LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095740.D
Acq On : 7 Jun 2017 10:25
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

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-BF060517.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	4.610	510	514	529	rBV2	62037	180746	8.13%	1.064%
2	5.281	624	628	663	rBV	1226193	2090388	93.97%	12.305%
3	6.945	906	911	922	rBV	1242567	1977316	88.89%	11.639%
4	7.045	922	928	944	rVB	1511197	2224465	100.00%	13.094%
5	7.381	982	985	1000	rBV	277956	381747	17.16%	2.247%
6	7.622	1020	1026	1048	rBV	1232031	1605179	72.16%	9.449%
7	8.304	1136	1142	1159	rBV	820248	1190962	53.54%	7.011%
8	9.416	1326	1331	1346	rBV	369026	484200	21.77%	2.850%
9	11.198	1627	1634	1648	rBV	1554930	1947134	87.53%	11.462%
10	11.886	1746	1751	1758	rBV	205454	238073	10.70%	1.401%
11	12.233	1805	1810	1816	rBV2	363969	459028	20.64%	2.702%
12	13.098	1951	1957	1961	rBV	22008	26681	1.20%	0.157%
13	13.527	2025	2030	2038	rBV	696182	907584	40.80%	5.342%
14	13.868	2082	2088	2090	rBV2	21483	29527	1.33%	0.174%
15	14.627	2213	2217	2223	rBV	300305	355931	16.00%	2.095%
16	15.645	2386	2390	2397	rBV3	68504	87107	3.92%	0.513%
17	16.451	2521	2527	2533	rVB	27462	38588	1.73%	0.227%
18	16.751	2574	2578	2585	rBV	38578	48093	2.16%	0.283%
19	17.004	2615	2621	2625	rVB	1125802	1290925	58.03%	7.599%
20	17.409	2687	2690	2697	rVB	24364	28348	1.27%	0.167%
21	17.856	2762	2766	2769	rVB	24118	26599	1.20%	0.157%
22	18.256	2830	2834	2844	rBV2	107710	208375	9.37%	1.227%
23	18.345	2844	2849	2854	rBV	322083	384985	17.31%	2.266%
24	18.674	2901	2905	2913	rVB	36454	46663	2.10%	0.275%
25	19.062	2966	2971	2979	rBV	94399	118520	5.33%	0.698%
26	19.427	3029	3033	3037	rBV3	26882	35786	1.61%	0.211%
27	19.780	3088	3093	3103	rBV2	56408	108467	4.88%	0.638%
28	20.009	3128	3132	3138	rBV	237859	274919	12.36%	1.618%
29	20.462	3204	3209	3212	rBV	39975	50119	2.25%	0.295%
30	20.503	3212	3216	3220	rVV4	20559	38892	1.75%	0.229%
31	20.545	3221	3223	3228	rVB3	18953	24505	1.10%	0.144%
32	21.597	3399	3402	3406	rVB6	14452	24732	1.11%	0.146%
33	21.780	3431	3433	3442	rVB10	14020	24015	1.08%	0.141%
34	21.956	3459	3463	3468	rVB7	15006	29653	1.33%	0.175%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095740.D
Acq On : 7 Jun 2017 10:25
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 16988252

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
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Acq On : 7 Jun 2017 10:25
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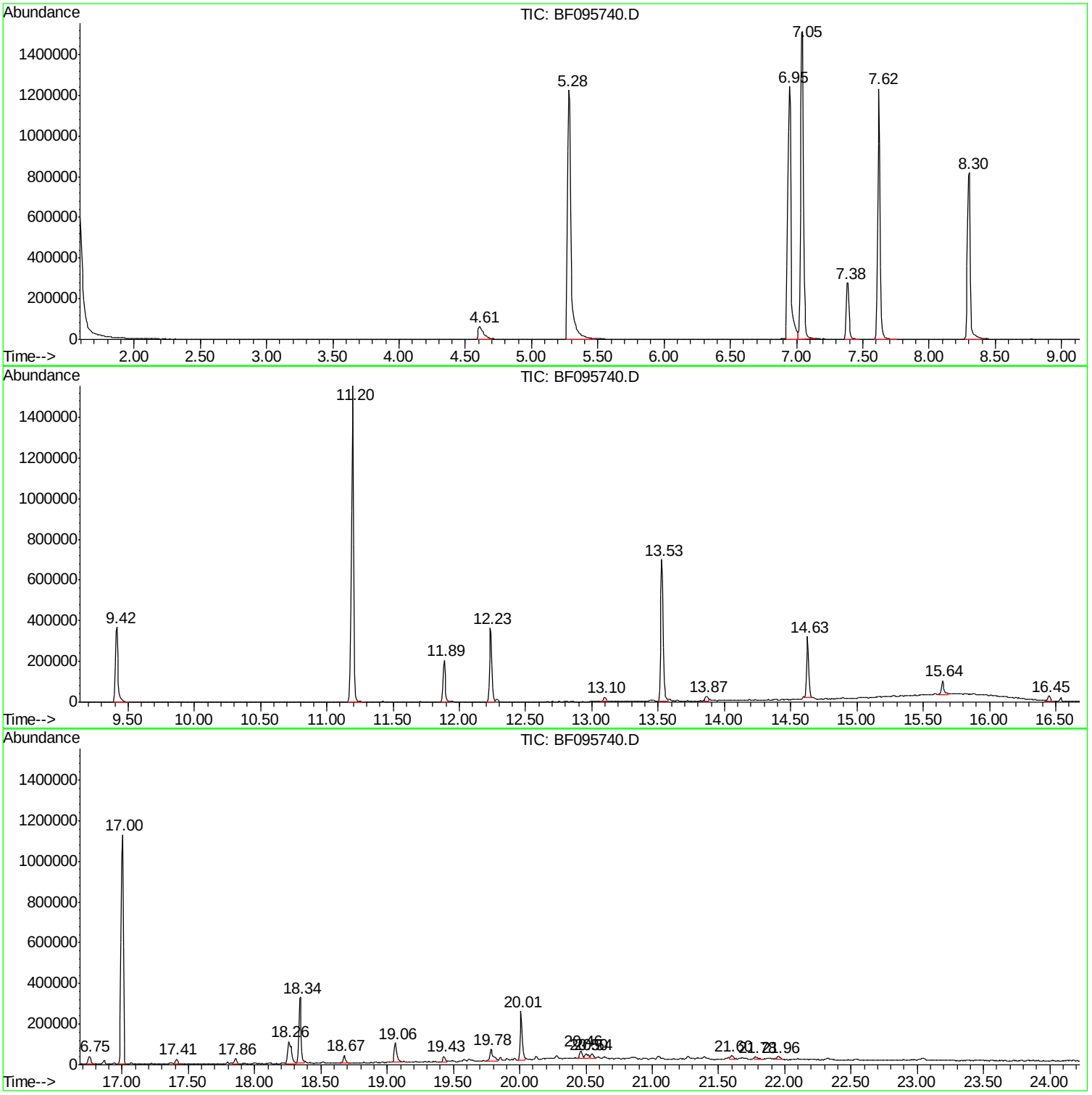
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

