LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

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-BF050217.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	4.801	500	504	522	rBV	68206	175020	8.43%	0.999%
2	5.472	614	618	651	rBV	901422	1915910	92.26%	10.931%
3	7.107	892	896	910	rBV	966786	1650364	79.47%	9.416%
4	7.213	910	914	933	rVB	1343074	2076645	100.00%	11.848%
5	7.554	968	972	985	rBV	438626	542607	26.13%	3.096%
6	7.789	1007	1012	1028	rVB	1184556	1546942	74.49%	8.826%
7	8.466	1122	1127	1145	rBV	775591	1182290	56.93%	6.745%
8	9.583	1313	1317	1328	rBV	506617	687368	33.10%	3.922%
9	11.360	1614	1619	1632	rBV	1488773	1766751	85.08%	10.080%
10	12.048	1732	1736	1748	rBV	246820	307630	14.81%	1.755%
11	12.407	1793	1797	1810	rBV2	481745	642349	30.93%	3.665%
12	13.254	1935	1941	1947	rBV2	26537	30651	1.48%	0.175%
13	13.707	2013	2018	2032	rBV	602520	867008	41.75%	4.947%
14	14.024	2067	2072	2079	rBV2	26314	38496	1.85%	0.220%
15	14.759	2190	2197	2201	rBV	18544	23743	1.14%	0.135%
