LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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	5.292	627	630	650	rBV	82564	222975	11.49%	2.226%
2	6.957	910	913	925	rBV	93784	218526	11.26%	2.181%
3	7.045	925	928	940	rVB	174581	321237	16.56%	3.206%
4	7.381	981	985	999	rBV	292699	389016	20.05%	3.883%
5	7.622	1022	1026	1047	rBB	166203	225574	11.63%	2.252%
6	8.298	1138	1141	1161	rBV	70196	141750	7.31%	1.415%
7	9.416	1326	1331	1345	rBV	419830	517639	26.68%	5.167%
8	11.192	1629	1633	1646	rVB	300123	347323	17.90%	3.467%
9	11.892	1748	1752	1757	rBV	32289	38415	1.98%	0.383%
10	12.239	1807	1811	1816	rBV2	405657	497729	25.66%	4.968%
11	12.286	1816	1819	1825	rVB2	17133	22911	1.18%	0.229%
12	13.098	1953	1957	1961	rVB2	18017	20264	1.04%	0.202%
13	13.539	2028	2032	2039	rBV2	86171	120101	6.19%	1.199%
14	13.868	2084	2088	2098	rVB2	19323	36201	1.87%	0.361%
15	14.045	2113	2118	2121	rBV	26424	30160	1.55%	0.301%
16	14.598	2208	2212	2214	rBV	19423	22488	1.16%	0.224%
17	14.633	2214	2218	2223	rVV	350012	432055	22.27%	4.312%
18	14.668	2223	2224	2231	rVB	21207	25746	1.33%	0.257%
19	15.280	2324	2328	2329	rBV	23342	27069	1.40%	0.270%
20	15.304	2329	2332	2336	rVB	56092	62631	3.23%	0.625%