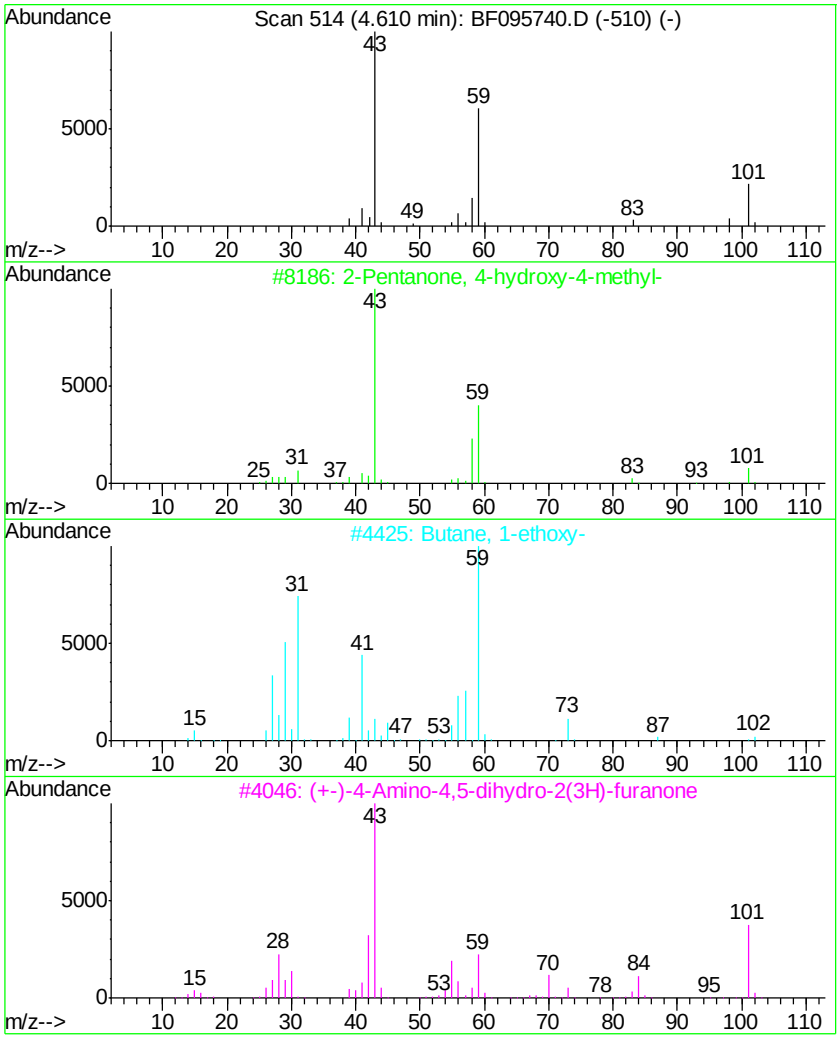
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

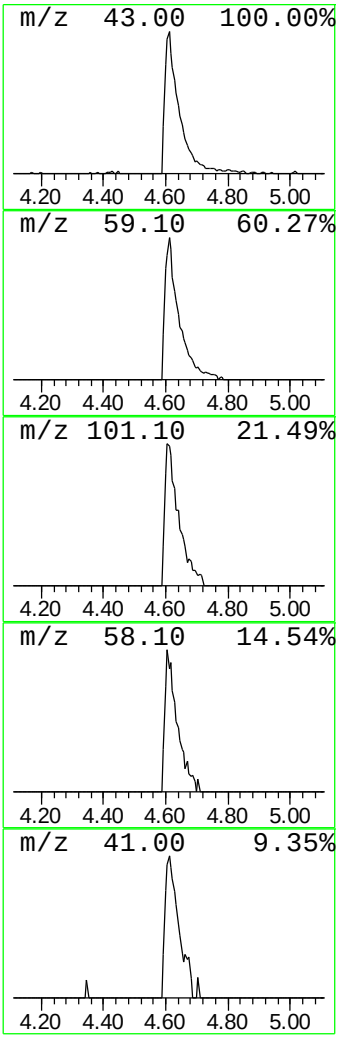
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	9.47 ng	180746	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095740.D
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Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

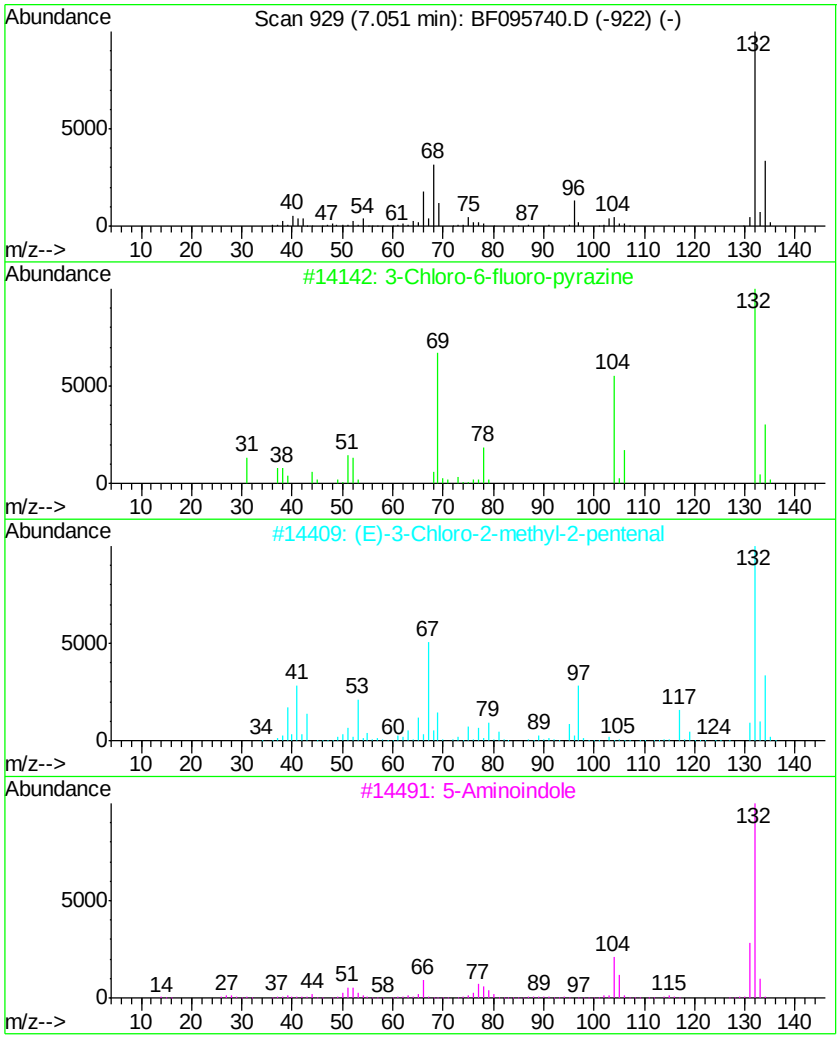
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