16	14.812	2201	2206	2211	rBV	392636	515026	24.80%	2.938%
17	15.583	2331	2337	2340	rBV	19404	24186	1.16%	0.138%
18	15.736	2359	2363	2367	rBV2	16860	23940	1.15%	0.137%
19	15.795	2370	2373	2381	rVB	78633	102606	4.94%	0.585%
20	16.577	2502	2506	2509	rVV2	26495	26232	1.26%	0.150%
21	16.612	2509	2512	2523	rVB	68515	87234	4.20%	0.498%
22	16.895	2556	2560	2561	rBV3	21460	23099	1.11%	0.132%
23	16.918	2561	2564	2573	rVB	75197	93613	4.51%	0.534%
24	17.077	2587	2591	2595	rBV	27007	31192	1.50%	0.178%
25	17.153	2600	2604	2610	rVB	1028187	1167212	56.21%	6.659%
26	17.547	2669	2671	2675	rVB2	23934	24658	1.19%	0.141%
27	17.853	2721	2723	2732	rVB	27734	33846	1.63%	0.193%
28	17.994	2744	2747	2751	rBV2	43195	45439	2.19%	0.259%
29	18.412	2812	2818	2825	rBV2	97993	164983	7.94%	0.941%
30	18.506	2829	2834	2838	rVV	443367	532972	25.67%	3.041%
31	18.565	2842	2844	2847	rVB2	28513	28367	1.37%	0.162%
32	18.818	2881	2887	2891	rBV	80559	89096	4.29%	0.508%
33	19.200	2948	2952	2961	rVB2	89655	110976	5.34%	0.633%
