LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095781.D
Acq On : 8 Jun 2017 13:56
Operator : SJ/MA
Sample : I3469-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(0-2)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	4.575	503	508	526	rBV	51032	148169	7.80%	0.905%
2	5.257	620	624	655	rBV	925298	1588695	83.62%	9.707%
3	6.928	903	908	920	rBV	1016498	1613966	84.95%	9.861%
4	7.022	920	924	935	rVB	1232795	1782759	93.83%	10.892%
5	7.369	979	983	998	rBV	278664	371692	19.56%	2.271%
6	7.604	1018	1023	1039	rVB	1003303	1273500	67.03%	7.781%
7	8.286	1133	1139	1157	rBV	693561	1006625	52.98%	6.150%
8	9.398	1323	1328	1342	rBV	414770	529089	27.85%	3.233%
9	11.180	1624	1631	1642	rBV	1491320	1899907	100.00%	11.608%
10	11.868	1744	1748	1754	rBV	220493	259268	13.65%	1.584%
11	12.221	1803	1808	1813	rBV2	462532	589724	31.04%	3.603%
12	12.268	1813	1816	1820	rVB2	26801	32543	1.71%	0.199%
13	13.080	1946	1954	1959	rBV2	37037	47668	2.51%	0.291%
14	13.445	2008	2016	2021	rBV4	9885	23312	1.23%	0.142%
15	13.515	2023	2028	2035	rBV	793591	1058487	55.71%	6.467%
16	13.851	2081	2085	2094	rBV	39729	61659	3.25%	0.377%
17	14.580	2206	2209	2210	rBV2	23186	22473	1.18%	0.137%
18	14.615	2210	2215	2219	rVV	428625	552965	29.10%	3.378%
19	14.651	2219	2221	2227	rVB	24823	31998	1.68%	0.195%
20	15.645	2387	2390	2393	rBV	95471	101865	5.36%	0.622%
21	16.439	2519	2525	2529	rVB	52760	72012	3.79%	0.440%
22	16.739	2571	2576	2582	rBV	75108	96241	5.07%	0.588%
23	16.992	2613	2619	2623	rVB	1271712	1452361	76.44%	8.874%
24	17.350	2675	2680	2684	rBV5	12086	19650	1.03%	0.120%
25	17.398	2684	2688	2691	rVB	24422	25009	1.32%	0.153%
26	17.845	2760	2764	2767	rVB	28595	31575	1.66%	0.193%
27	18.245	2827	2832	2841	rBV2	131754	223382	11.76%	1.365%
28	18.327	2842	2846	2851	rBV	367538	445127	23.43%	2.720%
29	18.662	2898	2903	2909	rBV	37450	49117	2.59%	0.300%
30	19.050	2965	2969	2975	rVB	67507	80372	4.23%	0.491%
31	19.415	3028	3031	3036	rBV3	18527	28391	1.49%	0.173%
32	19.568	3053	3057	3059	rBV3	16673	19319	1.02%	0.118%
33	19.603	3059	3063	3066	rBV	28035	40380	2.13%	0.247%
34	19.768	3088	3091	3101	rBV3	38935	89460	4.71%	0.547%

LSC Area Percent Report

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Acq On : 8 Jun 2017 13:56
Operator : SJ/MA
Sample : I3469-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(0-2)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

35	19.891	3108	3112	3115	rBV	16275	22103	1.16%	0.135%
36	19.944	3119	3121	3125	rVV	25492	28106	1.48%	0.172%
37	19.997	3126	3130	3140	rVB	329687	406975	21.42%	2.487%
38	20.268	3172	3176	3186	rVB9	20257	34352	1.81%	0.210%
39	20.444	3203	3206	3209	rBV	36116	45059	2.37%	0.275%
40	20.480	3209	3212	3218	rVV3	35731	57005	3.00%	0.348%
41	20.527	3218	3220	3227	rVB6	14570	21859	1.15%	0.134%
42	21.027	3302	3305	3309	rVB4	19574	23446	1.23%	0.143%
43	22.297	3516	3521	3531	rBV4	10595	38072	2.00%	0.233%
44	23.009	3640	3642	3649	rVB7	14964	21582	1.14%	0.132%

Sum of corrected areas: 16367319

LSC Report - Integrated Chromatogram

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Misc :
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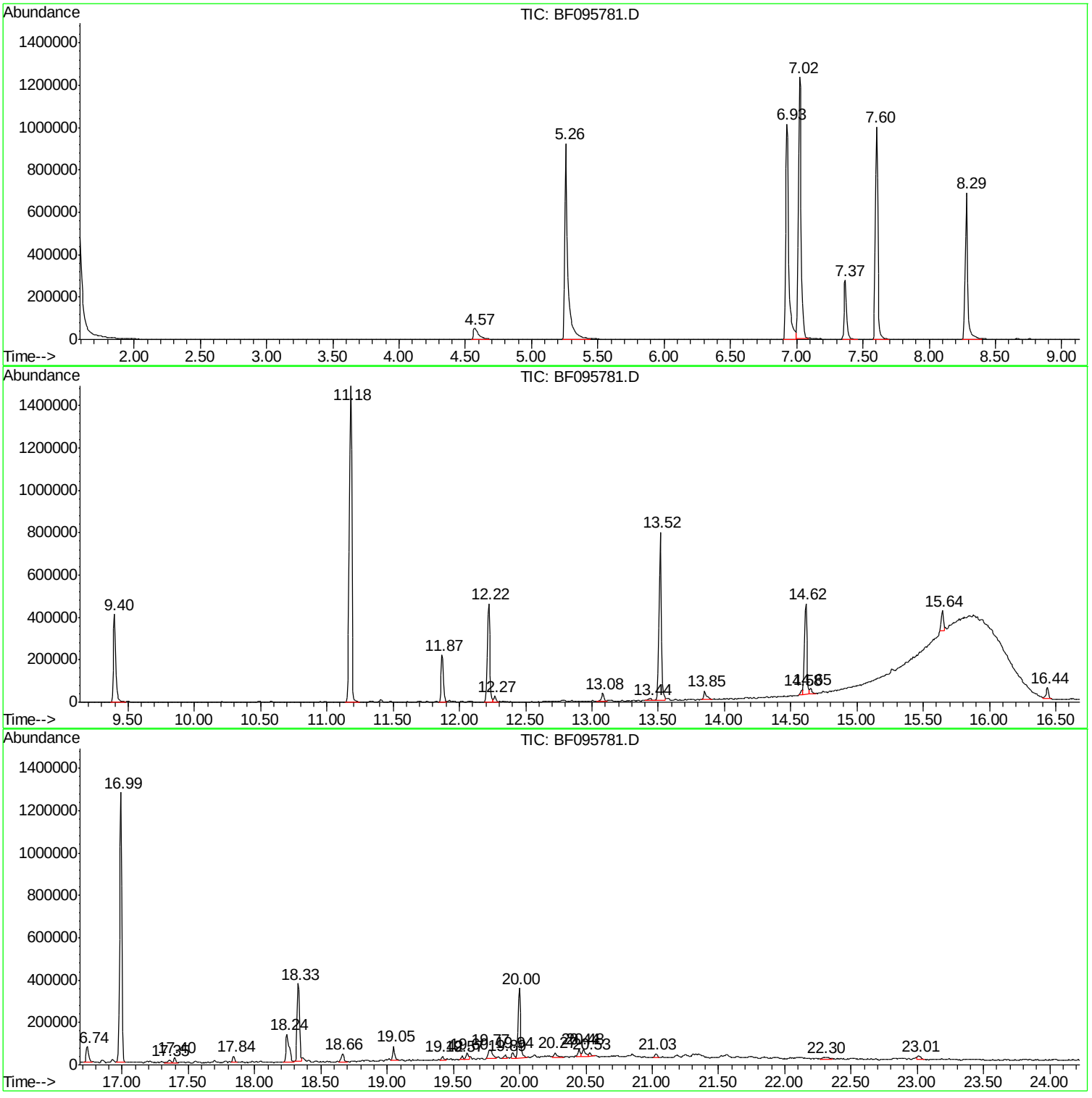
Instrument : BNA_F
ClientSampleId : SB-6(0-2)20170603

