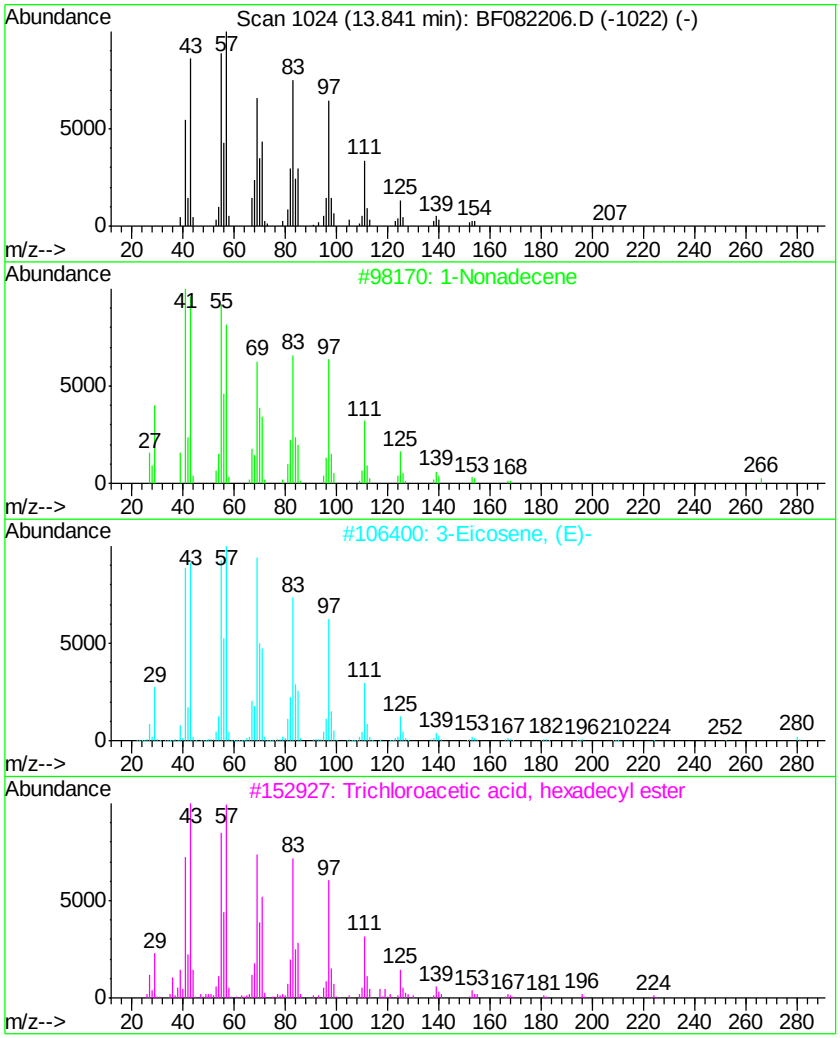
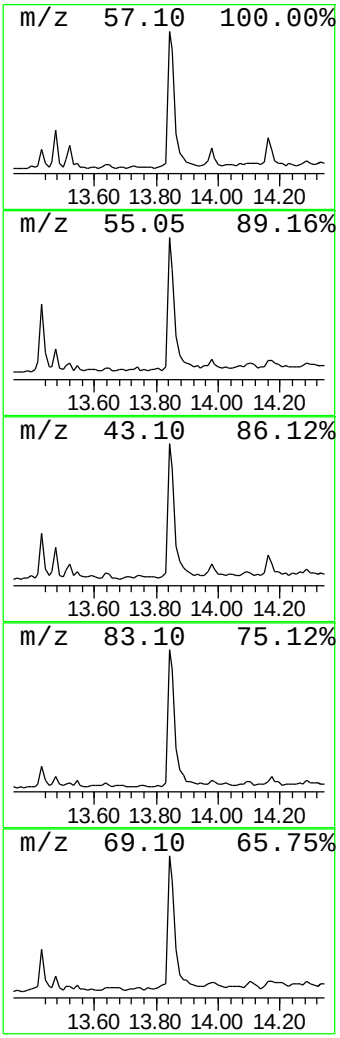
Peak Number 8 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	9.59 ng	230143	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
5	1-Docosene	308	C22H44	001599-67-3	91





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Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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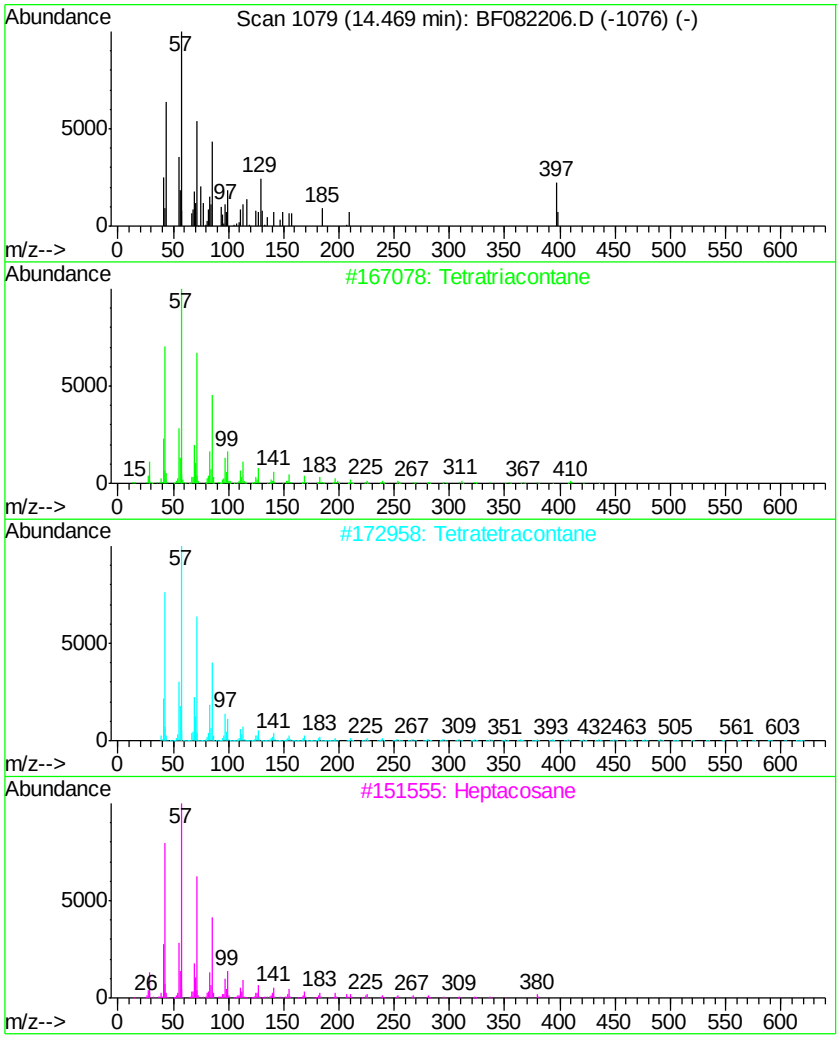
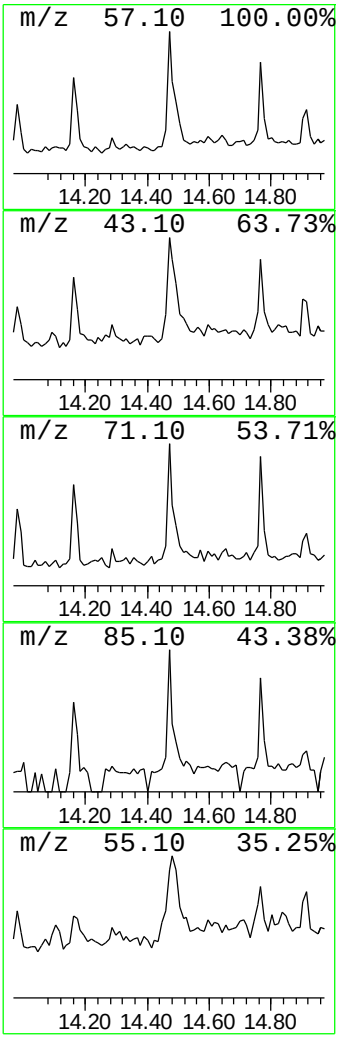
Peak Number 9 Tetratriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	3.34 ng	80285	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	53