34	19.571	3011	3015	3018	rVV	45351	53368	2.57%	0.304%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.636	3023	3026	3032	rVB2	22917	27892	1.34%	0.159%
36	19.783	3047	3051	3054	rBV	48504	69064	3.33%	0.394%
37	19.924	3072	3075	3081	rVV2	44699	62024	2.99%	0.354%
38	20.071	3097	3100	3106	rBV	30617	36626	1.76%	0.209%
39	20.130	3106	3110	3114	rBV	40910	55077	2.65%	0.314%
40	20.177	3114	3118	3127	rVV	368451	468662	22.57%	2.674%
41	20.265	3130	3133	3137	rVB2	24413	29945	1.44%	0.171%
42	20.618	3190	3193	3197	rBV	40525	47279	2.28%	0.270%
43	20.912	3238	3243	3251	rBV	30913	72031	3.47%	0.411%
44	21.447	3330	3334	3336	rBV3	18758	26860	1.29%	0.153%

Sum of corrected areas: 17527279

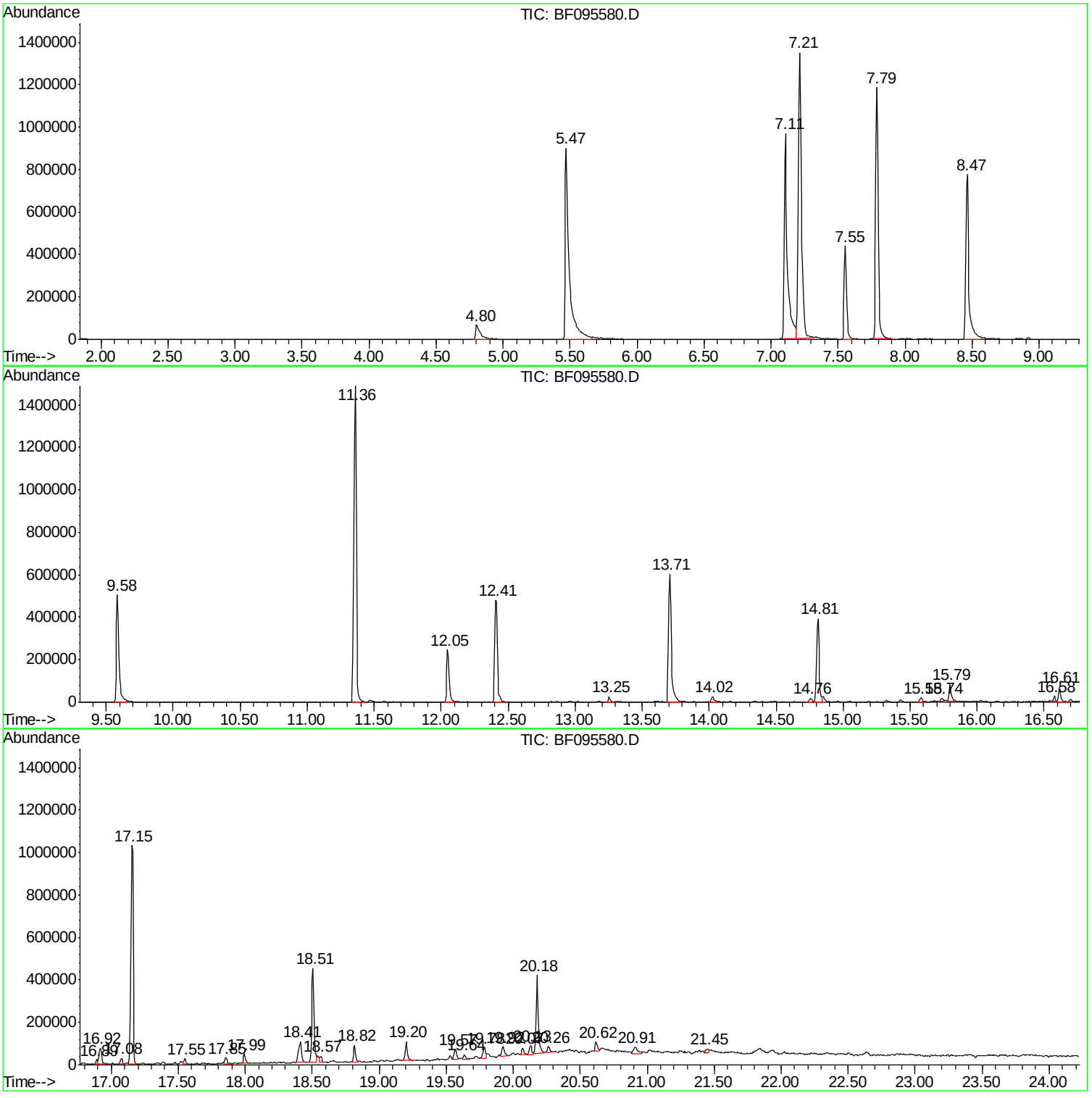
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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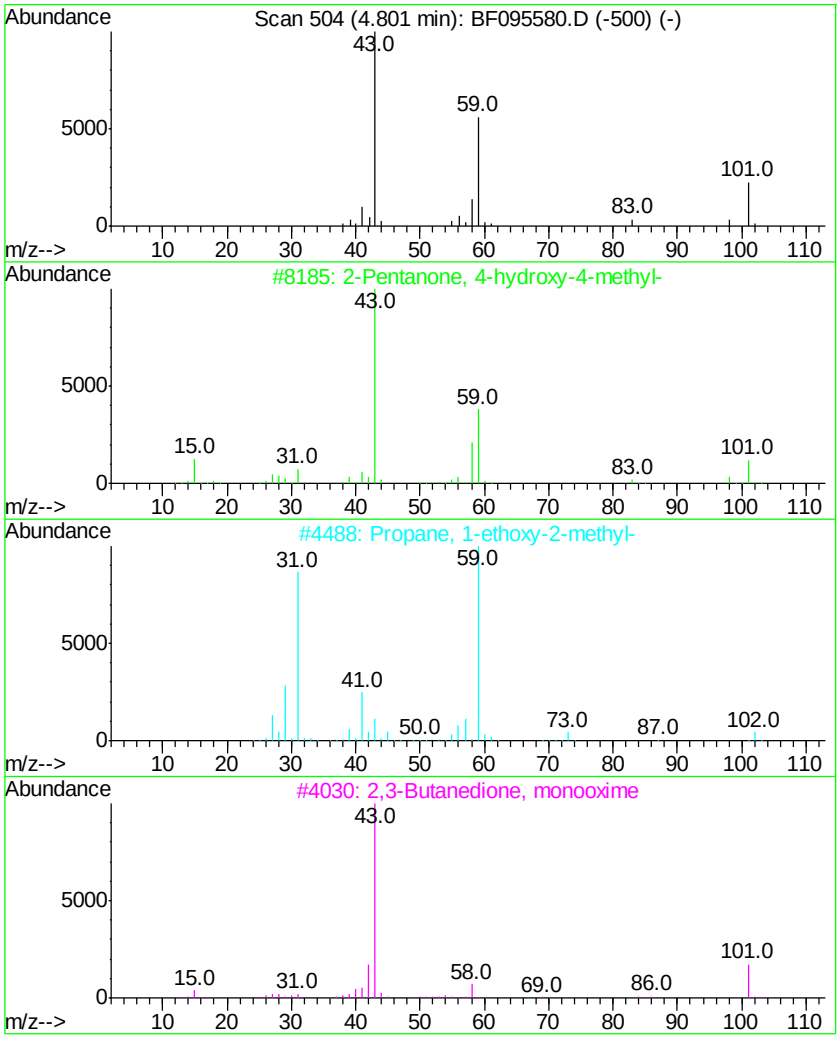
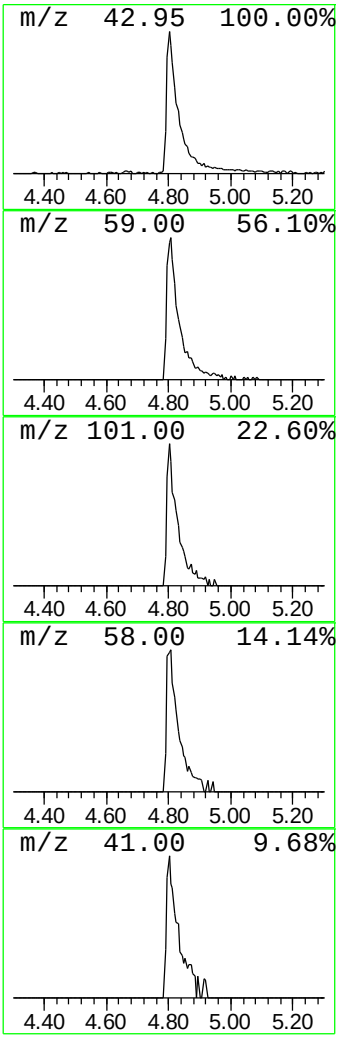