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\BF060817\
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Operator : SJ/MA
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Misc :
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Instrument : BNA_F
ClientSampleId : SB-6(0-2)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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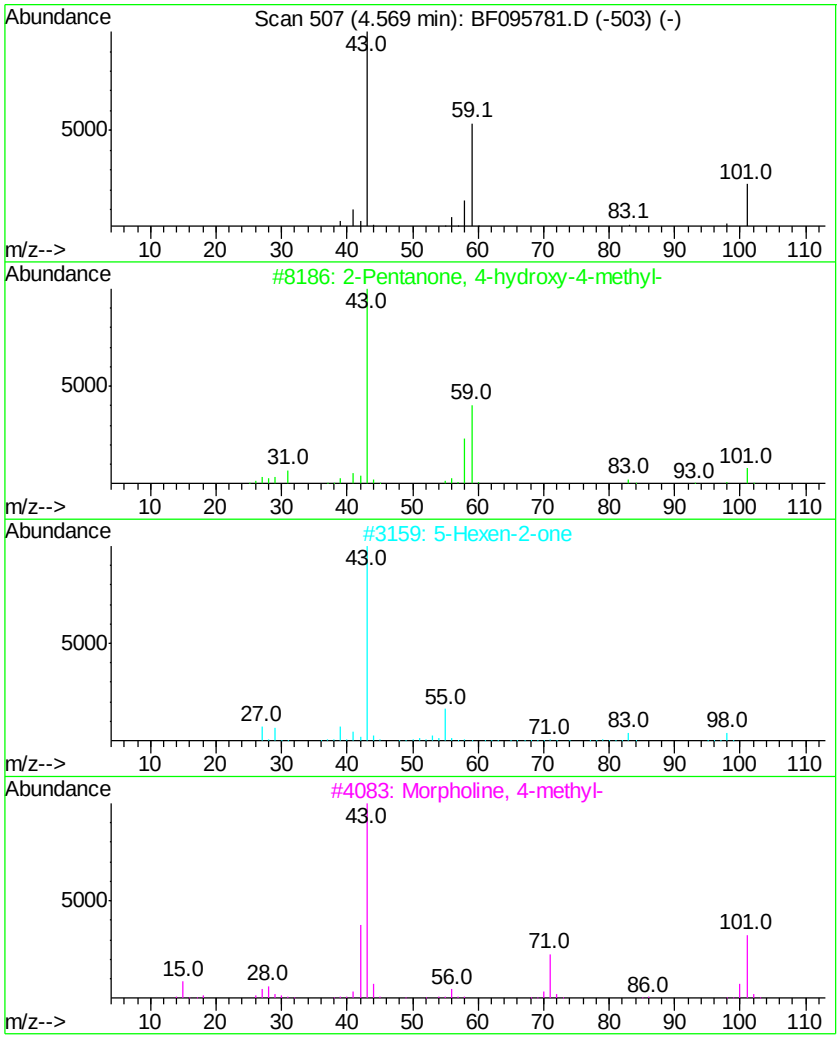
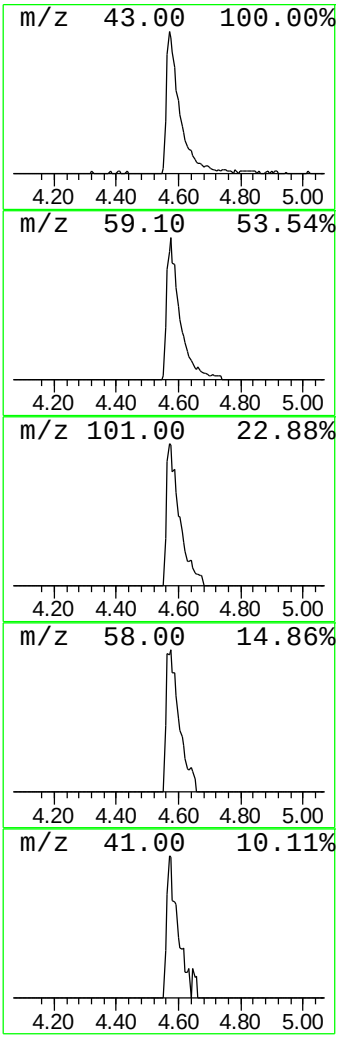
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	7.97 ng	148169	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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Operator : SJ/MA
Sample : I3469-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-6(0-2)20170603