21	15.433	2348	2354	2359	rBV	663855	764000	39.38%	7.626%
22	15.645	2386	2390	2399	rVB3	19040	29993	1.55%	0.299%
23	15.886	2427	2431	2436	rBV4	26430	35028	1.81%	0.350%
24	16.409	2514	2520	2522	rBV	1037547	1176280	60.63%	11.741%
25	16.445	2522	2526	2529	rVV	1693572	1940048	100.00%	19.364%
26	16.468	2529	2530	2535	rVB2	131962	116485	6.00%	1.163%
27	16.568	2543	2547	2552	rBV	330691	352859	18.19%	3.522%
28	16.756	2575	2579	2585	rVB	58361	67921	3.50%	0.678%
29	16.945	2607	2611	2617	rVV2	28739	37799	1.95%	0.377%
30	17.003	2617	2621	2629	rVB	260489	266263	13.72%	2.658%
31	17.415	2686	2691	2696	rVB3	44937	72024	3.71%	0.719%
32	17.533	2704	2711	2716	rBV5	20986	34950	1.80%	0.349%
33	17.856	2763	2766	2771	rBV	38401	41205	2.12%	0.411%
34	18.280	2831	2838	2845	rBV2	46737	80630	4.16%	0.805%

LSC Area Percent Report

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Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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	18.350	2845	2850	2854	rBV	356879	441006	22.73%	4.402%
36	18.680	2903	2906	2913	rVB2	48332	63472	3.27%	0.634%
37	19.068	2969	2972	2976	rVB	43629	40577	2.09%	0.405%
38	19.433	3031	3034	3038	rBV2	58213	73587	3.79%	0.734%