2	Tetratetracontane	619	C44H90	007098-22-8	53
3	Heptacosane	380	C27H56	000593-49-7	53
4	10-Methylnonadecane	282	C20H42	056862-62-5	53
5	Eicosane	282	C20H42	000112-95-8	49





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Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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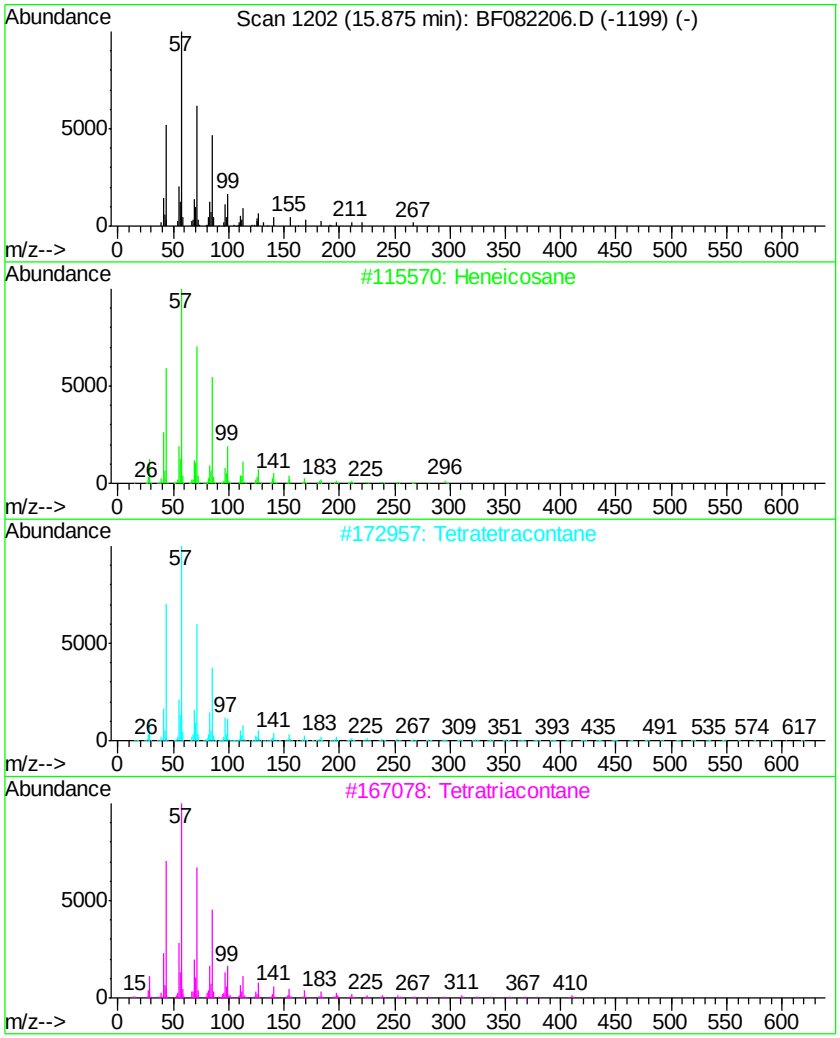
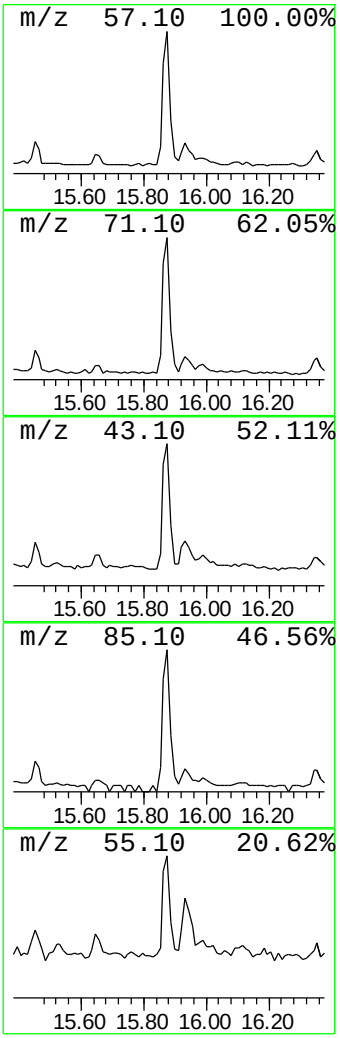
Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	5.05 ng	126813	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Tetratriacontane	479	C34H70	014167-59-0	