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

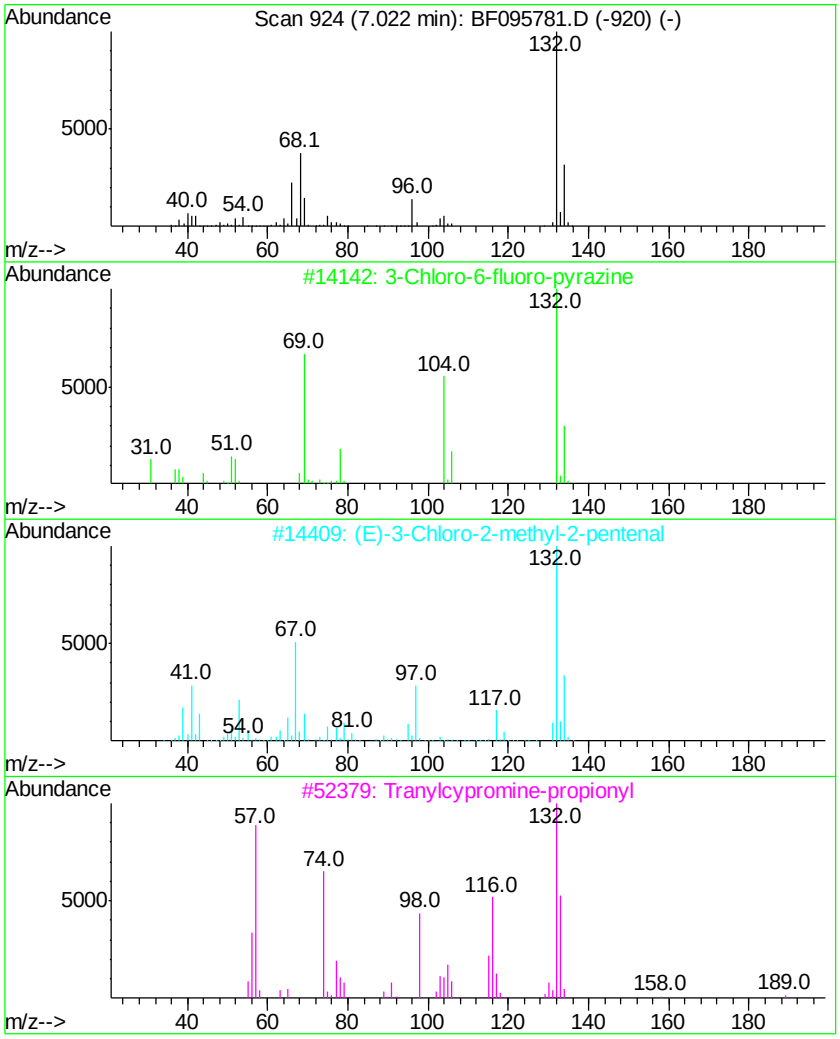
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

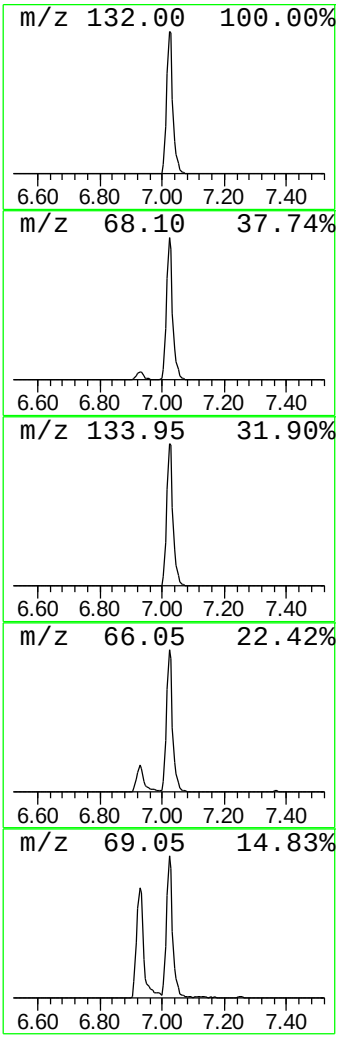
****

Peak Number 2 unknown7.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	95.93 ng	1782760	1,4-Dichlorobenzene-d4	7.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
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Acq On : 8 Jun 2017 13:56
Operator : SJ/MA
Sample : I3469-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-6(0-2)20170603

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

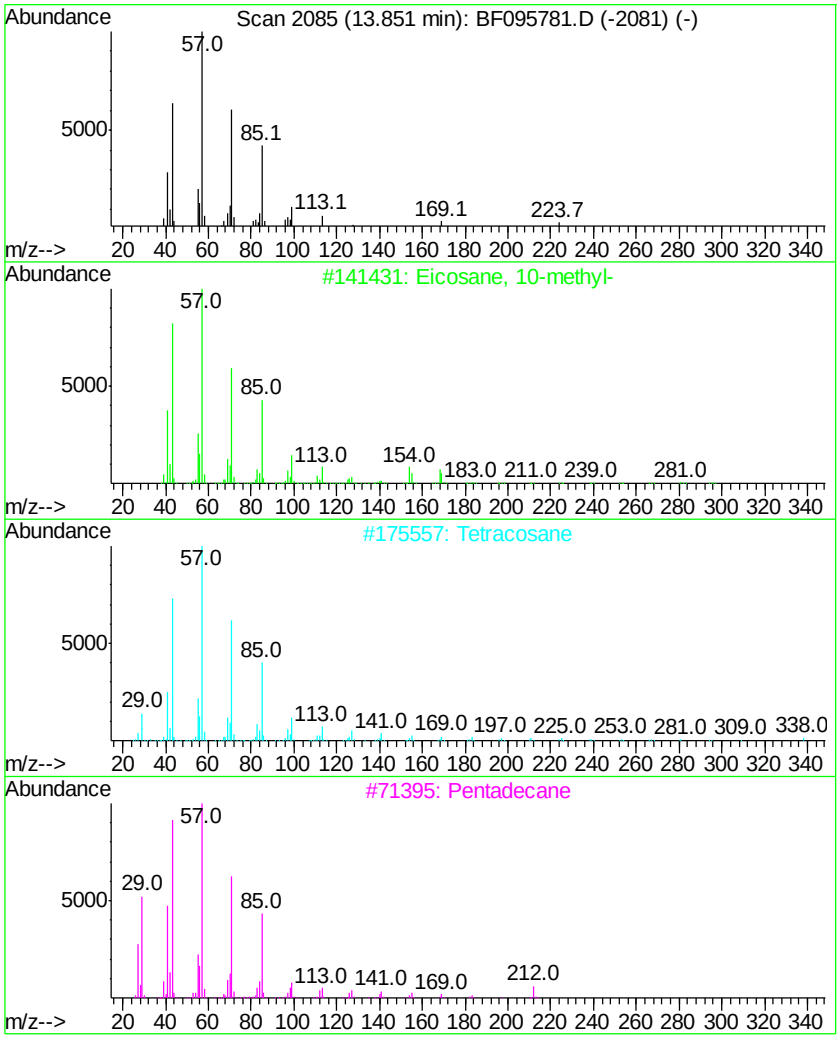
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