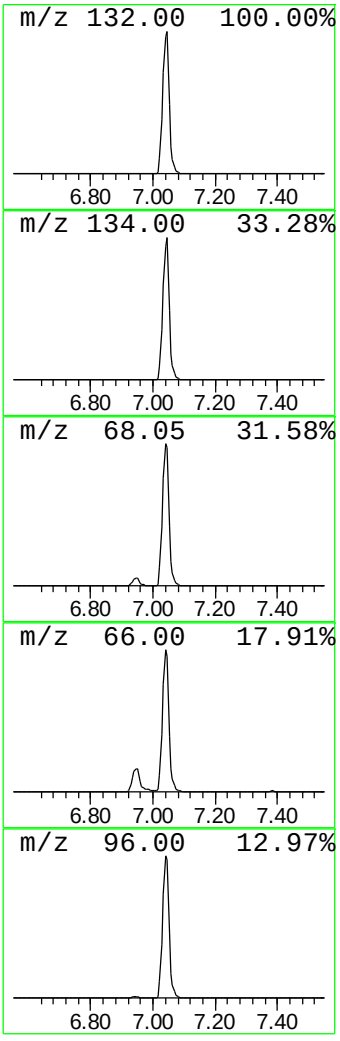
****

Peak Number 2 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	116.54 ng	2224470	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Acq On : 7 Jun 2017 10:25
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

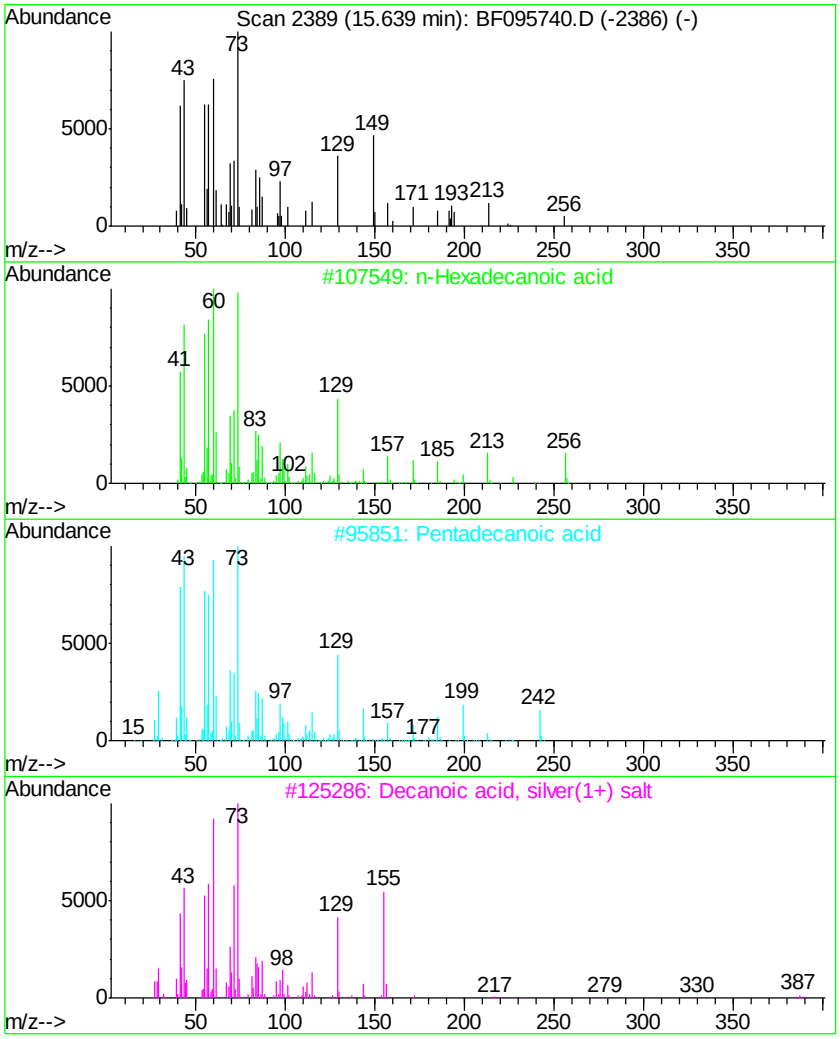
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

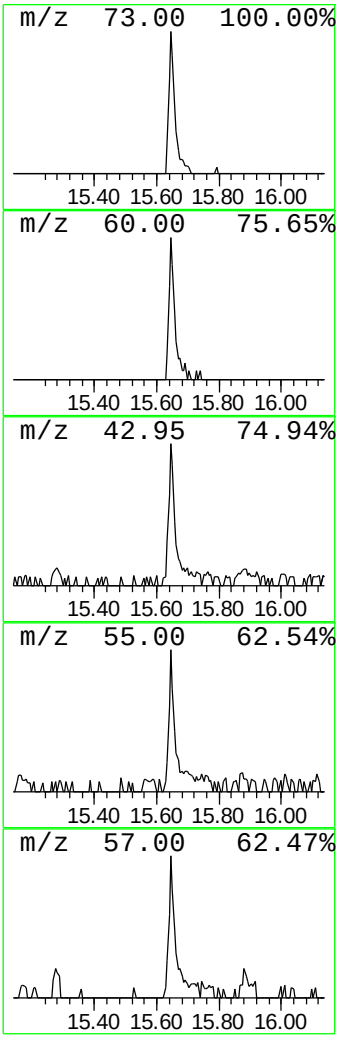
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	4.89 ng	87107	Phenanthrene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	59
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25