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	6.45 ng	175020	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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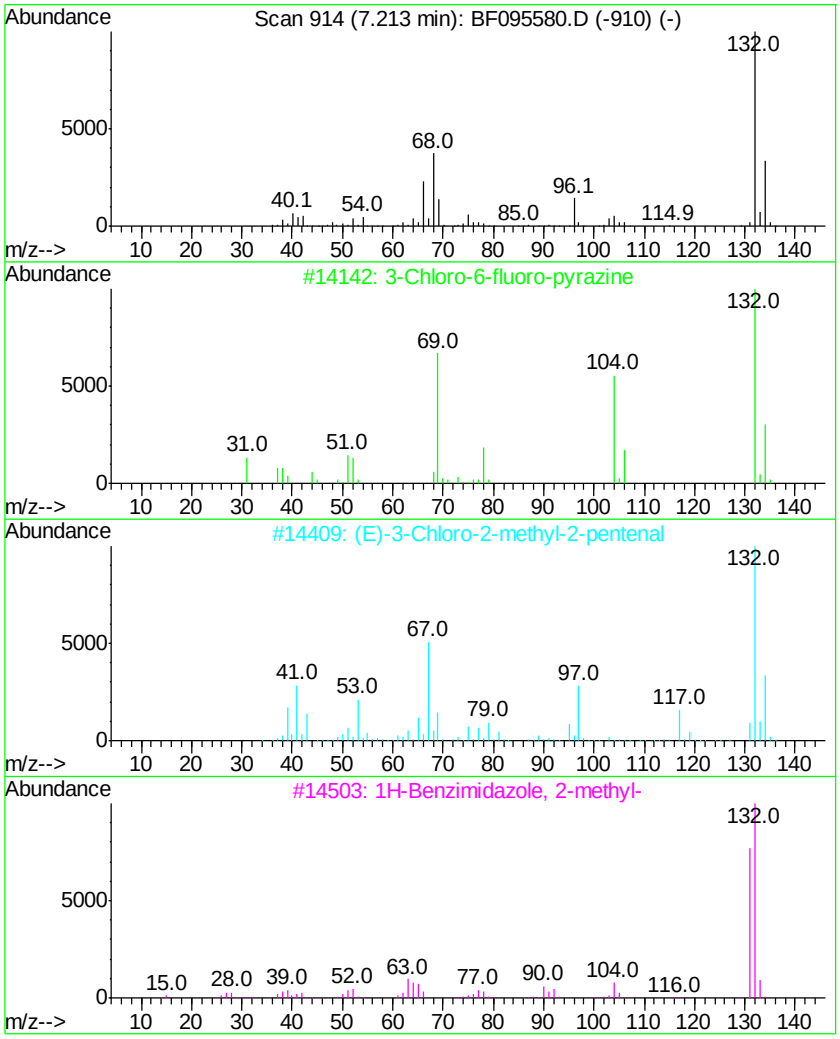
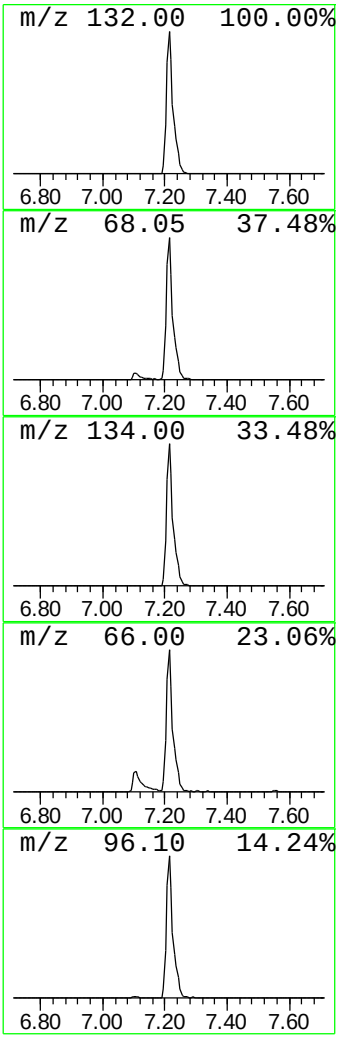
Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	76.54 ng	2076650	1,4-Dichlorobenzene-d4	7.55

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	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

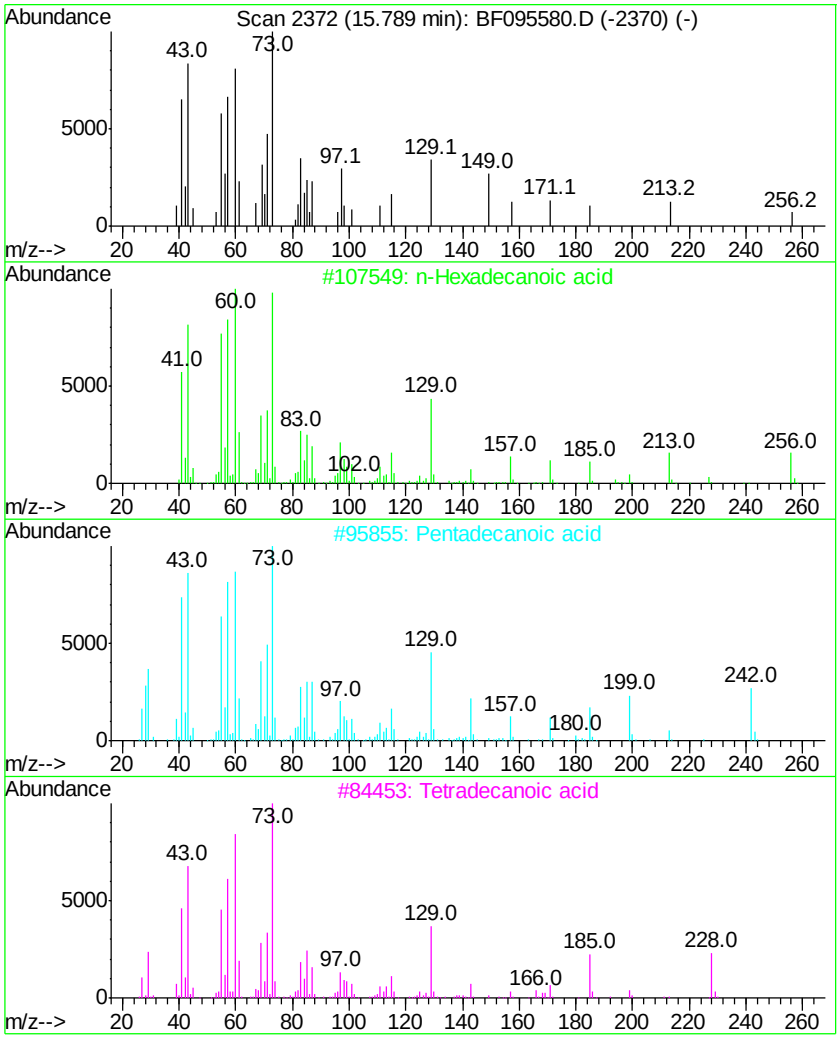
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

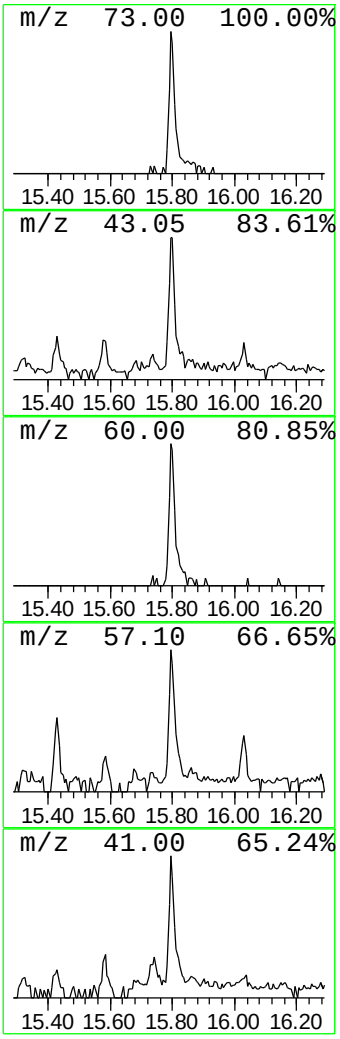
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	3.98 ng	102606	Phenanthrene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	20





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
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Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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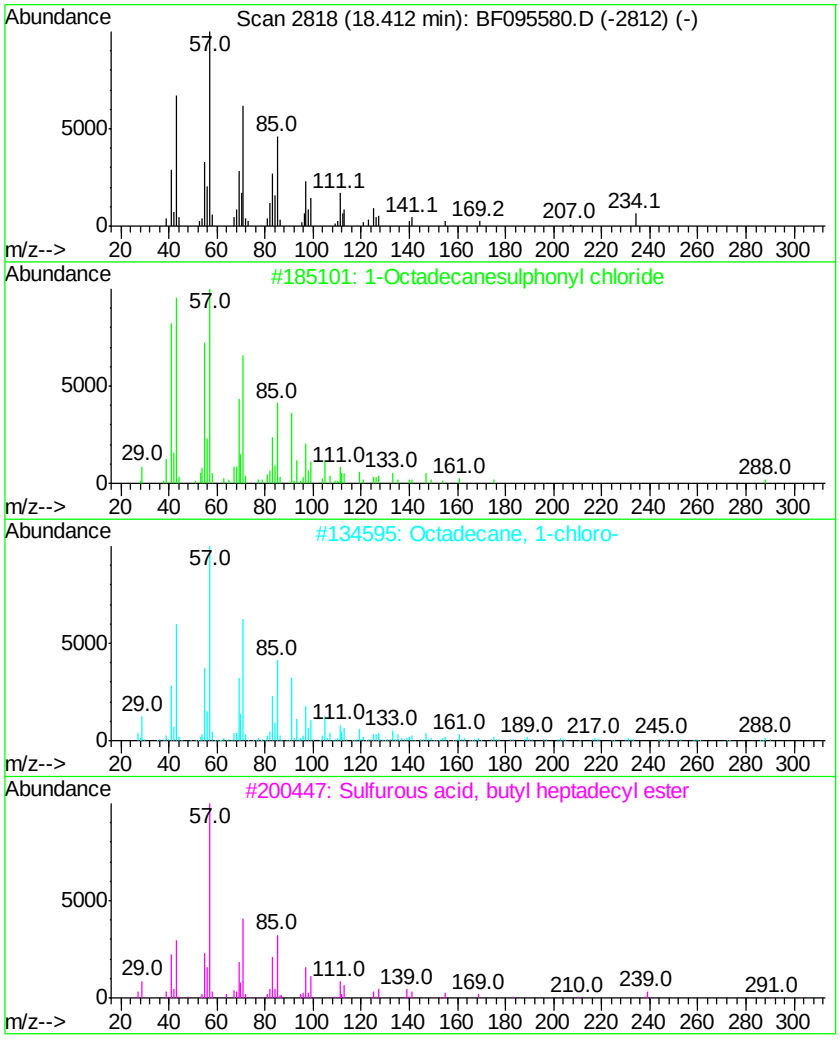
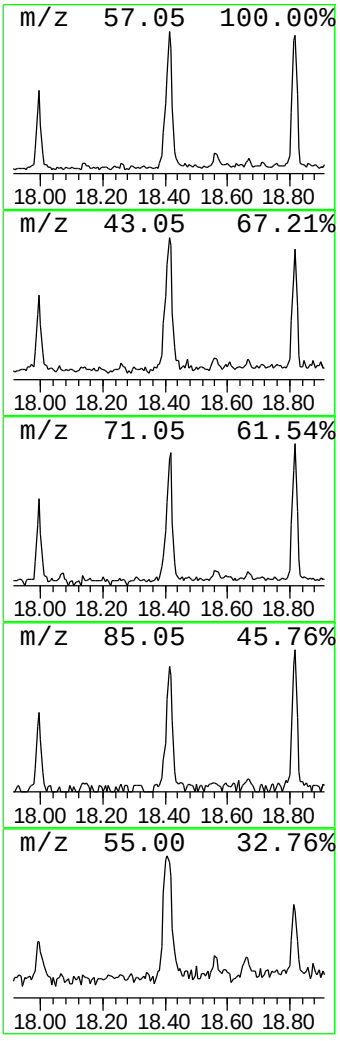