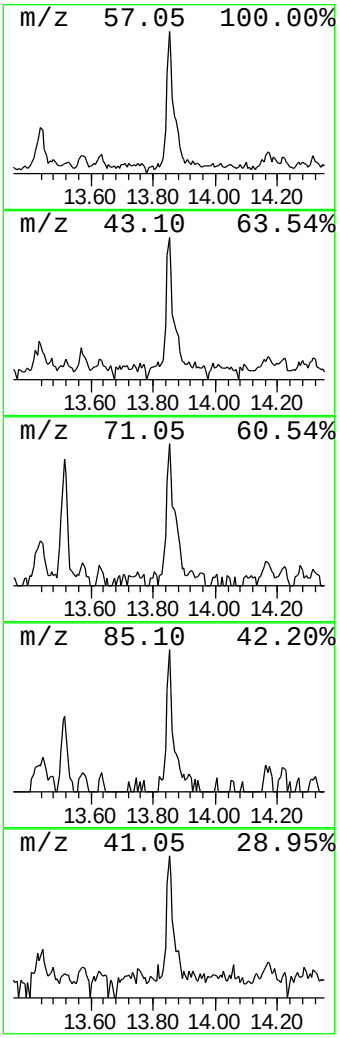
****

Peak Number 4 Eicosane, 10-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.23 ng	61659	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
2	Tetracosane	338	C24H50	000646-31-1	86
3	Pentadecane	212	C15H32	000629-62-9	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
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Operator : SJ/MA
Sample : I3469-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(0-2)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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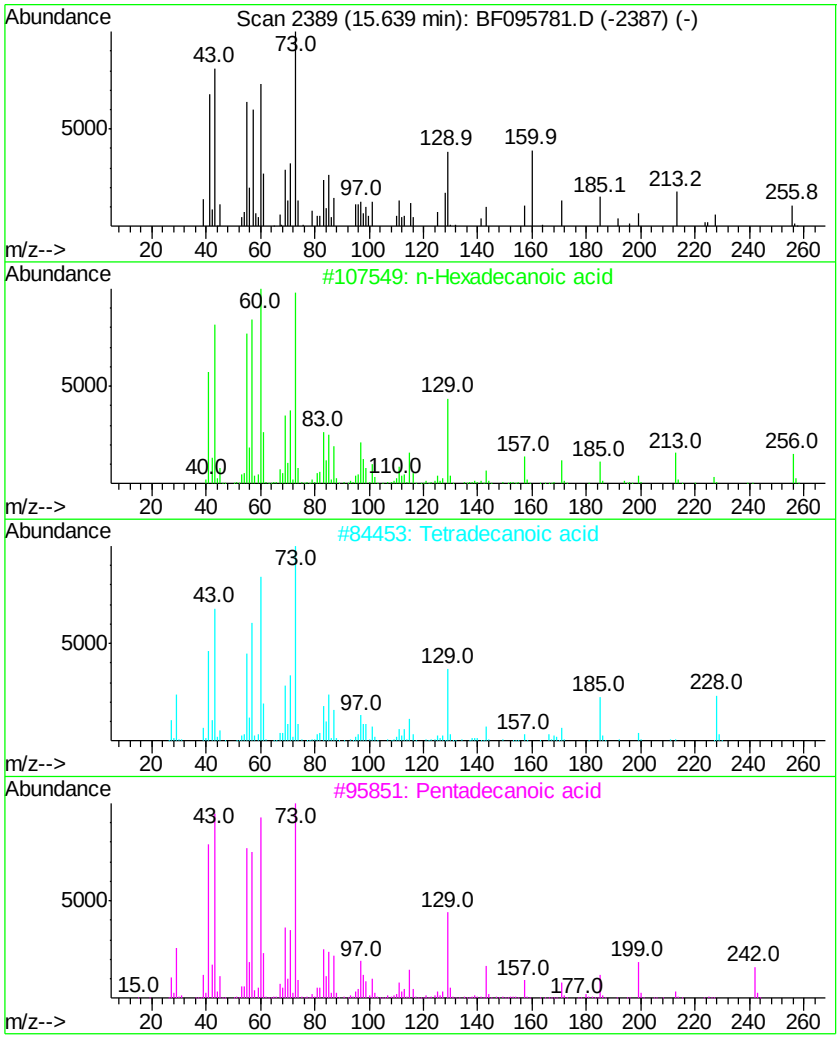
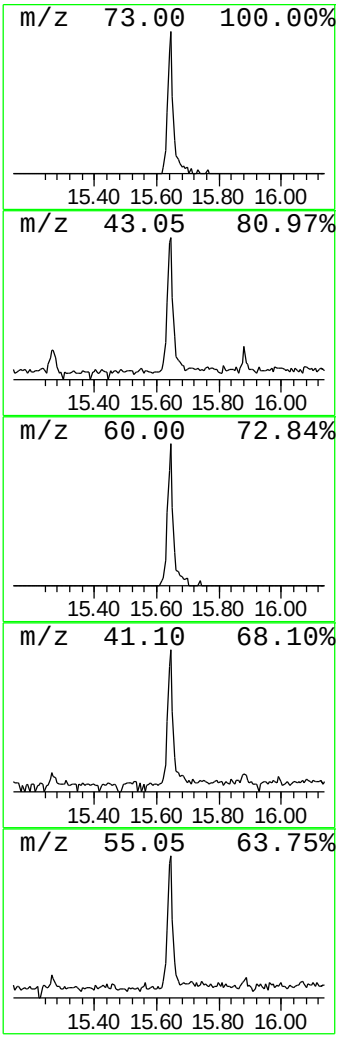
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	3.68 ng	101865	Phenanthrene-d10	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	60
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Tridecanoic acid	214	C13H26O2	000638-53-9	47