39	19.786	3091	3094	3098	rBV2	60816	70990	3.66%	0.709%
40	19.962	3122	3124	3128	rBV	24417	27324	1.41%	0.273%
41	20.015	3129	3133	3143	rVV	261051	347250	17.90%	3.466%
42	20.133	3150	3153	3158	rVB	73521	79978	4.12%	0.798%
43	20.468	3207	3210	3216	rVB	74743	91712	4.73%	0.915%
44	20.844	3272	3274	3278	rVB	44199	47633	2.46%	0.475%

Sum of corrected areas: 10018824

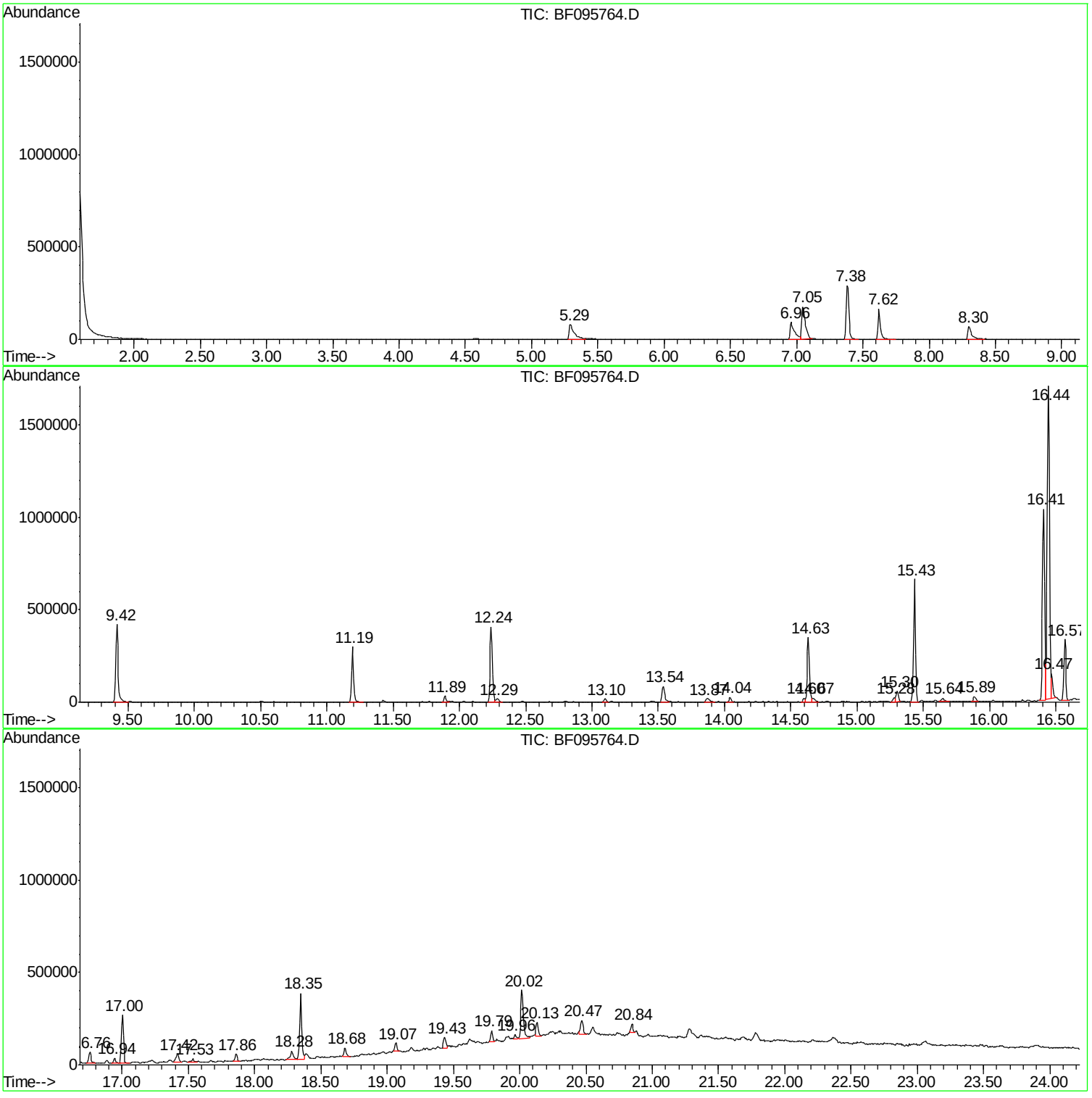
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-RO-45-060517

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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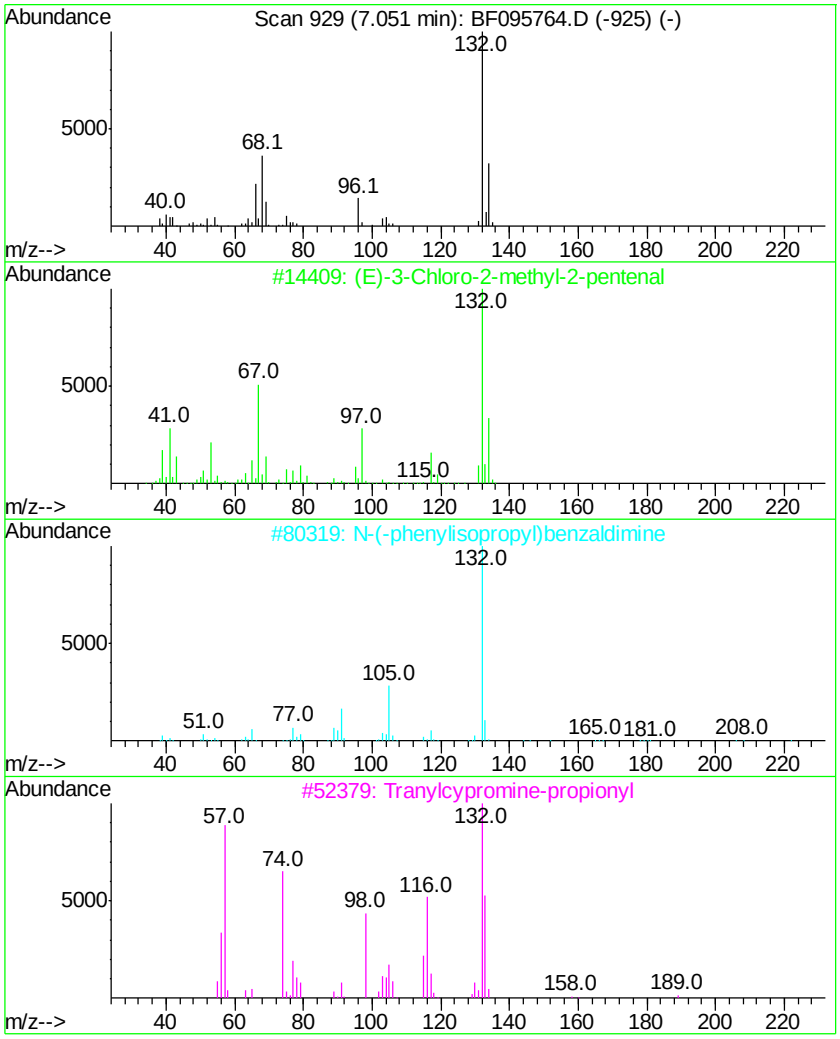
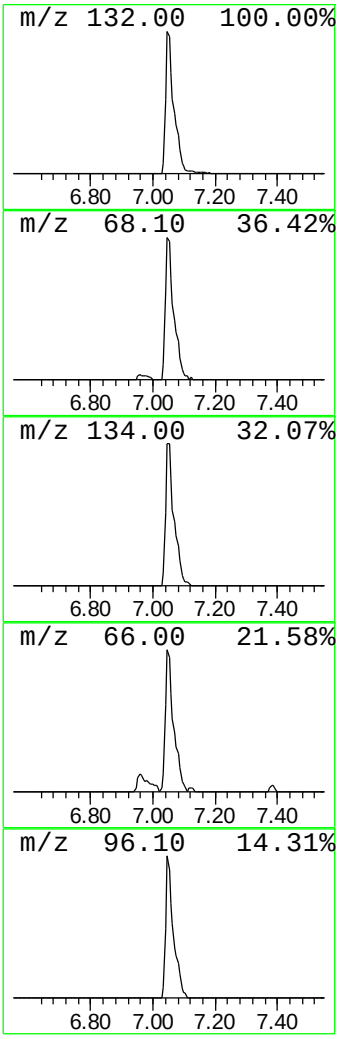
Peak Number 1 unknown7.05 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	16.52 ng	321237	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	N-(-phenylisopropyl)benzaldimine	223	C16H17N	1000379-01-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
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Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
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Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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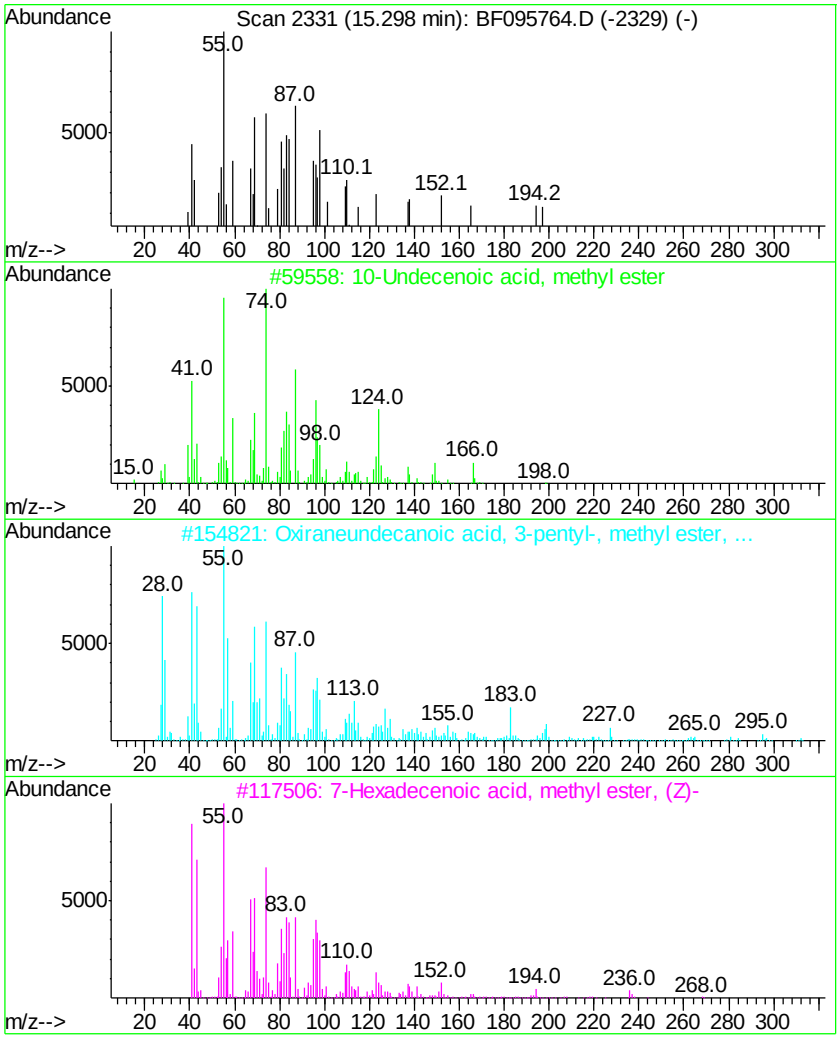