Peak Number 5 1-Octadecanesulphonyl chloride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	6.19 ng	164983	Chrysene-d12	18.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	87
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	86
4	Tritetracontane	605	C43H88	007098-21-7	72
5	Heptadecane	240	C17H36	000629-78-7	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
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Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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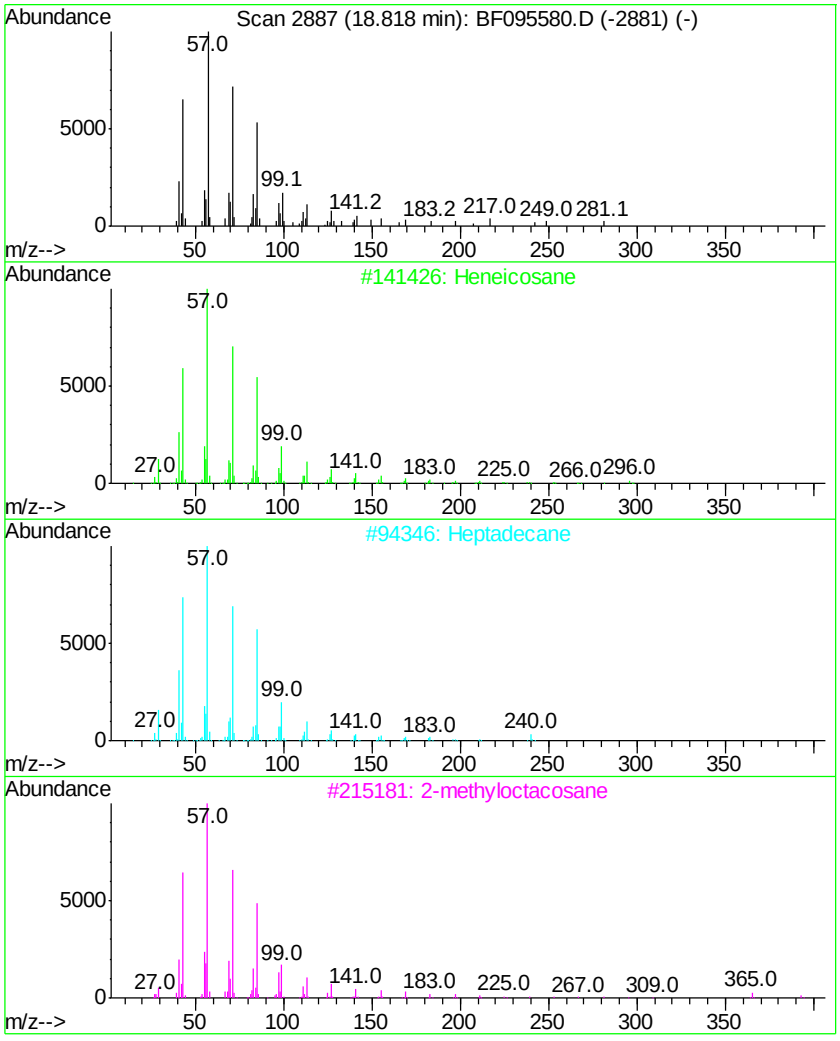
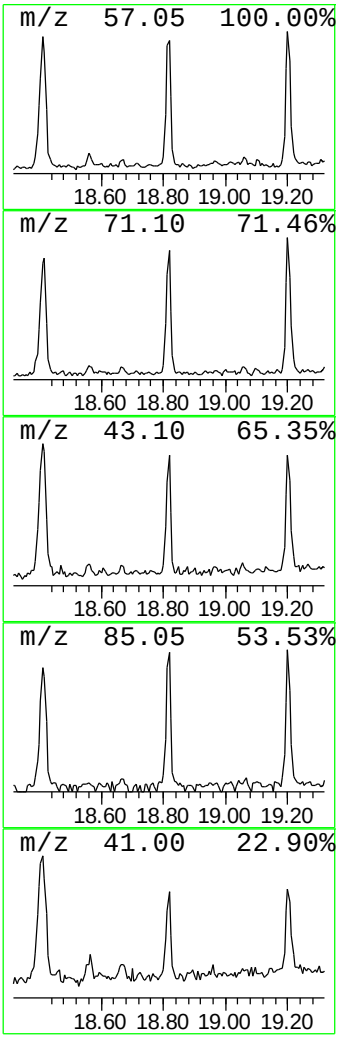
Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.82	3.34 ng	89096	Chrysene-d12	18.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





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Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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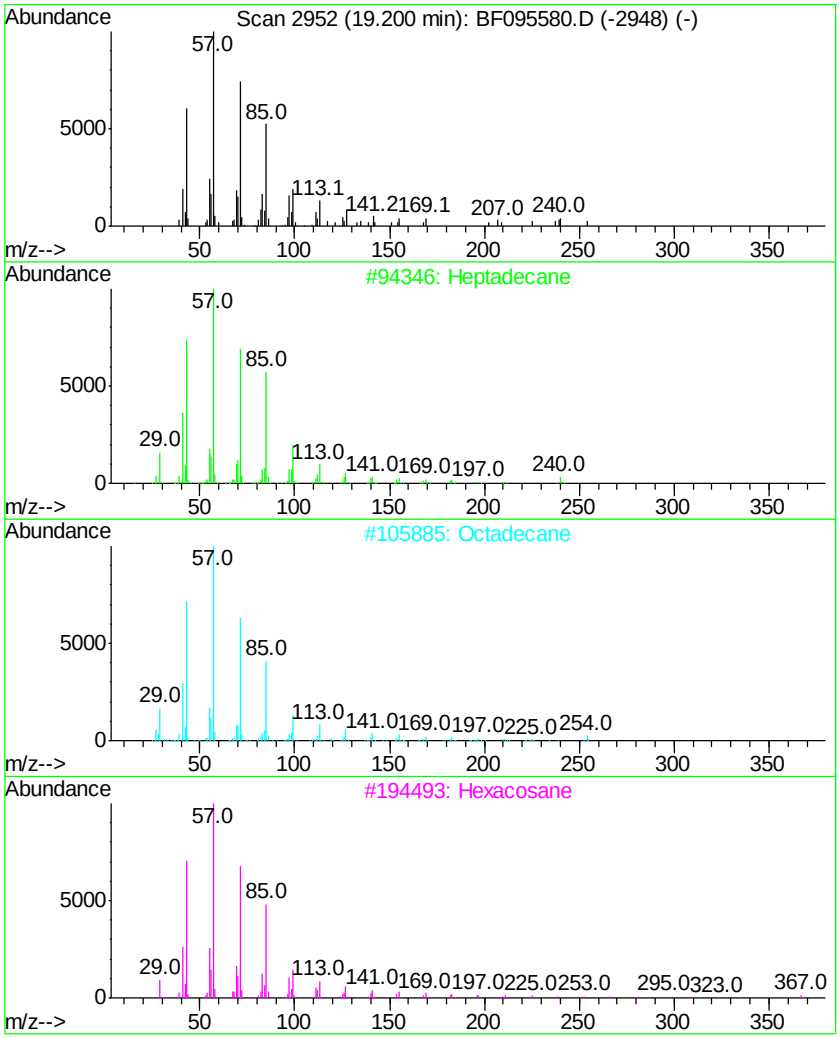
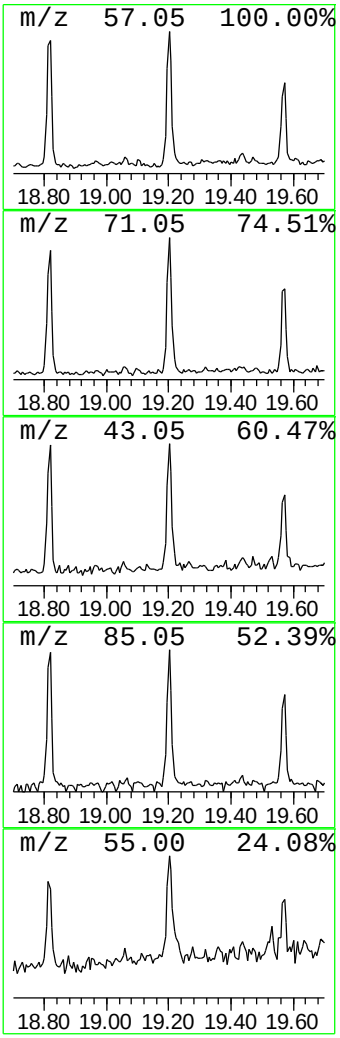