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Sample : I3469-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(0-2)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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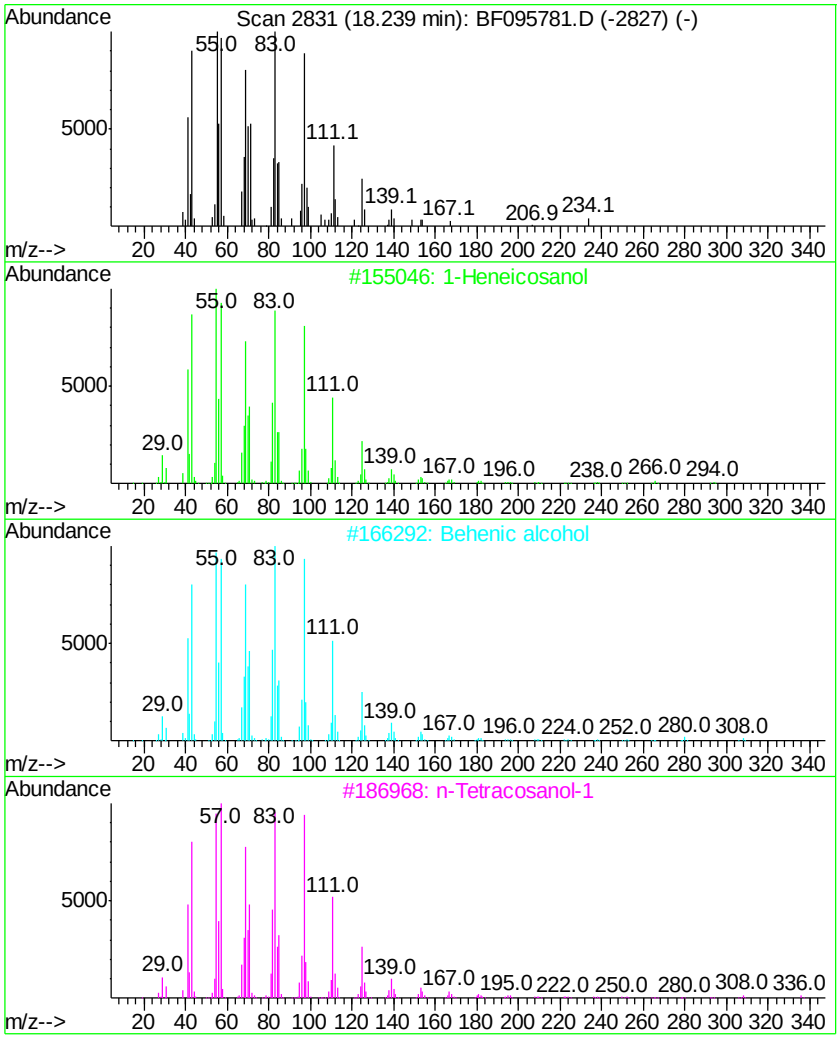
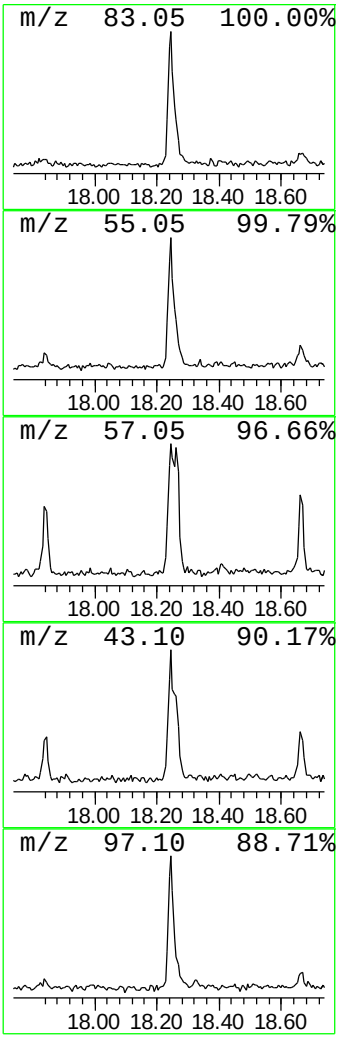
****

Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	10.04 ng	223382	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93





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Sample : I3469-10
Misc :
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Instrument : BNA_F
ClientSampleId : SB-6(0-2)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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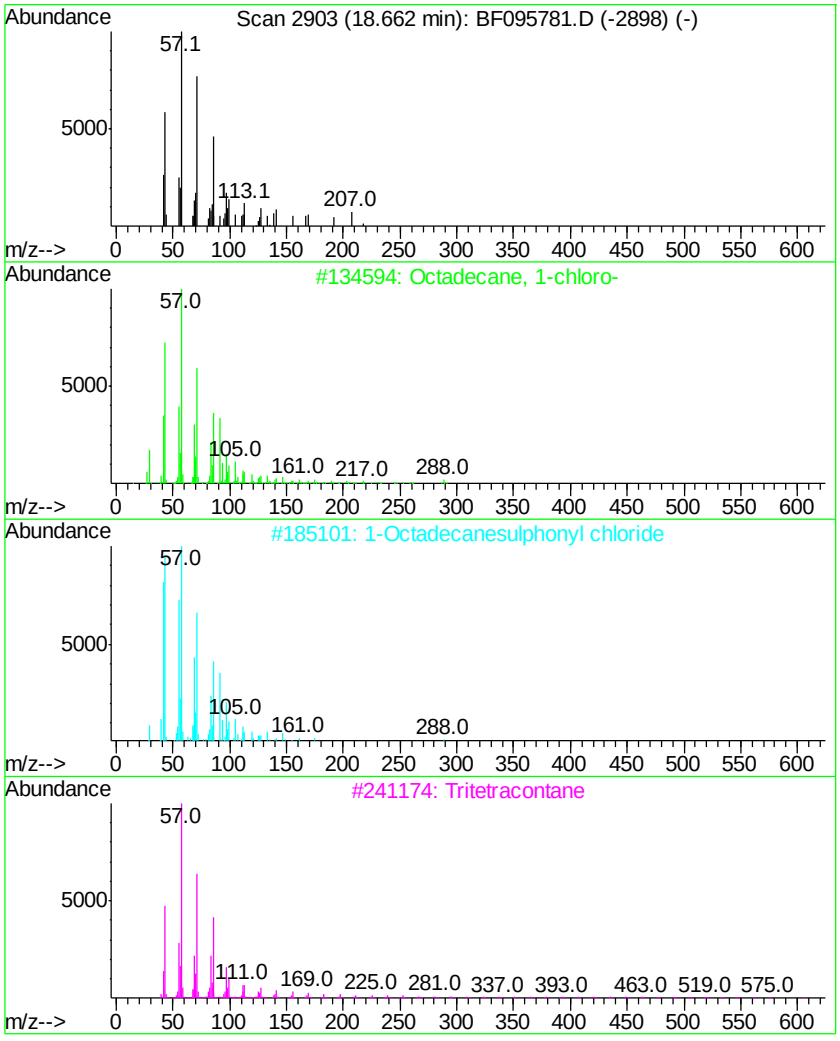
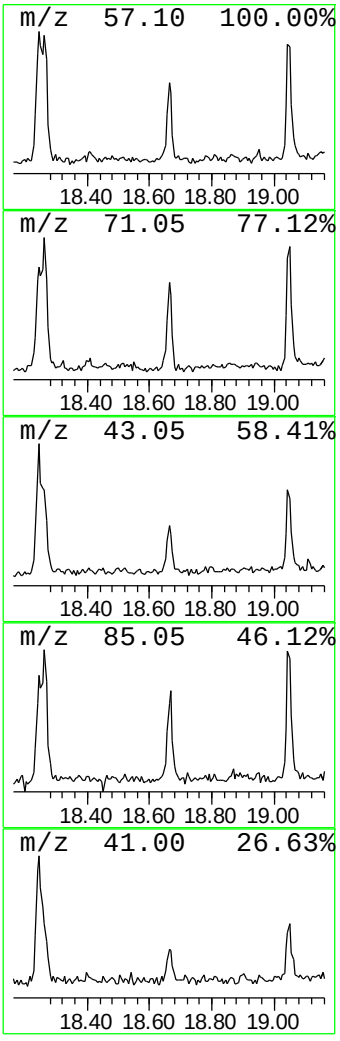
Peak Number 7 Octadecane, 1-chloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.66	2.21 ng	49117	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
3	Tritetracontane	605	C43H88	007098-21-7	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Tetradecane	198	C14H30	000629-59-4	90