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Data File : BF095740.D
Acq On : 7 Jun 2017 10:25
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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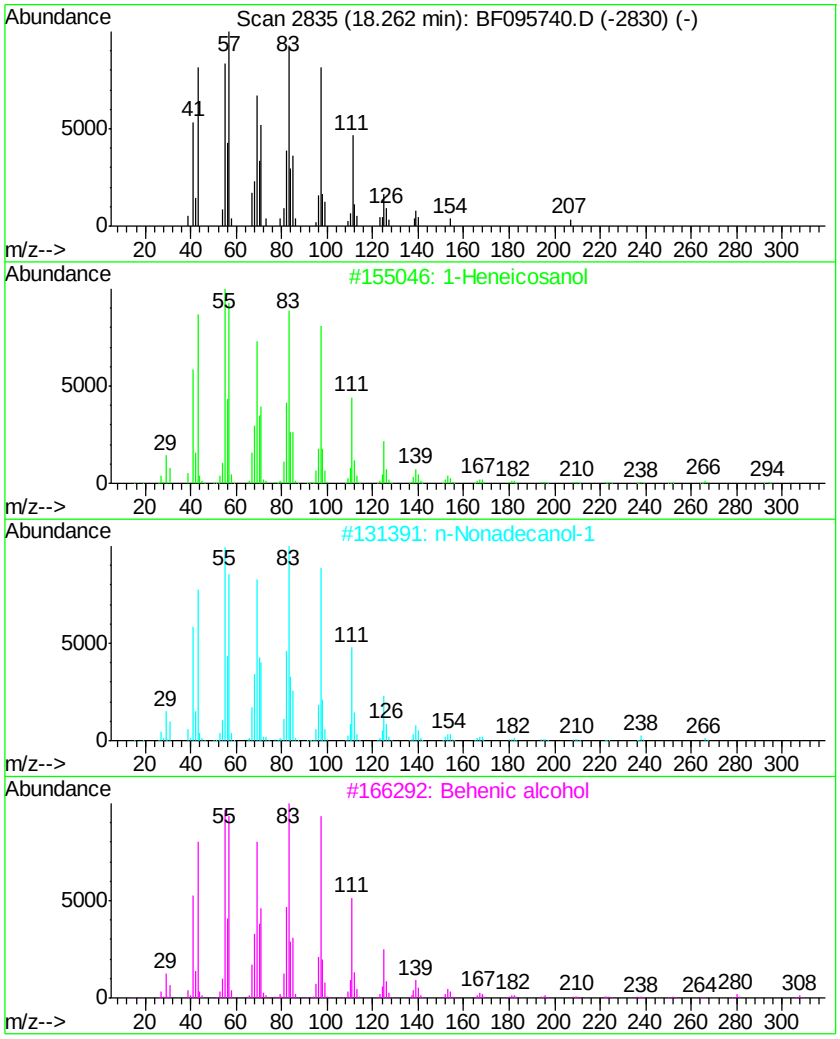
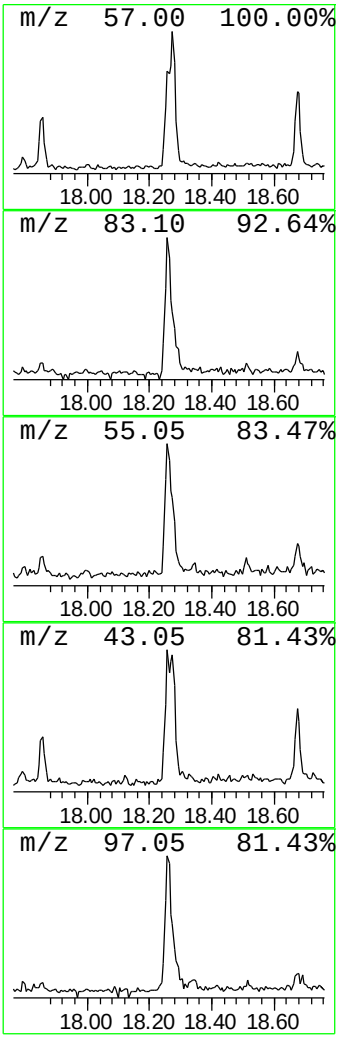
****

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	10.83 ng	208375	Chrysene-d12	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





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Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

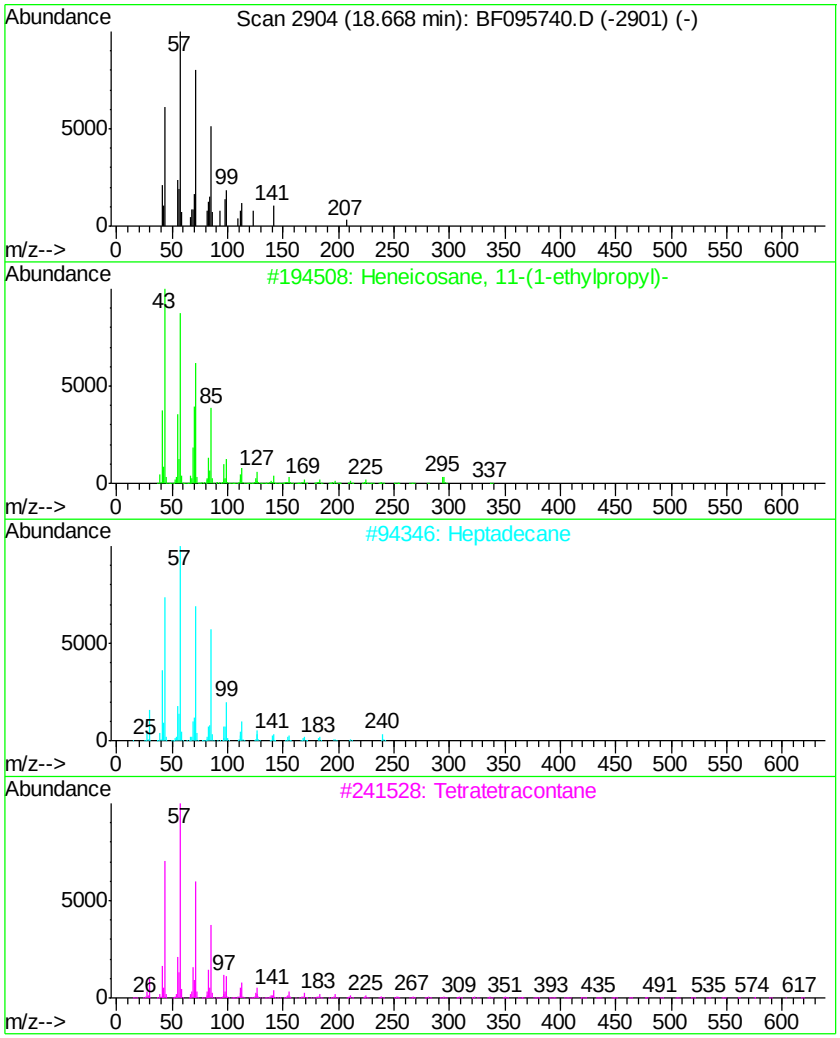
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

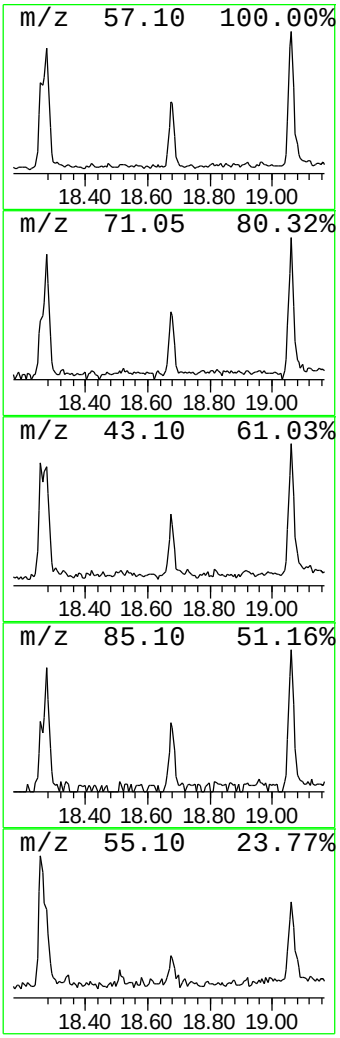
****

Peak Number 8 Heneicosane, 11-(1-ethylpro... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.67	2.42 ng	46663	Chrysene-d12	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
2	Heptadecane	240	C17H36	000629-78-7	83
3	Tetratetracontane	619	C44H90	007098-22-8	78
4	Heneicosane	296	C21H44	000629-94-7	72
5	Octadecane	254	C18H38	000593-45-3	72