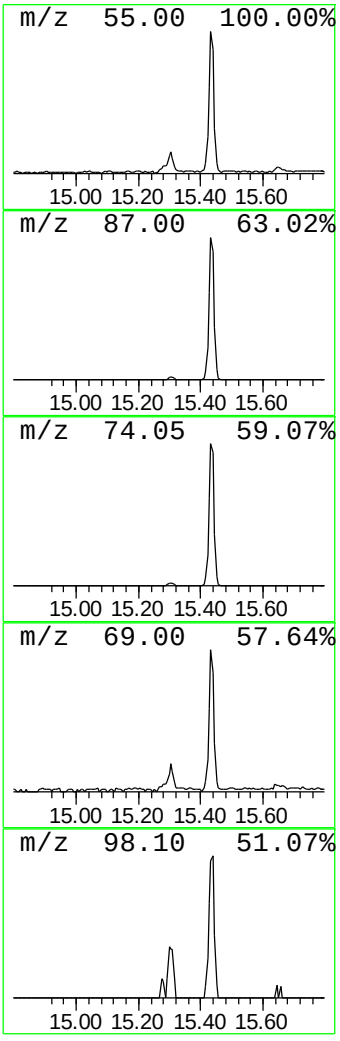
Peak Number 3 10-Undecenoic acid, methyl ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	2.90 ng	62631	Phenanthrene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Undecenoic acid, methyl ester	198	C12H22O2	000111-81-9	43
2	Oxiraneundecanoic acid, 3-pentyl...	312	C19H36O3	038520-31-9	38
3	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	35
4	Oxiraneundecanoic acid, 3-pentyl...	312	C19H36O3	038520-30-8	35
5	Methyl 6-methyloctanoate	172	C10H20O2	005129-62-4	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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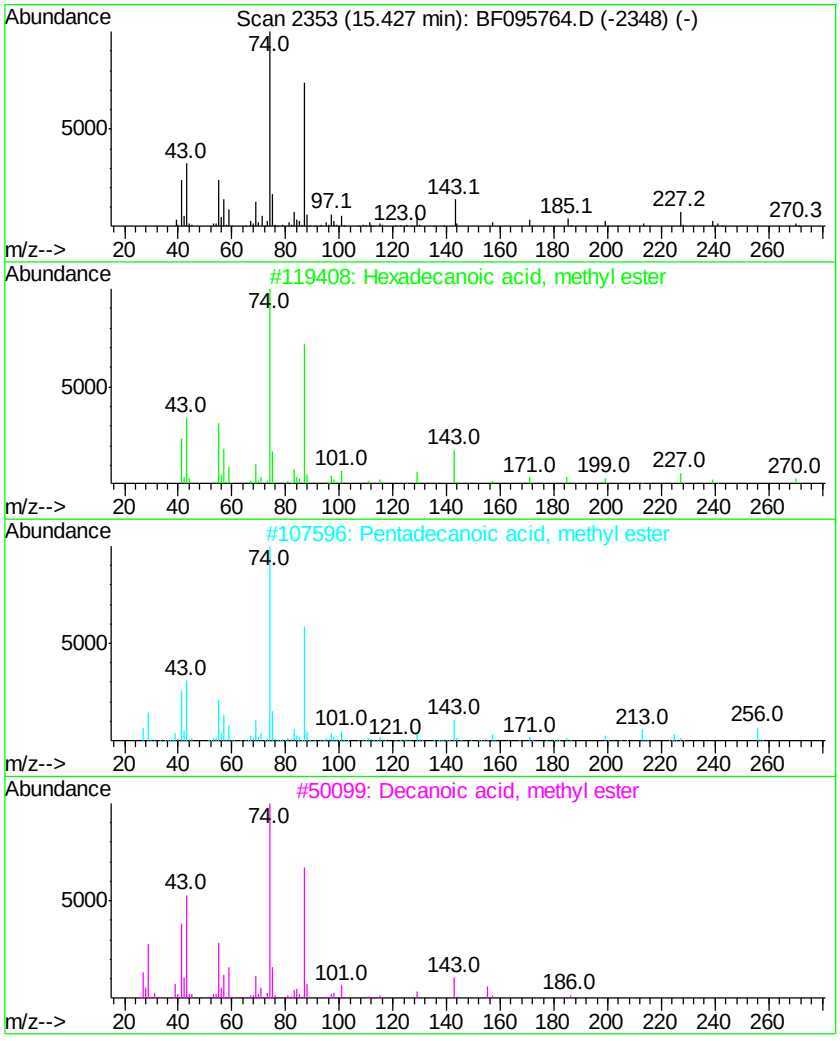
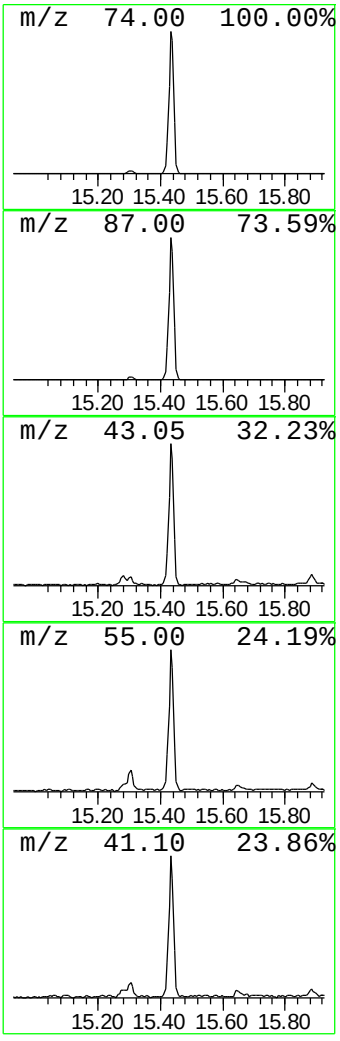
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.43	35.37 ng	764000	Phenanthrene-d10	14.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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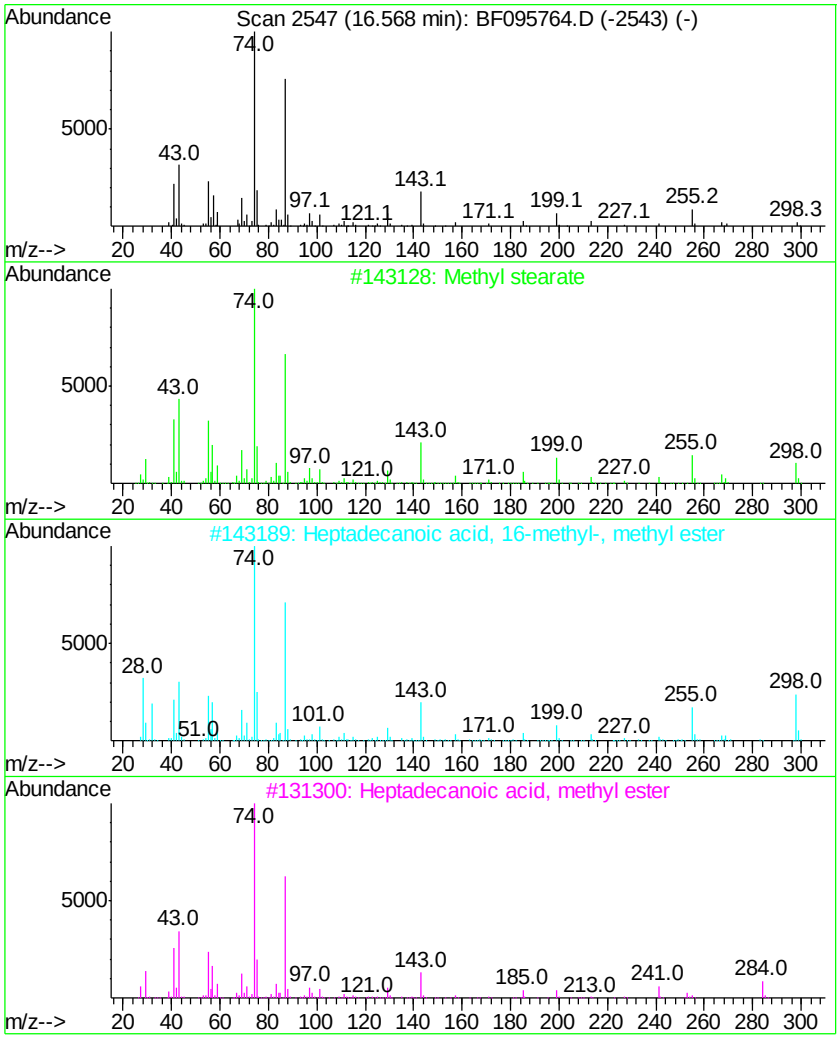
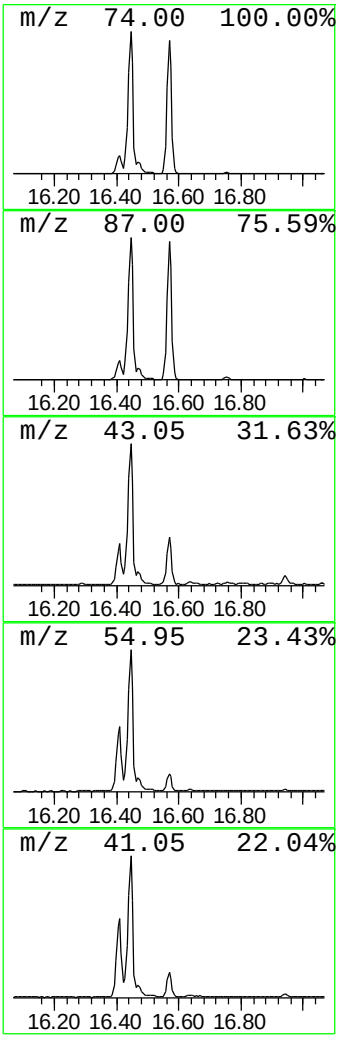
Peak Number 5 Methyl stearate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	16.00 ng	352859	Chrysene-d12	18.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86