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Instrument : BNA_F
ClientSampleId : SB-6(0-2)20170603

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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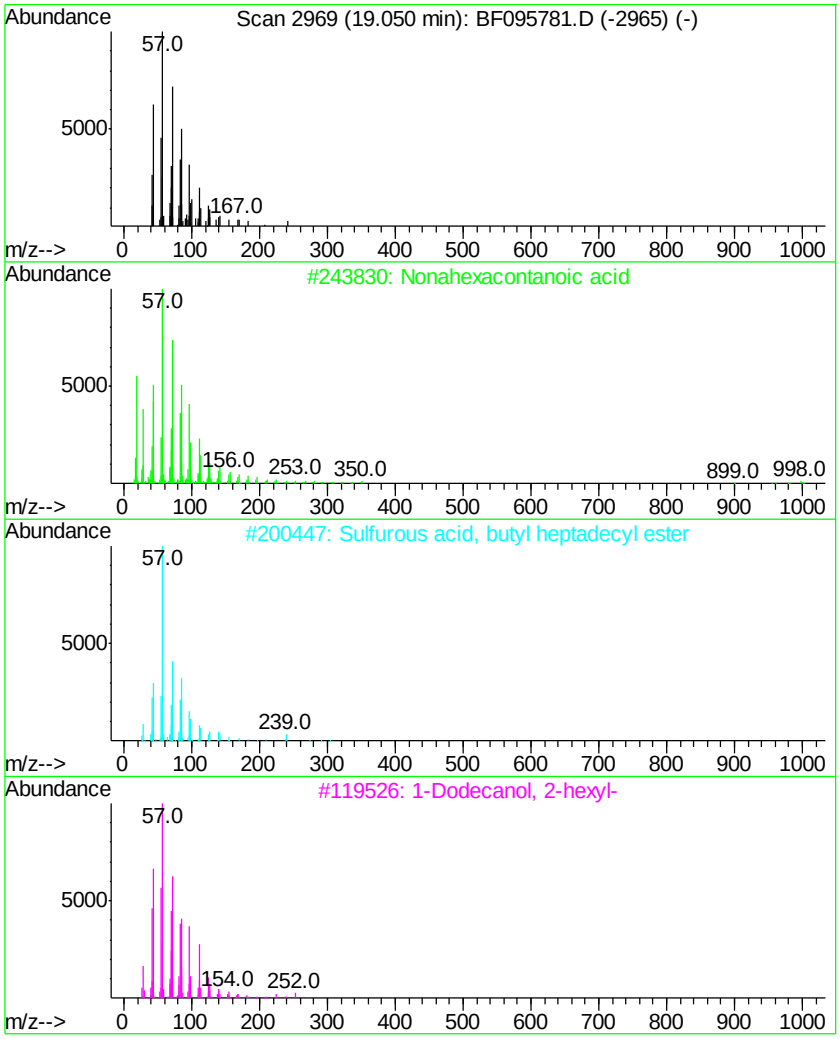
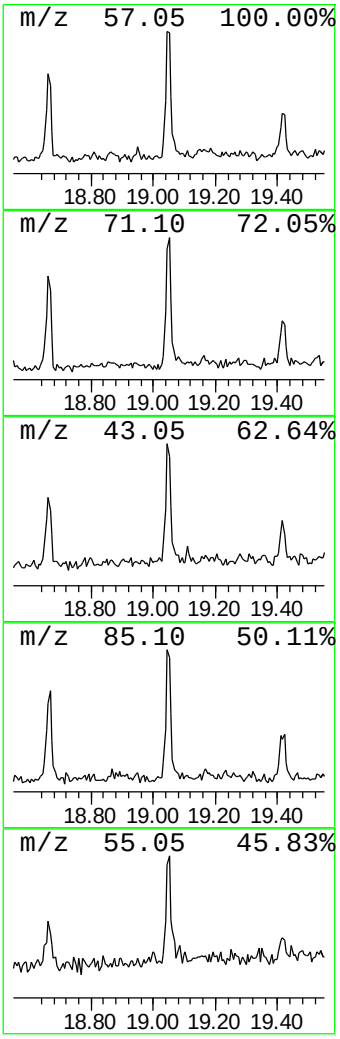
Peak Number 8 Nonahexacontanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.05	3.61 ng	80372	Chrysene-d12	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	91
2	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	86
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	83
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83