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Instrument :
BNA_F
ClientSampleId :
SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
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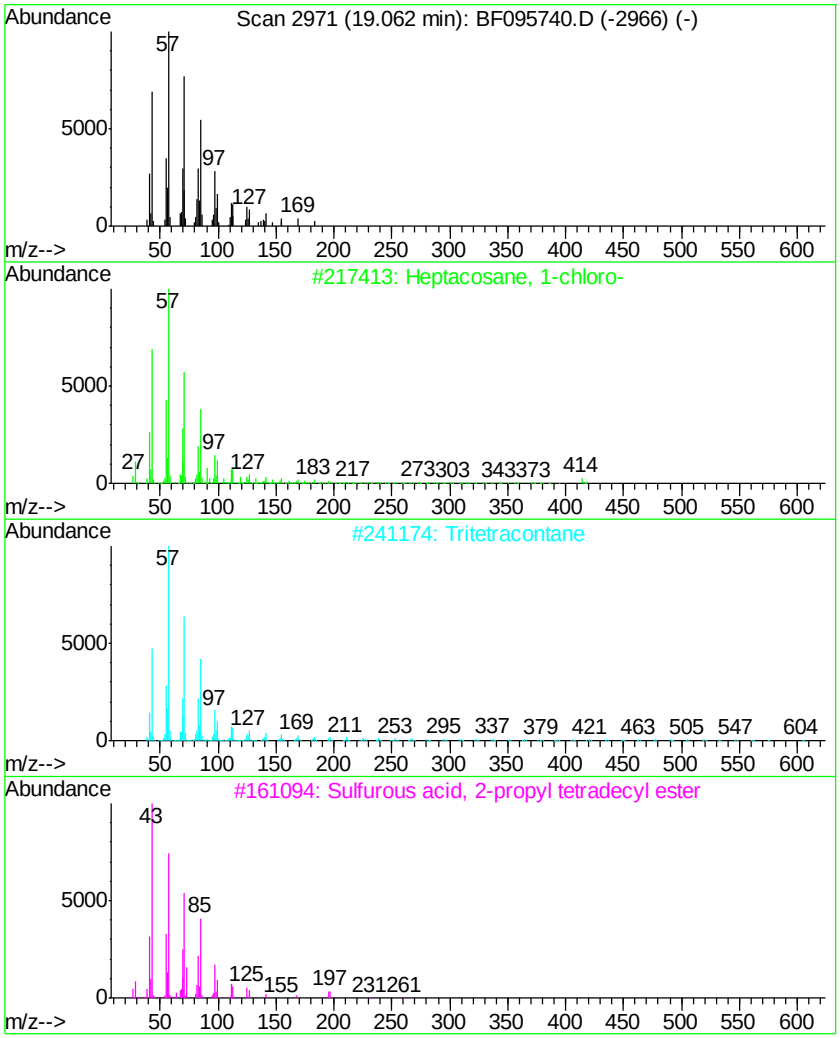
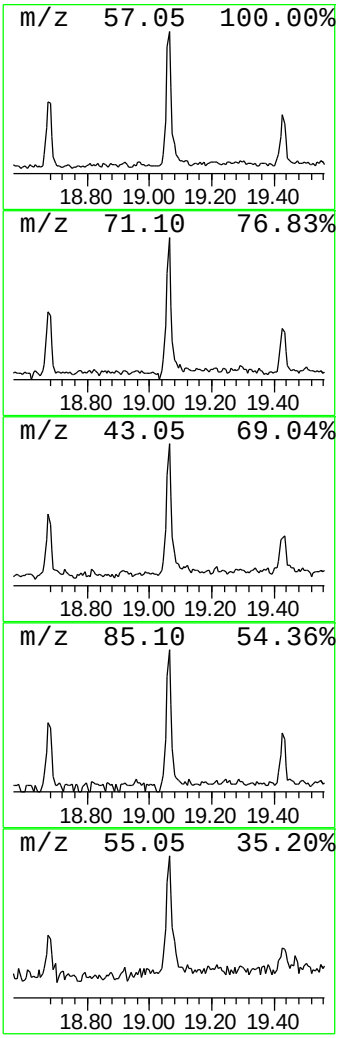
Peak Number 9 Heptacosane, 1-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.06	6.16 ng	118520	Chrysene-d12	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
2	Tritetracontane	605	C43H88	007098-21-7	91
3	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	91
4	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	87