Library Search Compound Report

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Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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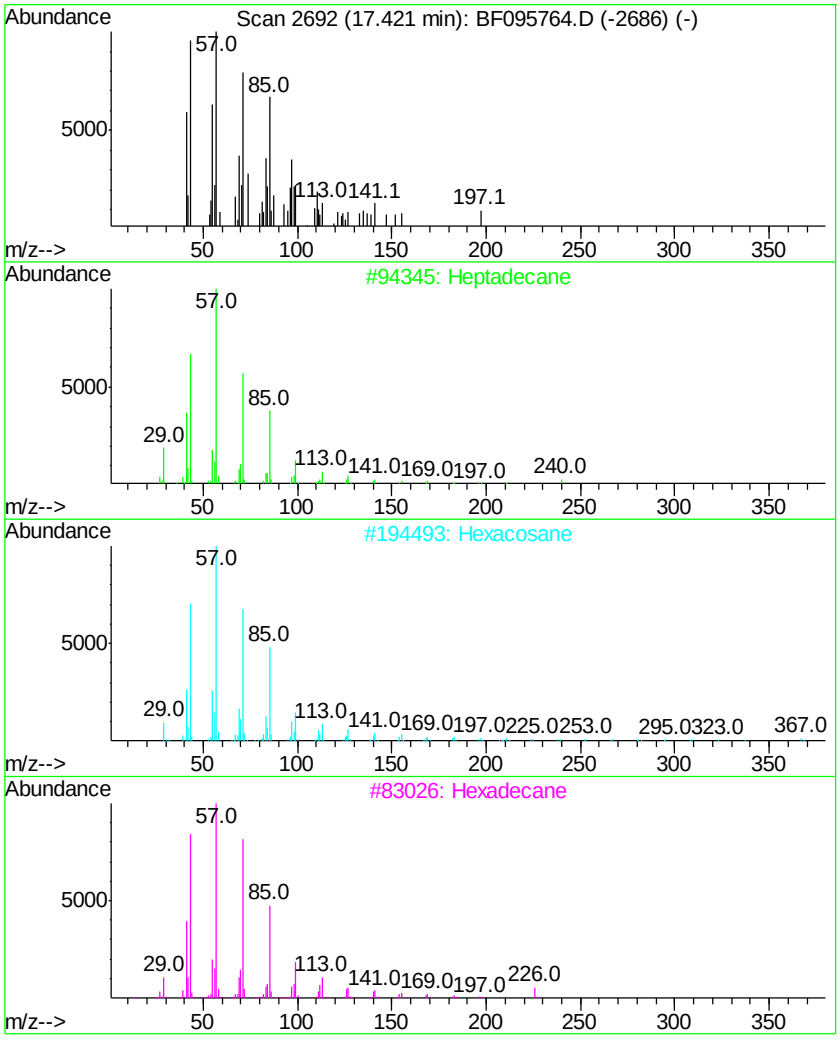
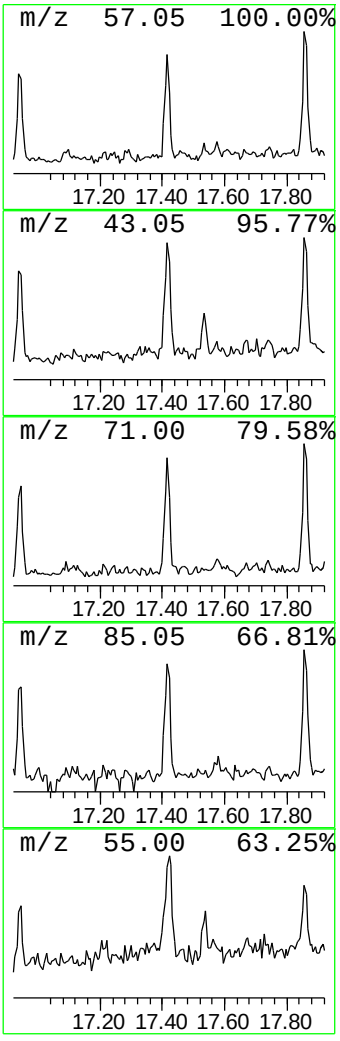
Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	3.27 ng	72024	Chrysene-d12	18.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Hexacosane	366	C26H54	000630-01-3	86
3	Hexadecane	226	C16H34	000544-76-3	80
4	Octacosane	394	C28H58	000630-02-4	80
5	Heneicosane	296	C21H44	000629-94-7	80





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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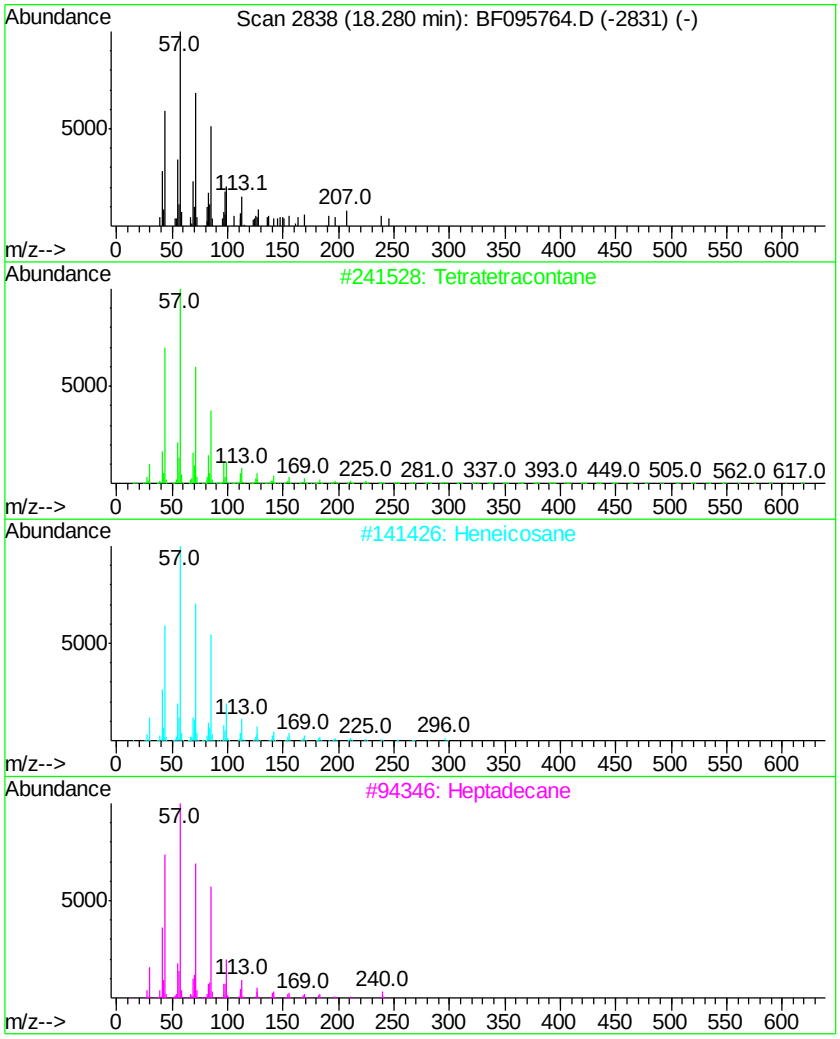
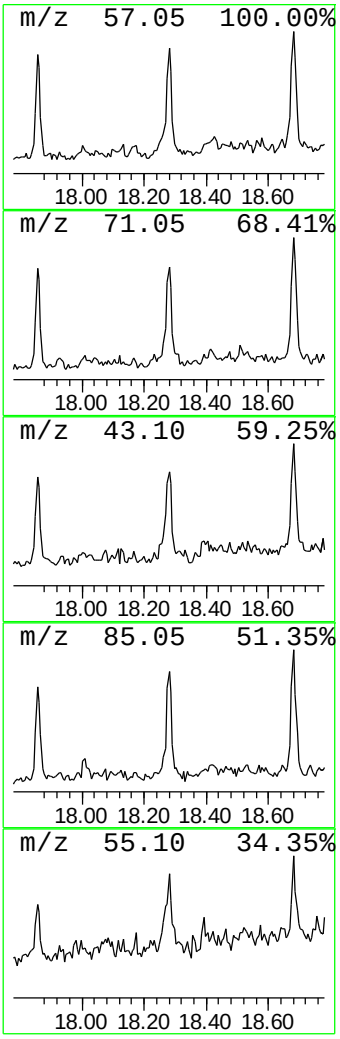
Peak Number 7 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	3.66 ng	80630	Chrysene-d12	18.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	86
2	Heneicosane	296	C21H44	000629-94-7	83
3	Heptadecane	240	C17H36	000629-78-7	83
4	Hexacosane	366	C26H54	000630-01-3	80
5	Hexadecane	226	C16H34	000544-76-3	80





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Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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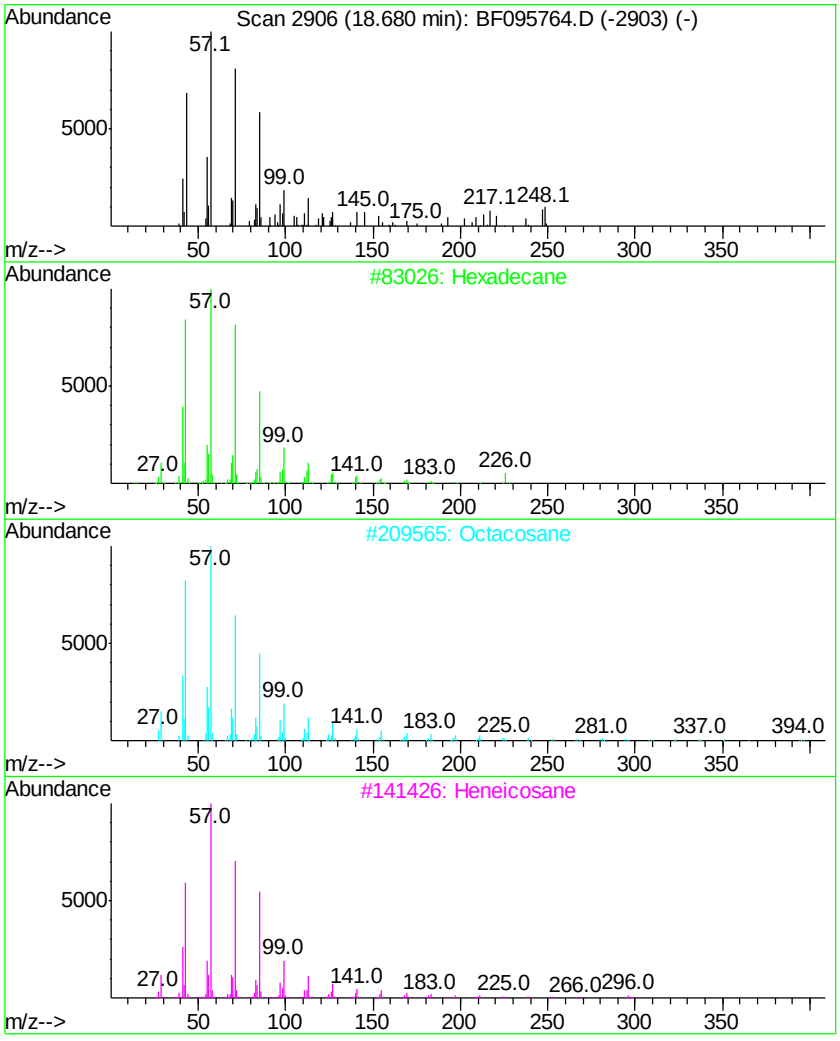