Peak Number 7 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.20	4.16 ng	110976	Chrysene-d12	18.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	97
2	Octadecane	254	C18H38	000593-45-3	96
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





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Acq On : 31 May 2017 23:53
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Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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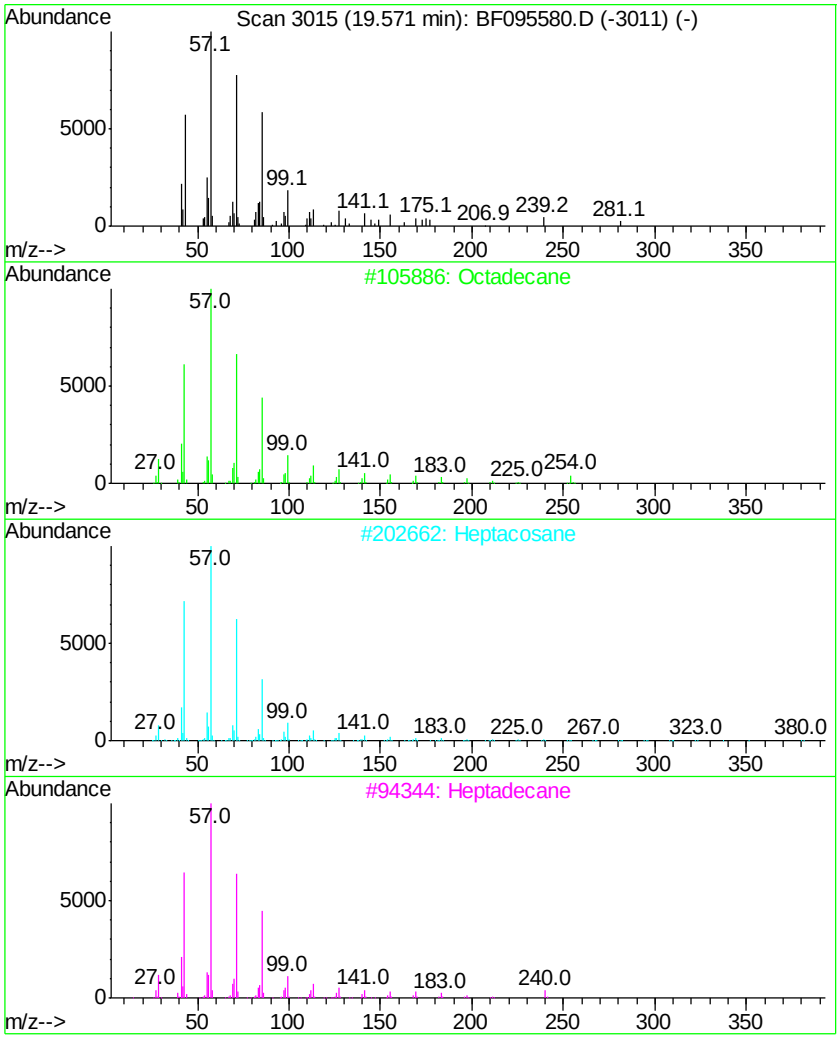
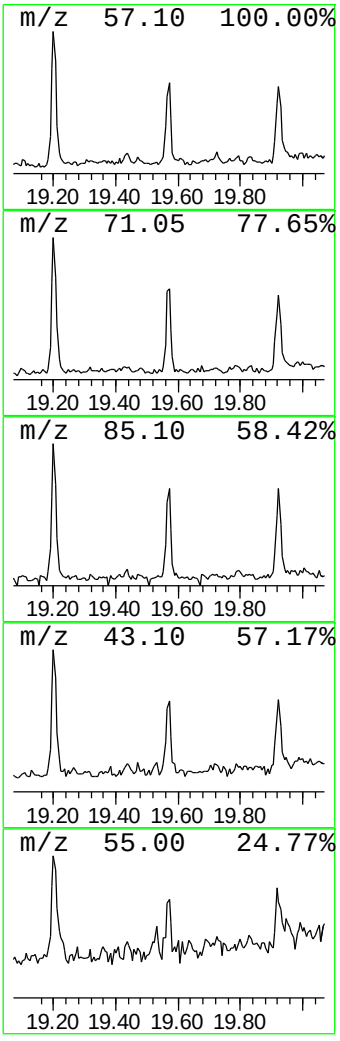
Peak Number 8 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.57	2.28 ng	53368	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	87
2	Heptacosane	380	C27H56	000593-49-7	86
3	Heptadecane	240	C17H36	000629-78-7	86
4	Docosane	310	C22H46	000629-97-0	86
5	Hexadecane	226	C16H34	000544-76-3	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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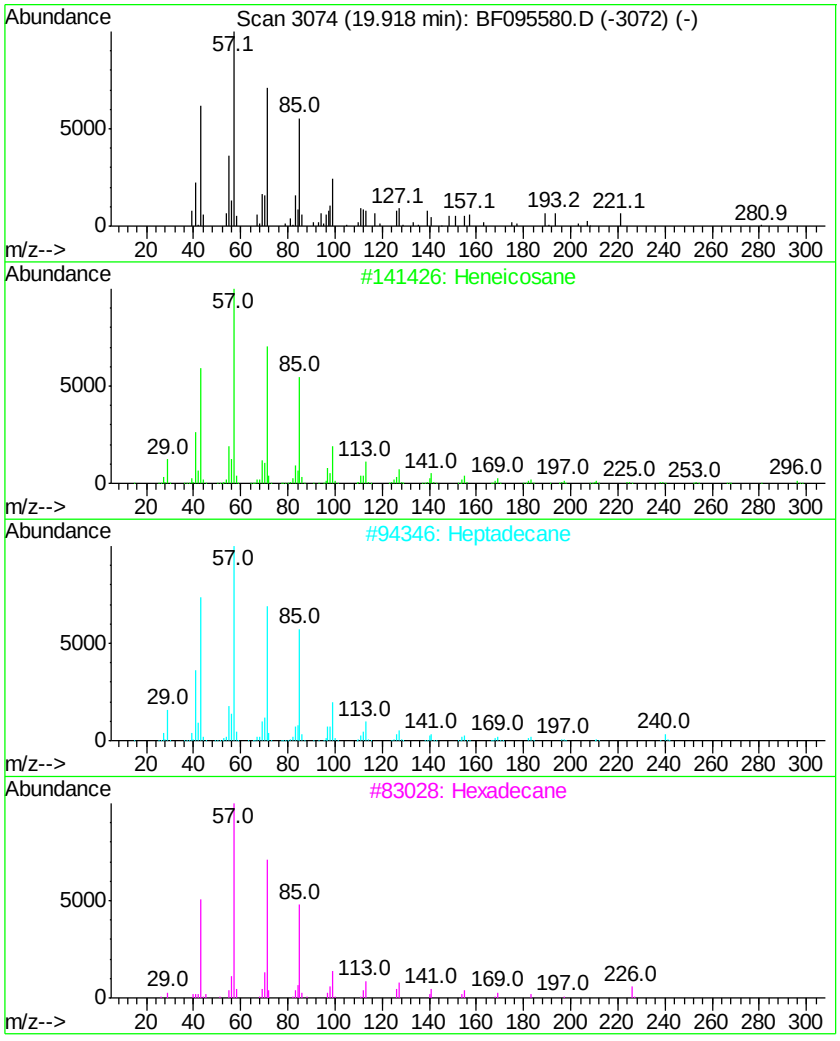