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hentriacontane	437	C31H64	000630-04-6	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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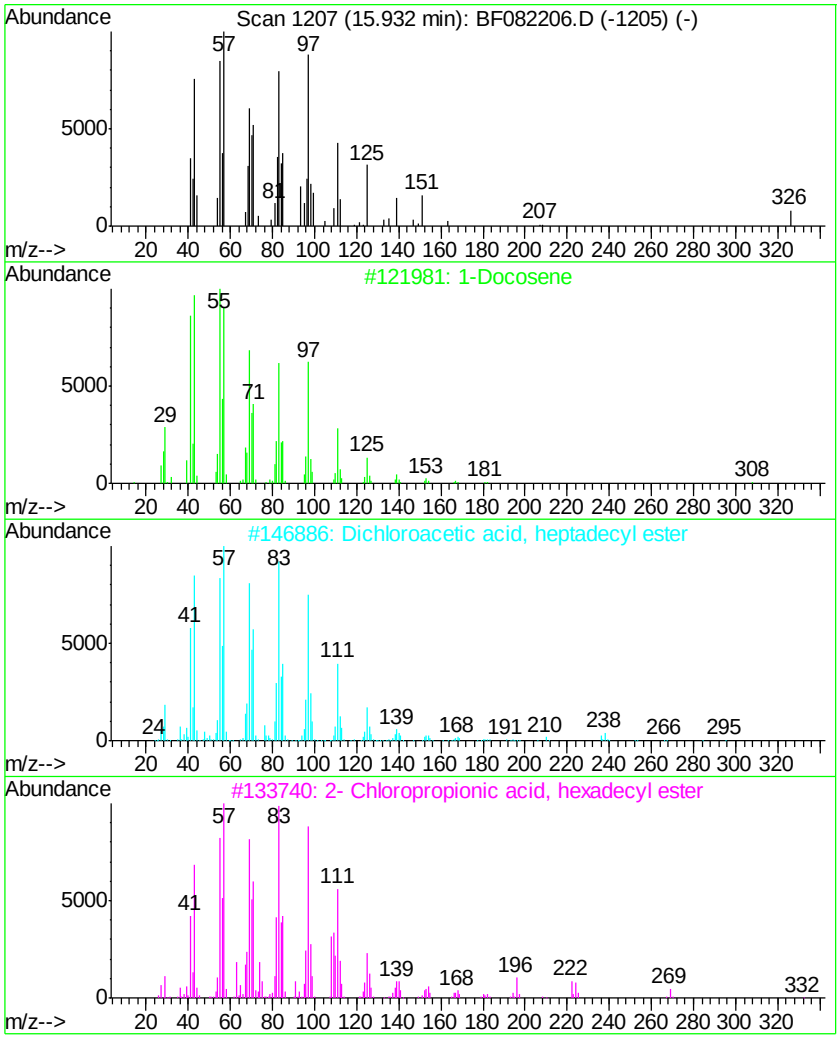
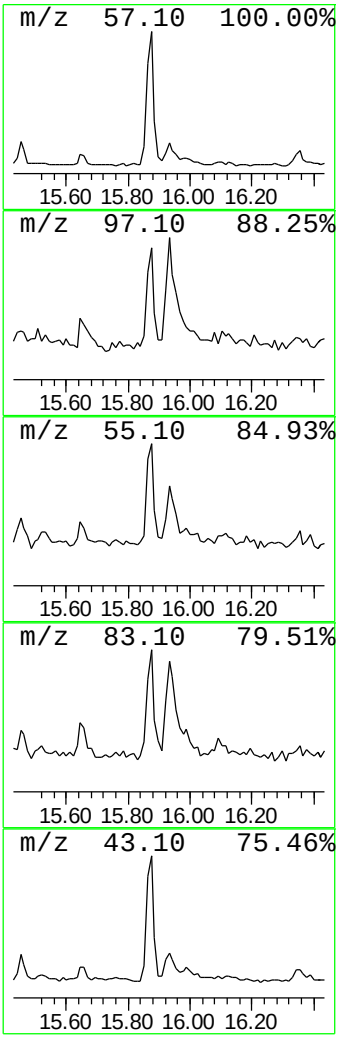
Peak Number 11 1-Docosene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.02 ng	50754	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
3	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082206.D
Acq On : 11 Oct 2015 6:10
Operator : UM/IZ
Sample : G3979-18
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A9COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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...	5.02	39.5	ng	950253	1	6.83	480756	20.0
unknown6.61	6.61	72.2	ng	1734390	1	6.83	480756	20.0
n-Hexadecanoic acid	11.90	2.9	ng	90100	4	11.36	612754	20.0
unknown12.66	12.66	3.3	ng	100719	4	11.36	612754	20.0
unknown12.77	12.77	9.8	ng	236283	5	14.00	480171	20.0
Hexadecanamide	13.43	3.3	ng	78112	5	14.00	480171	20.0
1-Nonadecene	13.84	9.6	ng	230143	5	14.00	480171	20.0
Tetratriacontane	14.47	3.3	ng	80285	5	14.00	480171	20.0
Heneicosane	15.88	5.0	ng	126813	6	15.44	501950	20.0
1-Docosene	15.93	2.0	ng	50754	6	15.44	501950	20.0