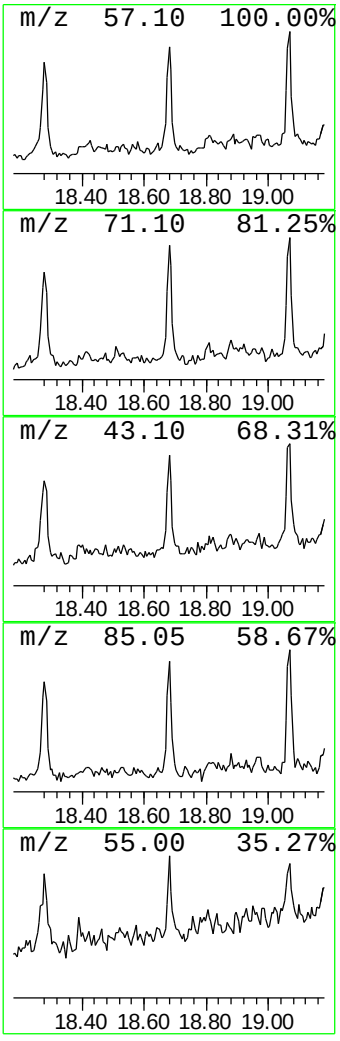
Peak Number 8 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.68	2.88 ng	63472	Chrysene-d12	18.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Octacosane	394	C28H58	000630-02-4	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Pentacosane	352	C25H52	000629-99-2	86
5	Hexacosane	366	C26H54	000630-01-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060717\
Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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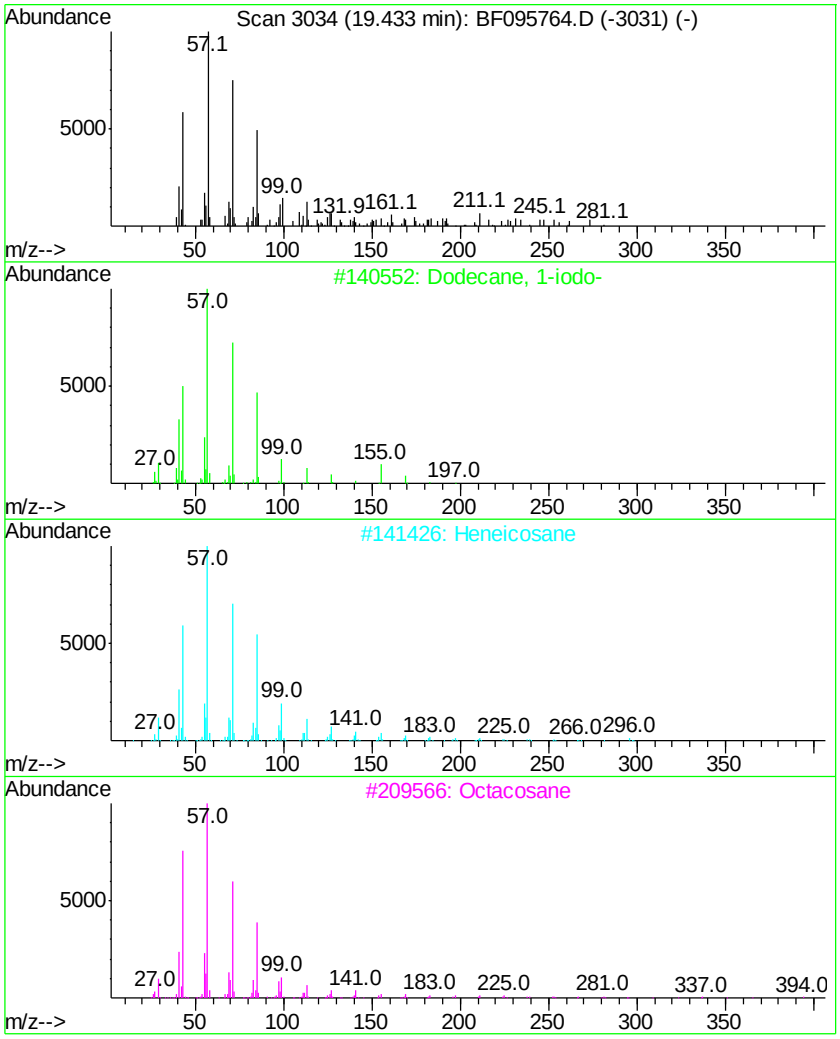
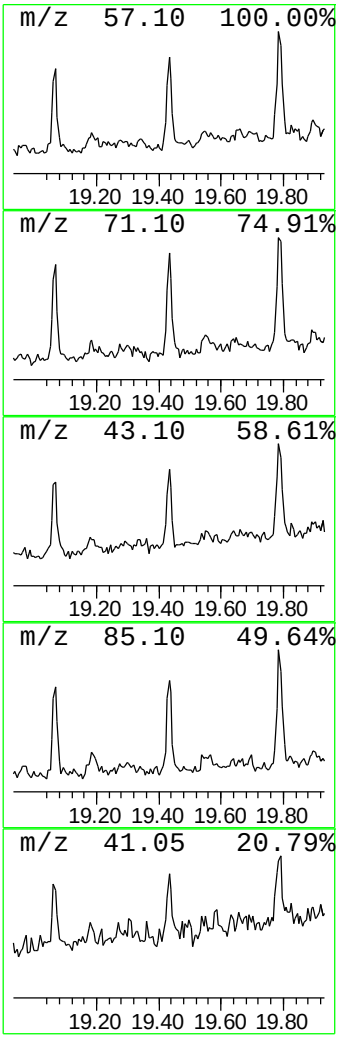
Peak Number 9 Dodecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	4.24 ng	73587	Perylene-d12	20.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
2	Heneicosane	296	C21H44	000629-94-7	64
3	Octacosane	394	C28H58	000630-02-4	64
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
5	Octadecane	254	C18H38	000593-45-3	64





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Data File : BF095764.D
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Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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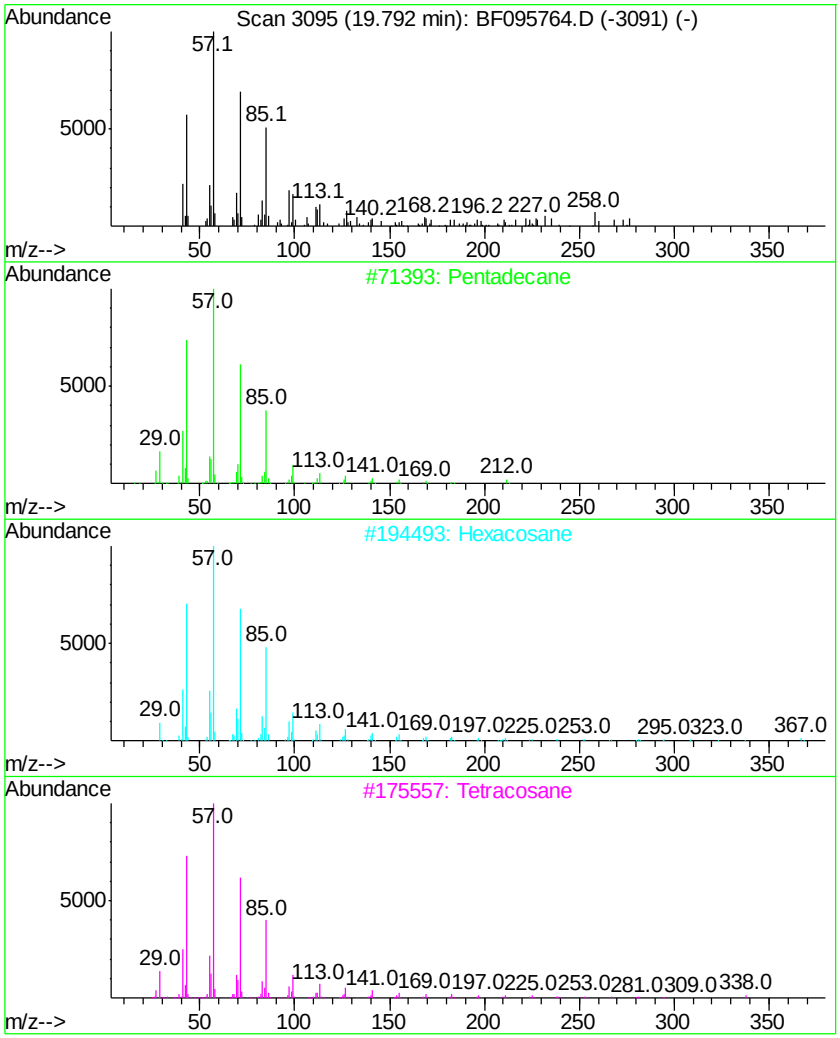