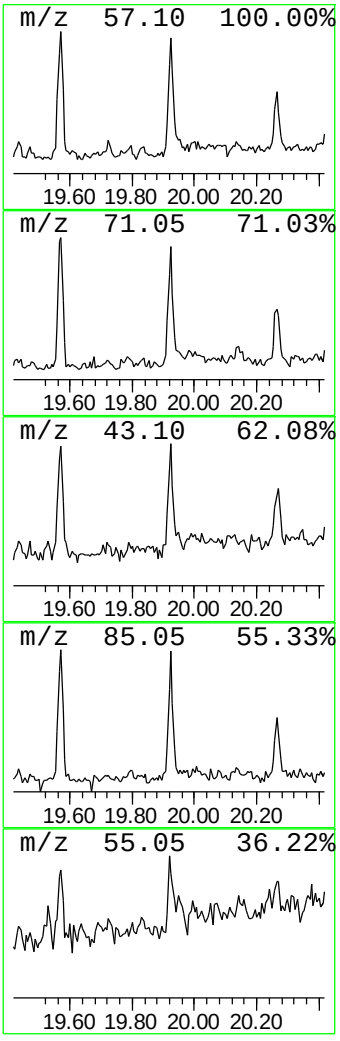
Peak Number 9 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	2.65 ng	62024	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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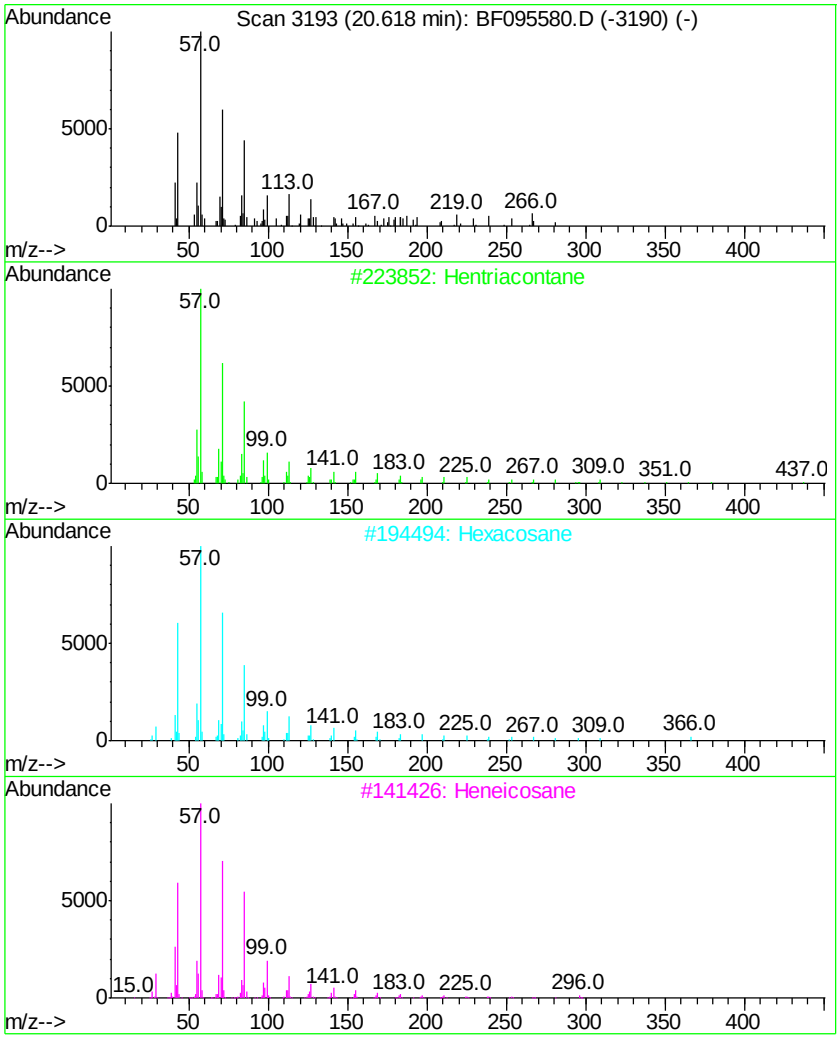
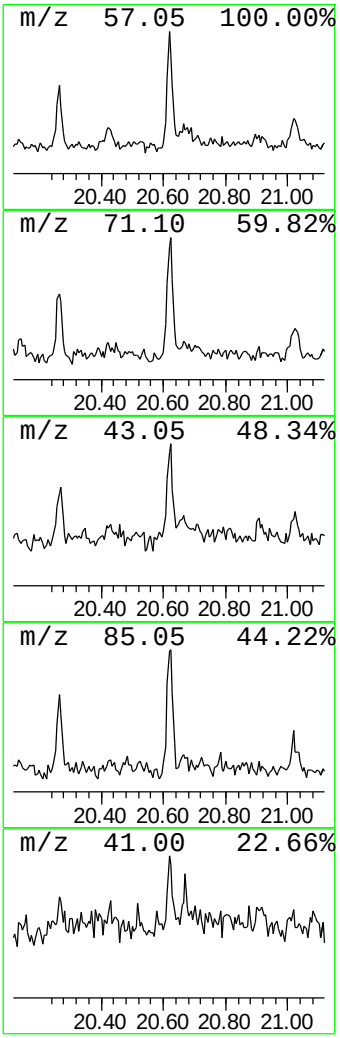
Peak Number 10 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.62	2.02 ng	47279	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	83
2	Hexacosane	366	C26H54	000630-01-3	80
3	Heneicosane	296	C21H44	000629-94-7	74
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

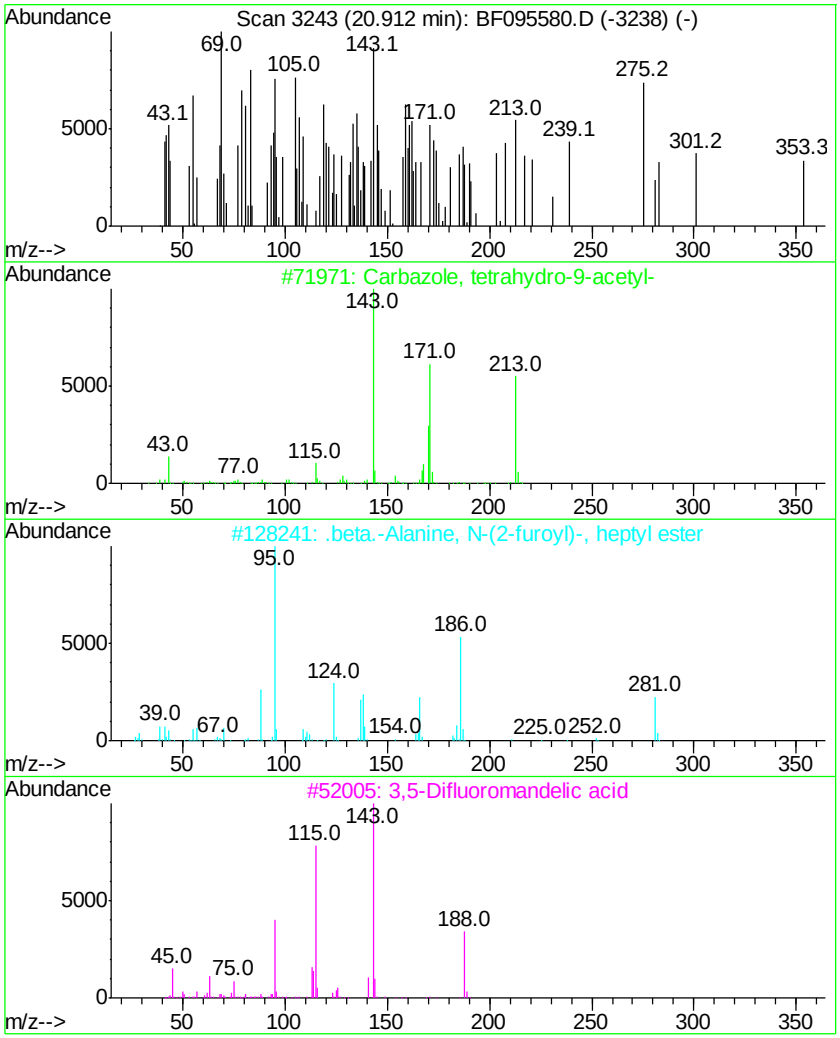
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

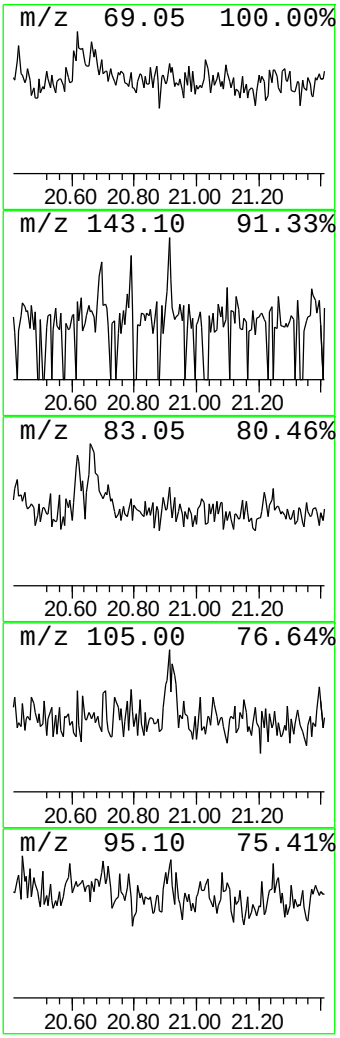
****

Peak Number 11 unknown20.91 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.91	3.07 ng	72031	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbazole, tetrahydro-9-acetyl-	213	C14H15NO	027236-49-3	10