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Sample : I3469-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(0-2)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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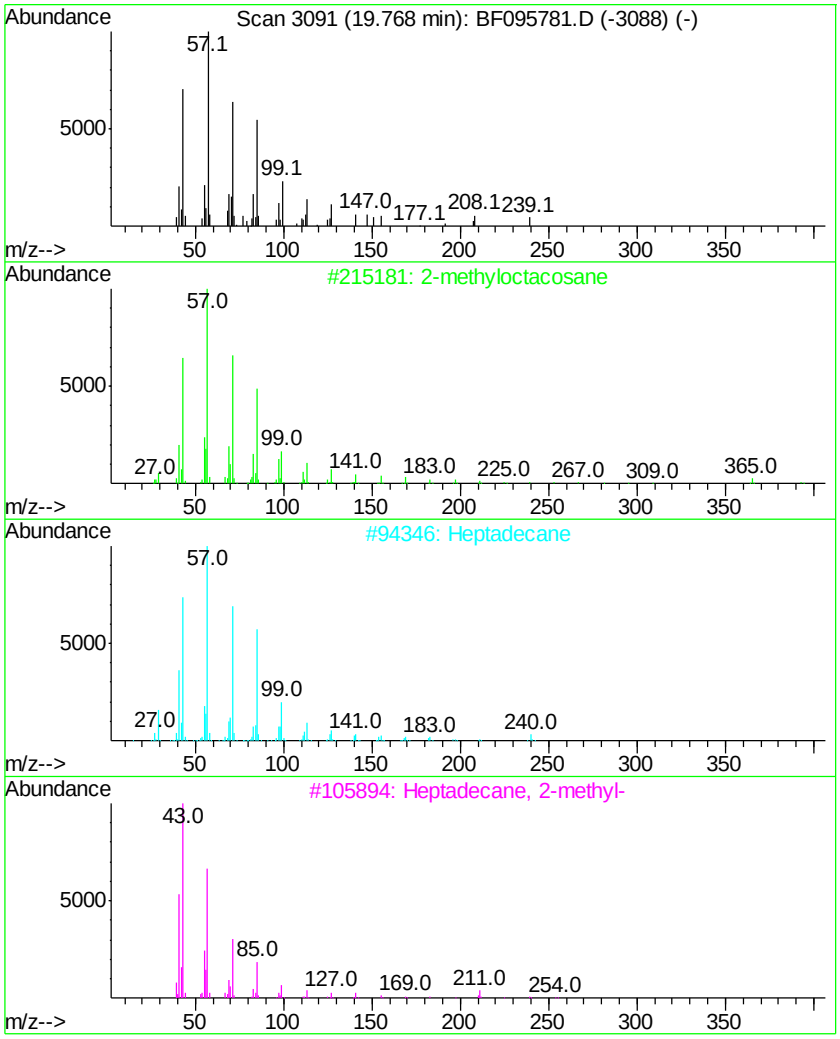
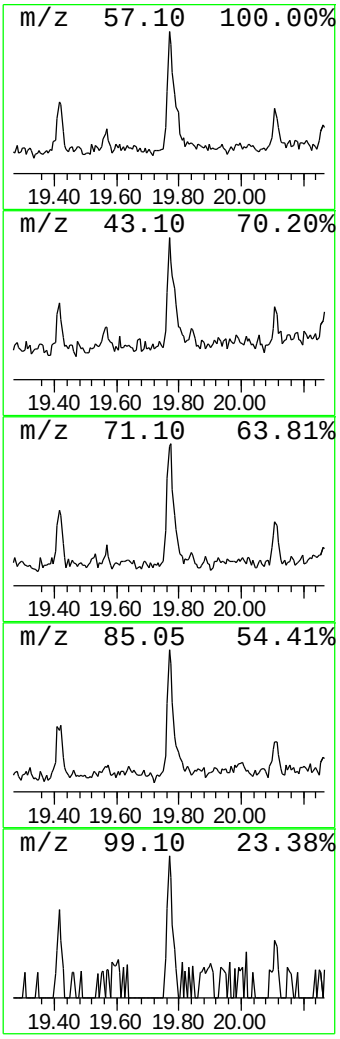
Peak Number 9 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	4.40 ng	89460	Perylene-d12	20.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	86
2	Heptadecane	240	C17H36	000629-78-7	80
3	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	80
4	Nonacosane	408	C29H60	000630-03-5	78
5	Tetracontane	563	C40H82	004181-95-7	78





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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(0-2)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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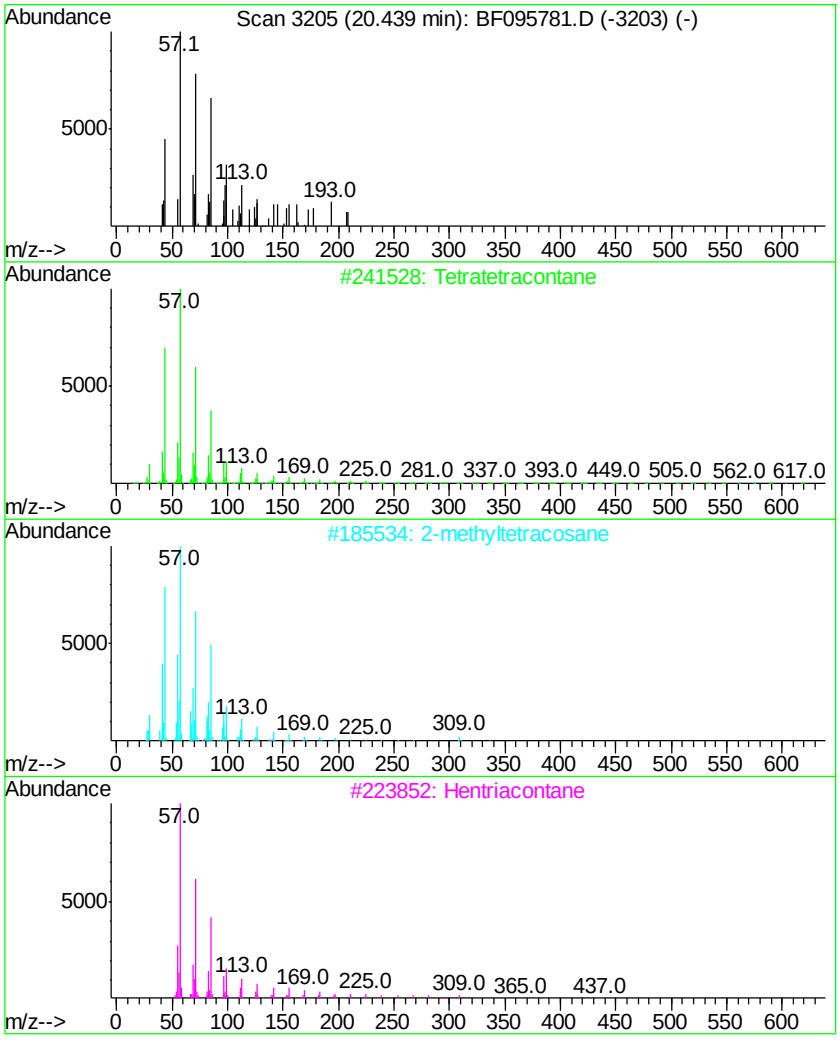
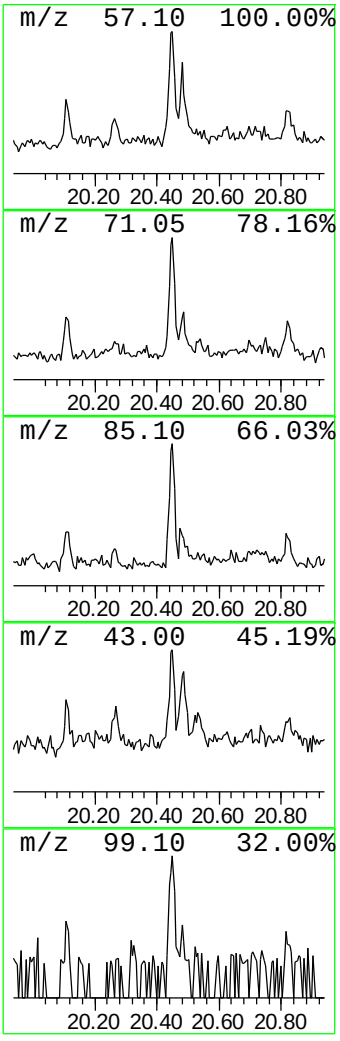
Peak Number 10 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.44	2.21 ng	45059	Perylene-d12	20.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	2-methyltetracosane	352	C25H52	1000376-72-6	90
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Tetrapentacontane	759	C54H110	005856-66-6	90
5	Heptacosane	380	C27H56	000593-49-7	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095781.D
Acq On : 8 Jun 2017 13:56
Operator : SJ/MA
Sample : I3469-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(0-2)20170603