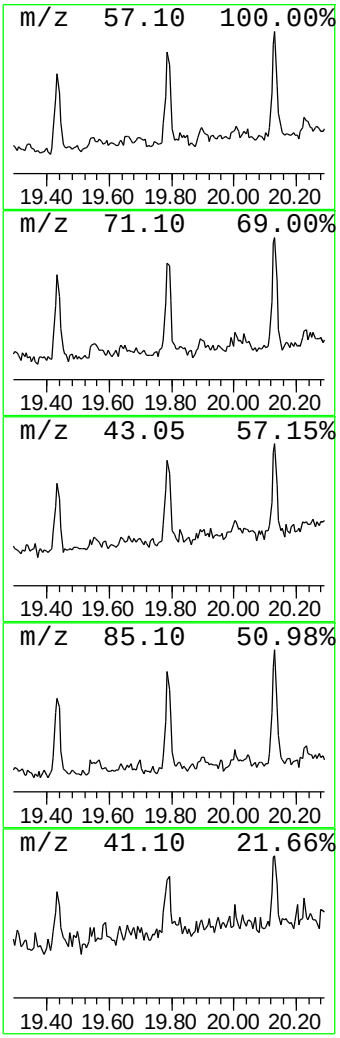
Peak Number 10 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	4.09 ng	70990	Perylene-d12	20.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Hexacosane	366	C26H54	000630-01-3	87
3	Tetracosane	338	C24H50	000646-31-1	74
4	Nonadecane	268	C19H40	000629-92-5	72
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	70





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Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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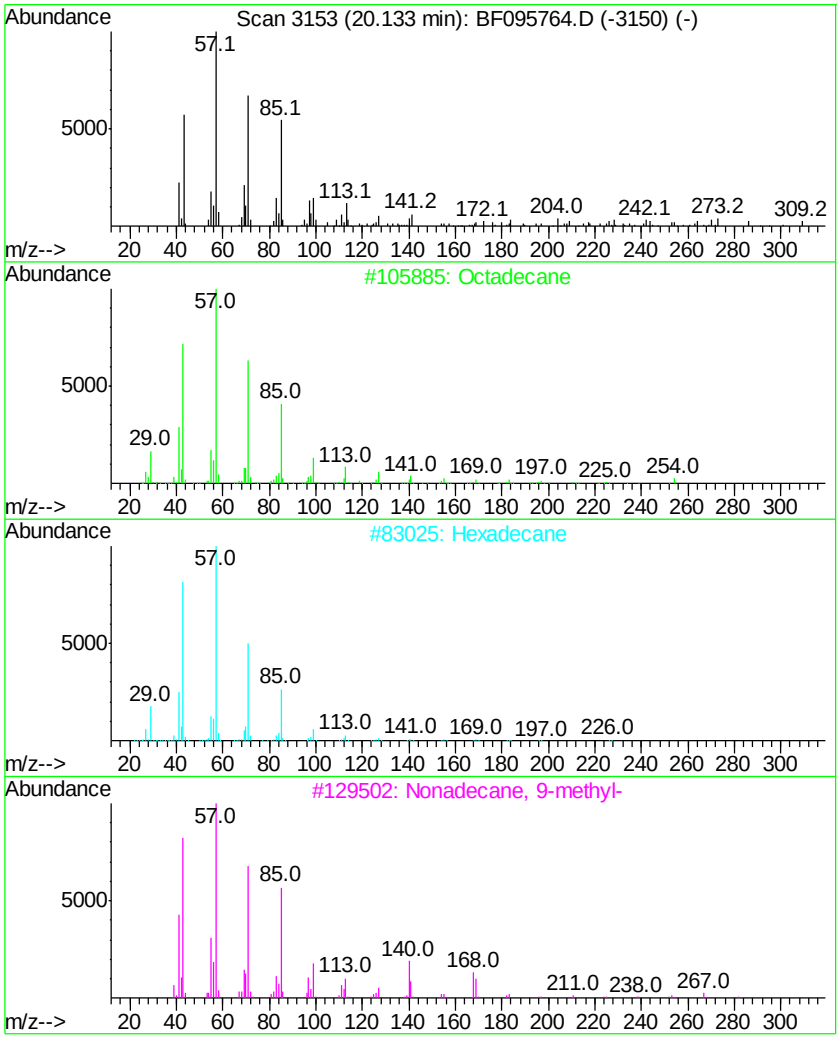
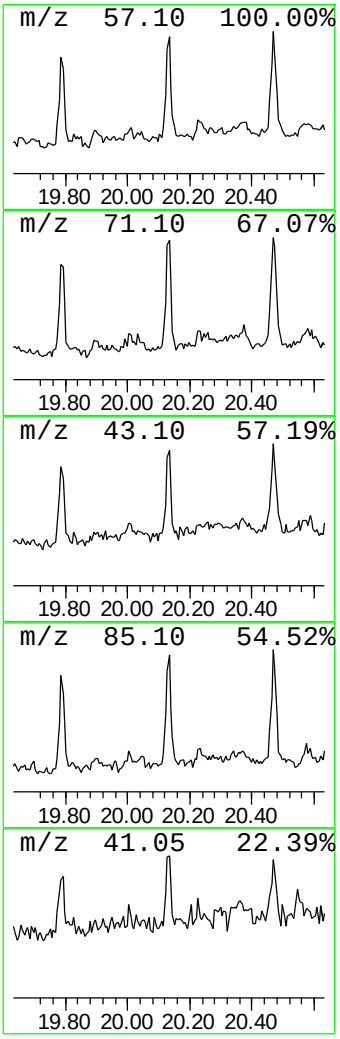
Peak Number 11 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.13	4.61 ng	79978	Perylene-d12	20.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Hexadecane	226	C16H34	000544-76-3	91
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane	296	C21H44	000629-94-7	87





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Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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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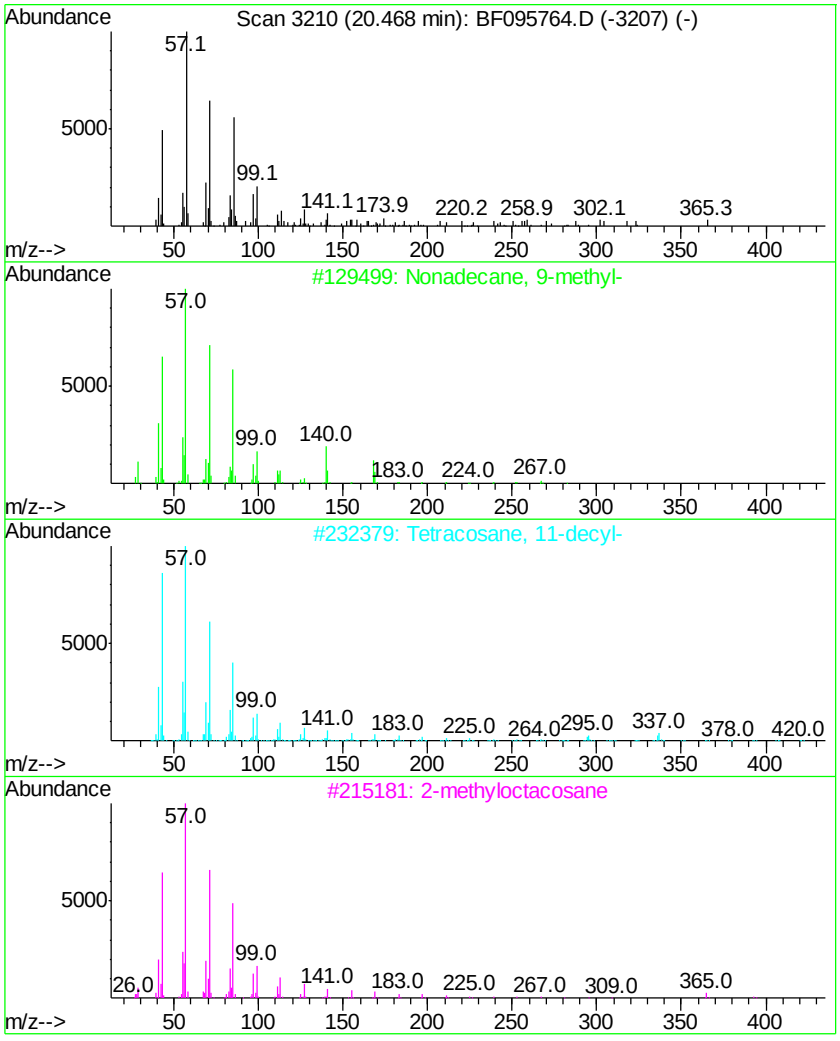