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Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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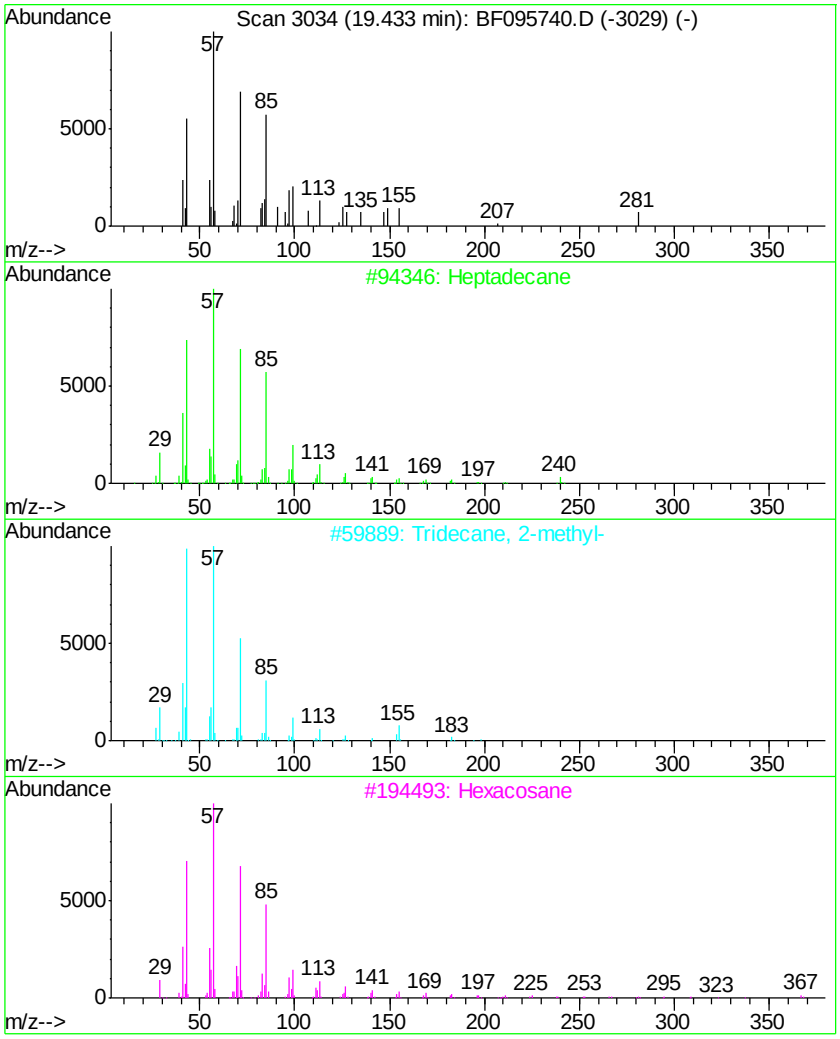
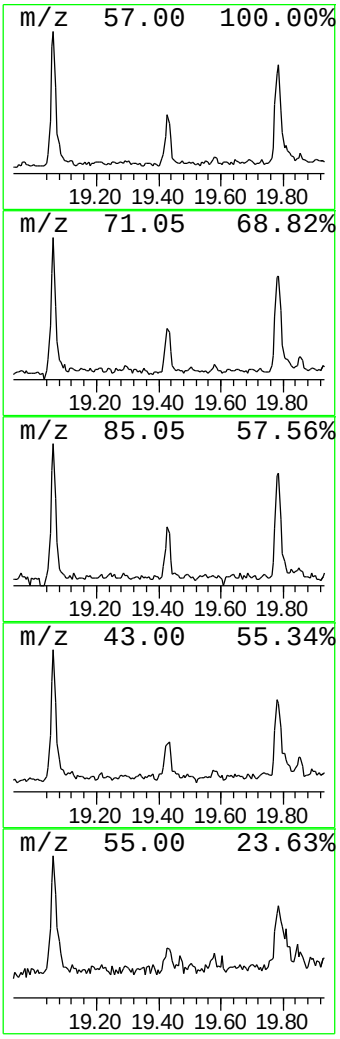
Peak Number 10 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	2.60 ng	35786	Perylene-d12	20.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	80
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9	72
3	Hexacosane	366	C26H54	000630-01-3	64
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	59
5	Octadecane	254	C18H38	000593-45-3	59





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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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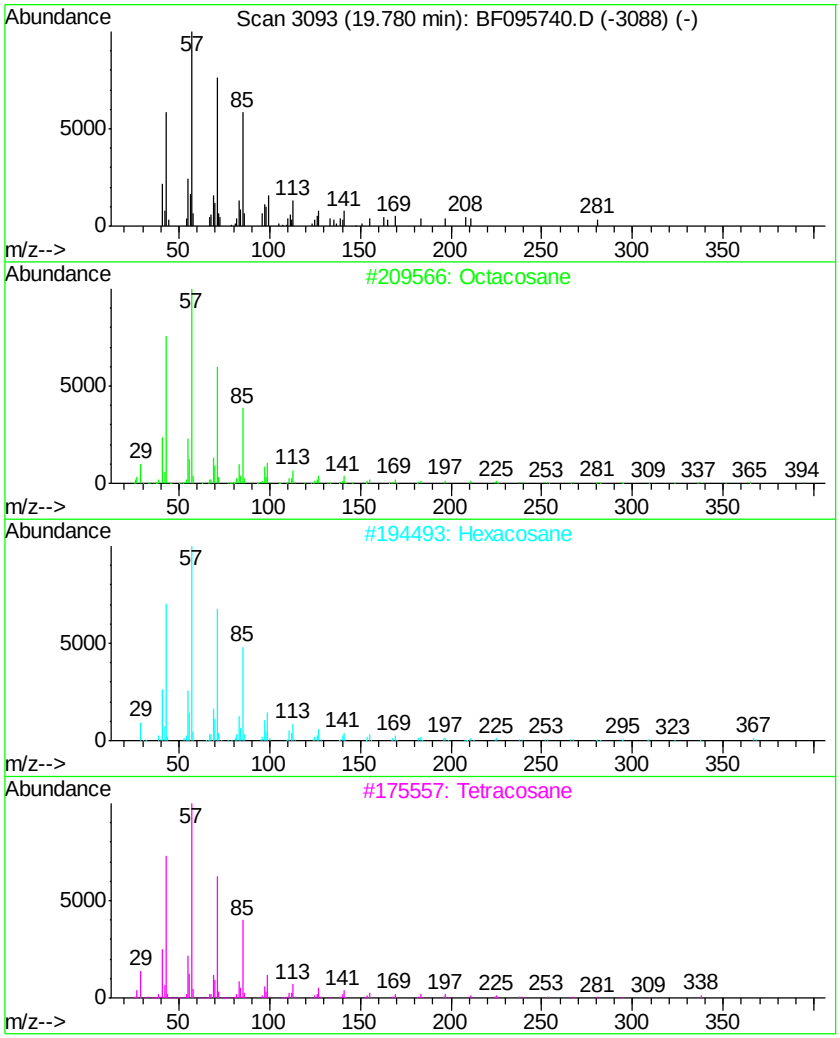
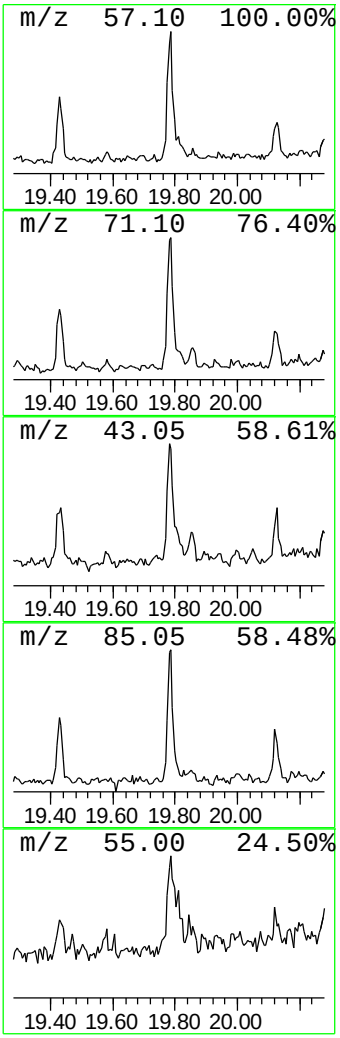
Peak Number 11 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	7.89 ng	108467	Perylene-d12	20.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	87
5	10-Methylnonadecane	282	C20H42	056862-62-5	87