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

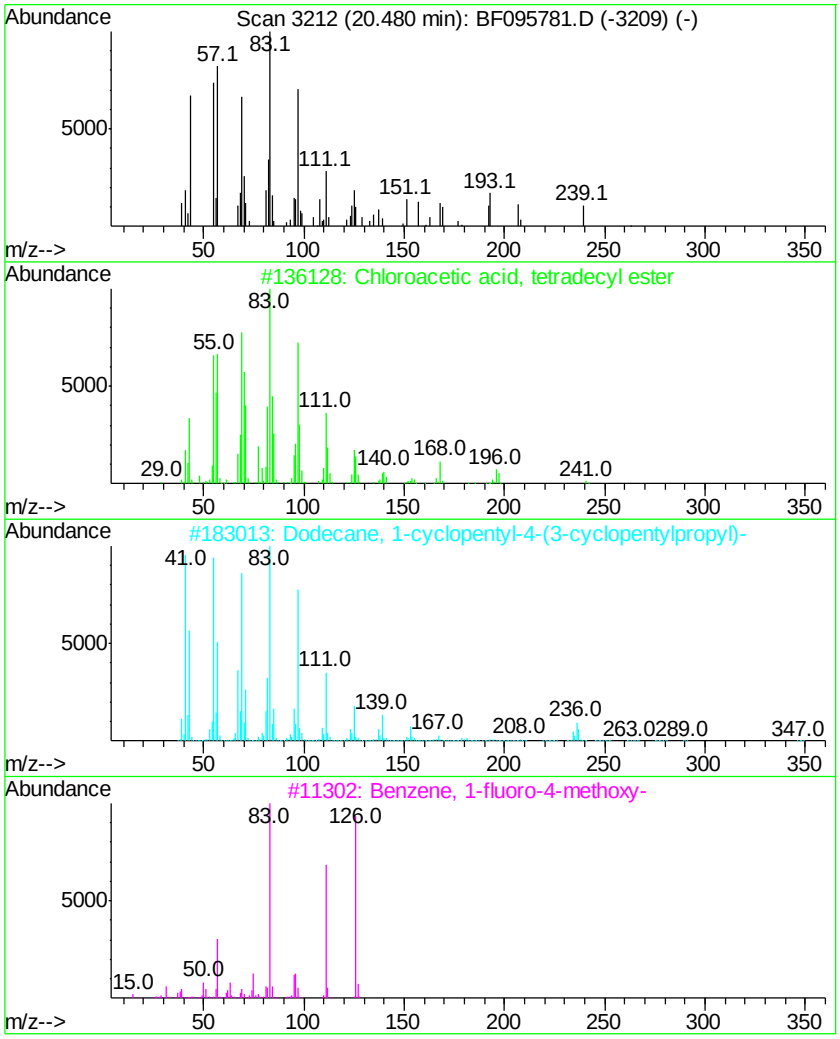
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

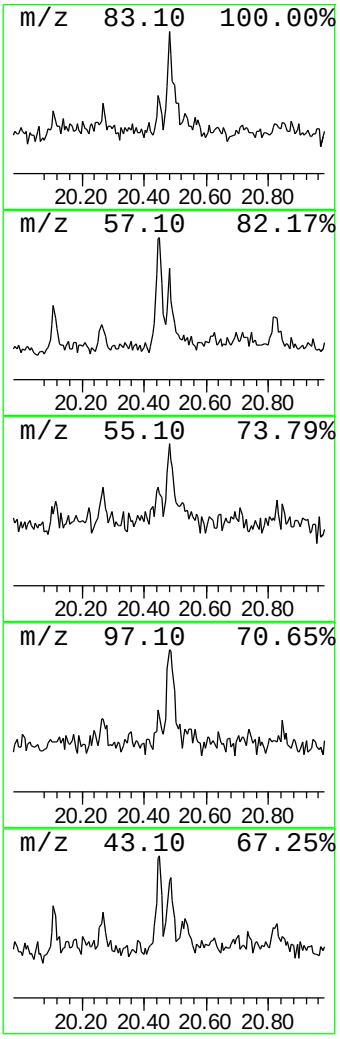
****

Peak Number 11 Chloroacetic acid, tetradec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.48	2.80 ng	57005	Perylene-d12	20.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	53
2	Dodecane, 1-cyclopentyl-4-(3-cyc...	348	C25H48	007225-68-5	52
3	Benzene, 1-fluoro-4-methoxy-	126	C7H7FO	000459-60-9	38
4	Cyclohexanecarbonyl chloride	146	C7H11ClO	002719-27-9	35
5	Oxalic acid, 1-menthyl pentadecy...	438	C27H50O4	1000314-98-2	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095781.D
Acq On : 8 Jun 2017 13:56
Operator : SJ/MA
Sample : I3469-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6(0-2)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...	4.57	8.0	ng	148169	1	7.37	371692	20.0
unknown7.02	7.02	95.9	ng	1782760	1	7.37	371692	20.0
Eicosane, 10-methyl-	13.85	2.2	ng	61659	4	14.62	552965	20.0
n-Hexadecanoic acid	15.64	3.7	ng	101865	4	14.62	552965	20.0
1-Heneicosanol	18.24	10.0	ng	223382	5	18.33	445127	20.0
Octadecane, 1-chl...	18.66	2.2	ng	49117	5	18.33	445127	20.0
Nonahexacontanoic...	19.05	3.6	ng	80372	5	18.33	445127	20.0
2-methyloctacosane	19.77	4.4	ng	89460	6	20.00	406975	20.0
Tetratetracontane	20.44	2.2	ng	45059	6	20.00	406975	20.0
Chloroacetic acid...	20.48	2.8	ng	57005	6	20.00	406975	20.0