2	.beta.-Alanine, N-(2-furoyl)-, h...	281	C15H23NO4	1000321-97-7	9
3	3,5-Difluoromandelic acid	188	C8H6F2O3	1000211-67-2	9
4	Imidazole[4,5-c]pyridine, 4,5,6,...	191	C7H8F3N3	113306-69-7	9
5	2,5-Difluoromandelic acid	188	C8H6F2O3	207853-61-0	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095580.D
Acq On : 31 May 2017 23:53
Operator : SJ/MA
Sample : I3341-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM1-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	4.80	6.5	ng	175020	1	7.55	542607	20.0
unknown7.21	7.21	76.5	ng	2076650	1	7.55	542607	20.0
n-Hexadecanoic acid	15.79	4.0	ng	102606	4	14.81	515026	20.0
1-Octadecanesulph...	18.41	6.2	ng	164983	5	18.51	532972	20.0
Heneicosane	18.82	3.3	ng	89096	5	18.51	532972	20.0
Heptadecane	19.20	4.2	ng	110976	5	18.51	532972	20.0
Octadecane	19.57	2.3	ng	53368	6	20.18	468662	20.0
Hexadecane	19.92	2.6	ng	62024	6	20.18	468662	20.0
Hentriacontane	20.62	2.0	ng	47279	6	20.18	468662	20.0
unknown20.91	20.91	3.1	ng	72031	6	20.18	468662	20.0