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Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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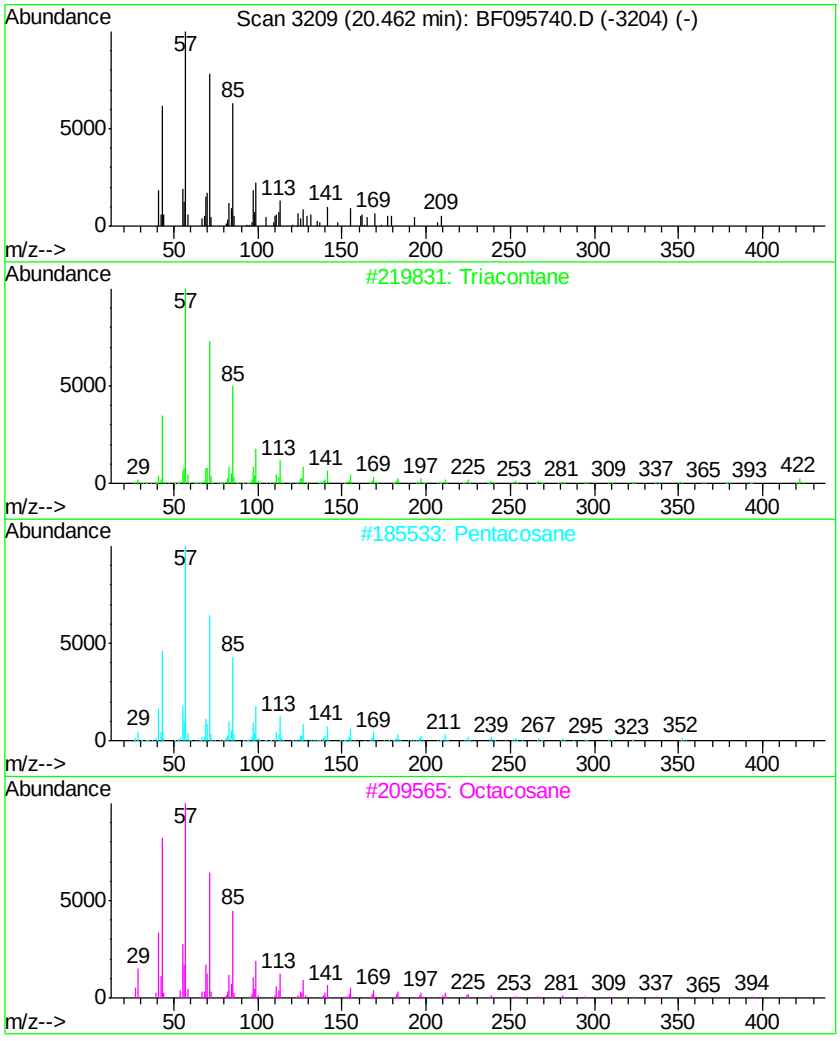
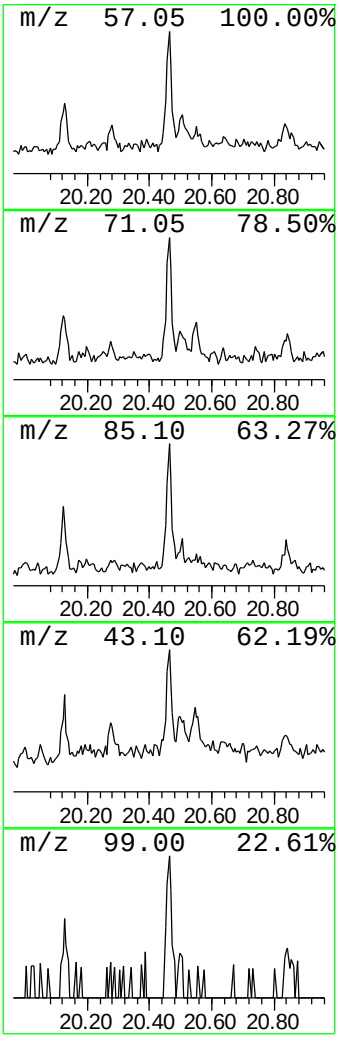
Peak Number 12 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.46	3.65 ng	50119	Perylene-d12	20.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	87
5	Heptadecane	240	C17H36	000629-78-7	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095740.D
Acq On : 7 Jun 2017 10:25
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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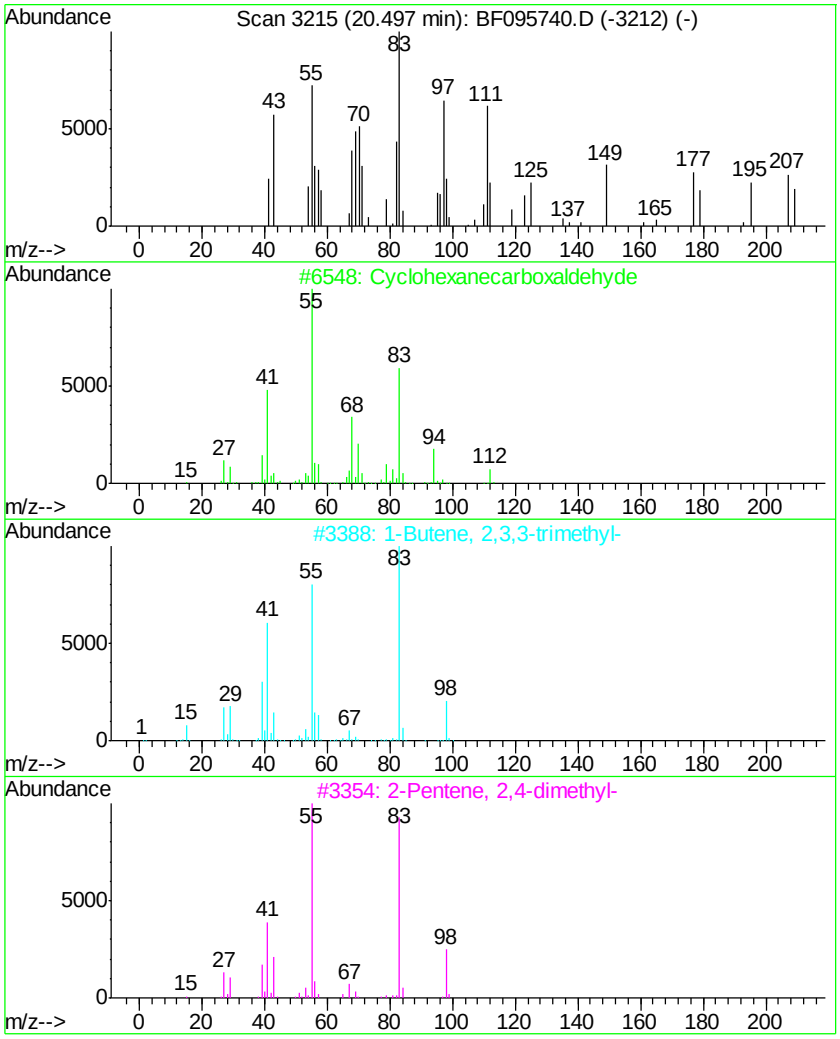
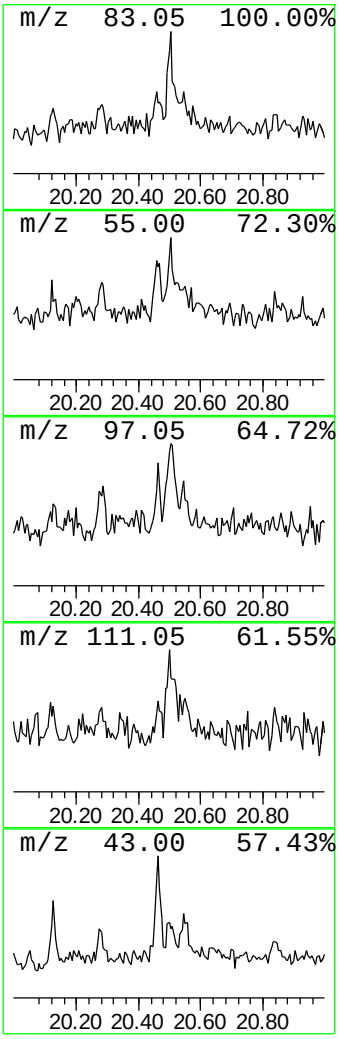
Peak Number 13 unknown20.50 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.50	2.83 ng	38892	Perylene-d12	20.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanecarboxaldehyde	112	C7H12O	002043-61-0	27
2	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	25
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	25
4	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	002207-01-4	25
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095740.D
Acq On : 7 Jun 2017 10:25
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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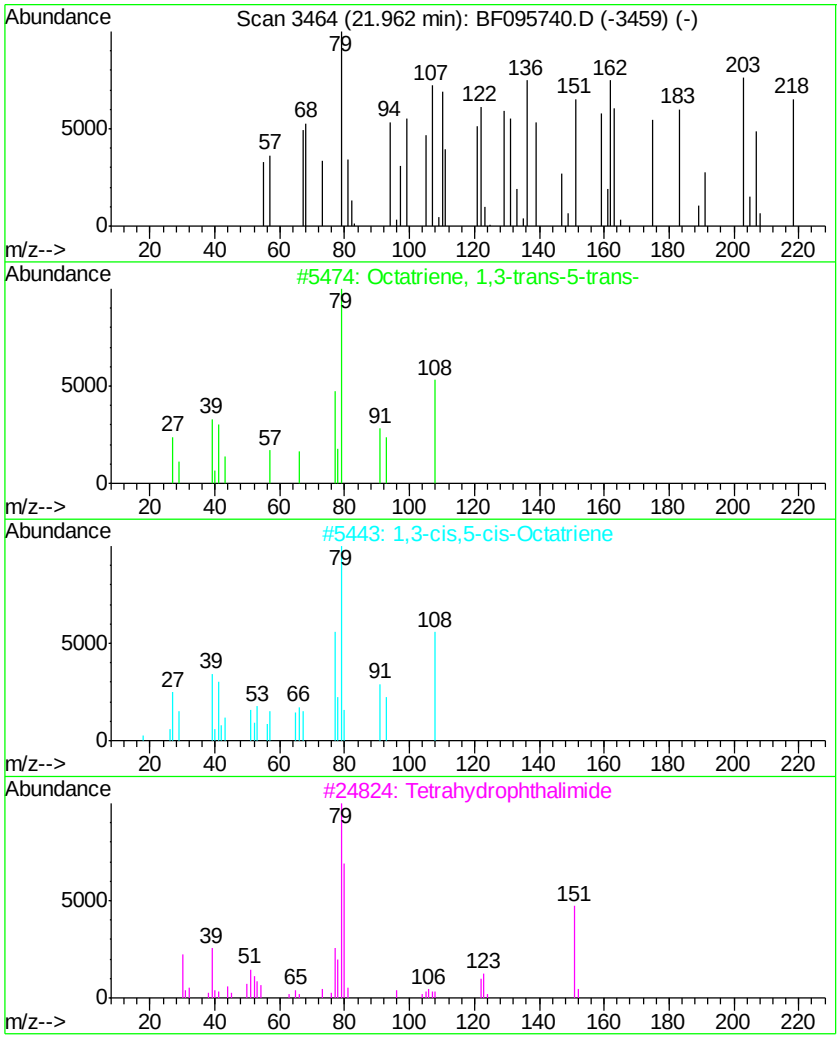