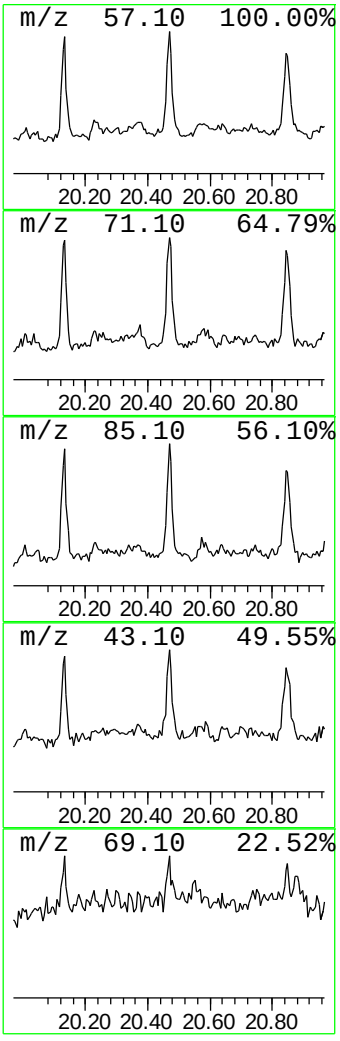
Peak Number 12 Nonadecane, 9-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.47	5.28 ng	91712	Perylene-d12	20.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Pentacosane	352	C25H52	000629-99-2	86
5	1-Iodoundecane	282	C11H23I	004282-44-4	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060717\
Data File : BF095764.D
Acq On : 8 Jun 2017 00:51
Operator : SJ/MA
Sample : I3488-13 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-RO-45-060517

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
unknown7.05	7.05	16.5	ng	321237	1	7.38	389016	20.0
10-Undecenoic aci...	15.30	2.9	ng	62631	4	14.63	432055	20.0
Hexadecanoic acid...	15.43	35.4	ng	764000	4	14.63	432055	20.0
Methyl stearate	16.57	16.0	ng	352859	5	18.35	441006	20.0
Heptadecane	17.42	3.3	ng	72024	5	18.35	441006	20.0
Tetratetracontane	18.28	3.7	ng	80630	5	18.35	441006	20.0
Hexadecane	18.68	2.9	ng	63472	5	18.35	441006	20.0
Dodecane, 1-iodo-	19.43	4.2	ng	73587	6	20.02	347250	20.0
Pentadecane	19.79	4.1	ng	70990	6	20.02	347250	20.0
Octadecane	20.13	4.6	ng	79978	6	20.02	347250	20.0
Nonadecane, 9-met...	20.47	5.3	ng	91712	6	20.02	347250	20.0