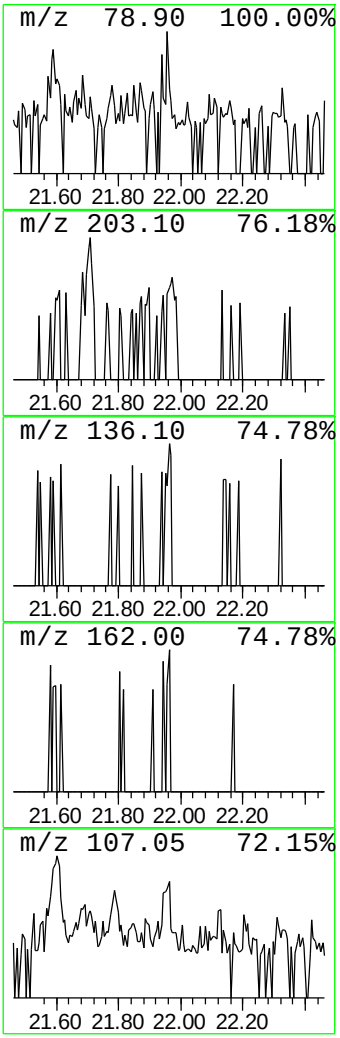
Peak Number 14 unknown21.96 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.96	2.16 ng	29653	Perylene-d12	20.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octatriene, 1,3-trans-5-trans-	108	C8H12	033580-04-0	14
2	1,3-cis,5-cis-Octatriene	108	C8H12	040087-62-5	10
3	Tetrahydrophthalimide	151	C8H9NO2	027813-21-4	9
4	1,3-Cyclohexadiene, 5-butyl-	136	C10H16	030168-57-1	9
5	4-Decen-6-yne, (E)-	136	C10H16	013343-77-6	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095740.D
Acq On : 7 Jun 2017 10:25
Operator : SJ/MA
Sample : I3469-13
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(7-9)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.61	9.5	ng	180746	1	7.39	381747	20.0
unknown7.05	7.05	116.5	ng	2224470	1	7.39	381747	20.0
n-Hexadecanoic acid	15.64	4.9	ng	87107	4	14.63	355931	20.0
1-Heneicosanol	18.26	10.8	ng	208375	5	18.34	384985	20.0
Heneicosane, 11-(...	18.67	2.4	ng	46663	5	18.34	384985	20.0
Heptacosane, 1-ch...	19.06	6.2	ng	118520	5	18.34	384985	20.0
Heptadecane	19.43	2.6	ng	35786	6	20.01	274919	20.0
Octacosane	19.78	7.9	ng	108467	6	20.01	274919	20.0
Triacontane	20.46	3.6	ng	50119	6	20.01	274919	20.0
unknown20.50	20.50	2.8	ng	38892	6	20.01	274919	20.0
unknown21.96	21.96	2.2	ng	29653	6	20.01	274919	20.0