LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061317\
Data File : BF095902.D
Acq On : 13 Jun 2017 19:39
Operator : SJ/MA
Sample : I3643-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-VNJ217

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	4.563	503	506	530	rBV	43374	141804	7.85%	0.890%
2	5.245	618	622	646	rBV	663790	1382250	76.53%	8.672%
3	6.910	901	905	917	rBV	840201	1353410	74.93%	8.491%
4	7.004	917	921	940	rVB	1062358	1731030	95.84%	10.860%
5	7.351	976	980	998	rVB	273118	384627	21.30%	2.413%
6	7.586	1015	1020	1038	rBV	858999	1191498	65.97%	7.475%
7	8.269	1132	1136	1156	rBV	554019	886960	49.11%	5.565%
8	9.380	1321	1325	1349	rBV	346938	539232	29.86%	3.383%
9	11.163	1622	1628	1646	rBV	1350828	1806144	100.00%	11.331%
10	11.863	1743	1747	1758	rBV	97514	148703	8.23%	0.933%
11	12.204	1800	1805	1810	rBV2	436532	589542	32.64%	3.699%
12	12.245	1810	1812	1819	rVB3	21312	33087	1.83%	0.208%
13	12.627	1864	1877	1881	rBV5	5351	18995	1.05%	0.119%
14	13.057	1944	1950	1956	rBV	24593	32608	1.81%	0.205%
15	13.115	1956	1960	1968	rBV8	10408	22432	1.24%	0.141%
16	13.409	2000	2010	2016	rBV6	17616	48169	2.67%	0.302%
17	13.498	2020	2025	2038	rBV	631384	967797	53.58%	6.072%
18	13.827	2077	2081	2083	rBV	29711	38951	2.16%	0.244%
19	14.598	2207	2212	2217	rBV	419882	600464	33.25%	3.767%
20	14.639	2217	2219	2228	rVB	70854	109436	6.06%	0.687%
21	14.751	2235	2238	2242	rBV2	19197	27757	1.54%	0.174%
22	15.415	2348	2351	2355	rBV4	15630	19275	1.07%	0.121%
23	15.462	2355	2359	2363	rBV	15270	22844	1.26%	0.143%
24	15.615	2381	2385	2393	rVB2	74560	106025	5.87%	0.665%
25	16.227	2486	2489	2492	rBV3	13251	18680	1.03%	0.117%
26	16.421	2518	2522	2534	rVB	146674	211258	11.70%	1.325%
27	16.721	2569	2573	2581	rBV	160727	249653	13.82%	1.566%
28	16.939	2606	2610	2611	rBV2	20516	20490	1.13%	0.129%
29	16.974	2611	2616	2623	rVB	1217069	1447597	80.15%	9.082%
30	17.203	2653	2655	2663	rVB2	18159	22489	1.25%	0.141%
31	17.339	2675	2678	2683	rBV4	16616	27502	1.52%	0.173%
32	18.233	2825	2830	2839	rVB4	36960	63638	3.52%	0.399%
33	18.315	2839	2844	2850	rVV2	350466	482830	26.73%	3.029%
34	18.392	2854	2857	2865	rVB	71680	87930	4.87%	0.552%

LSC Area Percent Report

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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-VNJ217

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	19.350	3015	3020	3029	rBV	368107	424318	23.49%	2.662%
36	19.456	3036	3038	3044	rVB3	17941	20031	1.11%	0.126%
37	19.597	3058	3062	3065	rBV	51042	69462	3.85%	0.436%
38	19.627	3065	3067	3071	rVB	20687	20902	1.16%	0.131%
39	19.886	3105	3111	3115	rVB2	32970	41899	2.32%	0.263%
40	19.944	3117	3121	3124	rBV	45909	51556	2.85%	0.323%
41	19.986	3124	3128	3139	rBV	235461	344358	19.07%	2.160%
42	20.480	3206	3212	3213	rBV5	13089	18268	1.01%	0.115%
43	21.185	3327	3332	3341	rBV3	22382	46495	2.57%	0.292%
44	21.527	3382	3390	3399	rBV2	26808	67080	3.71%	0.421%

Sum of corrected areas: 15939476

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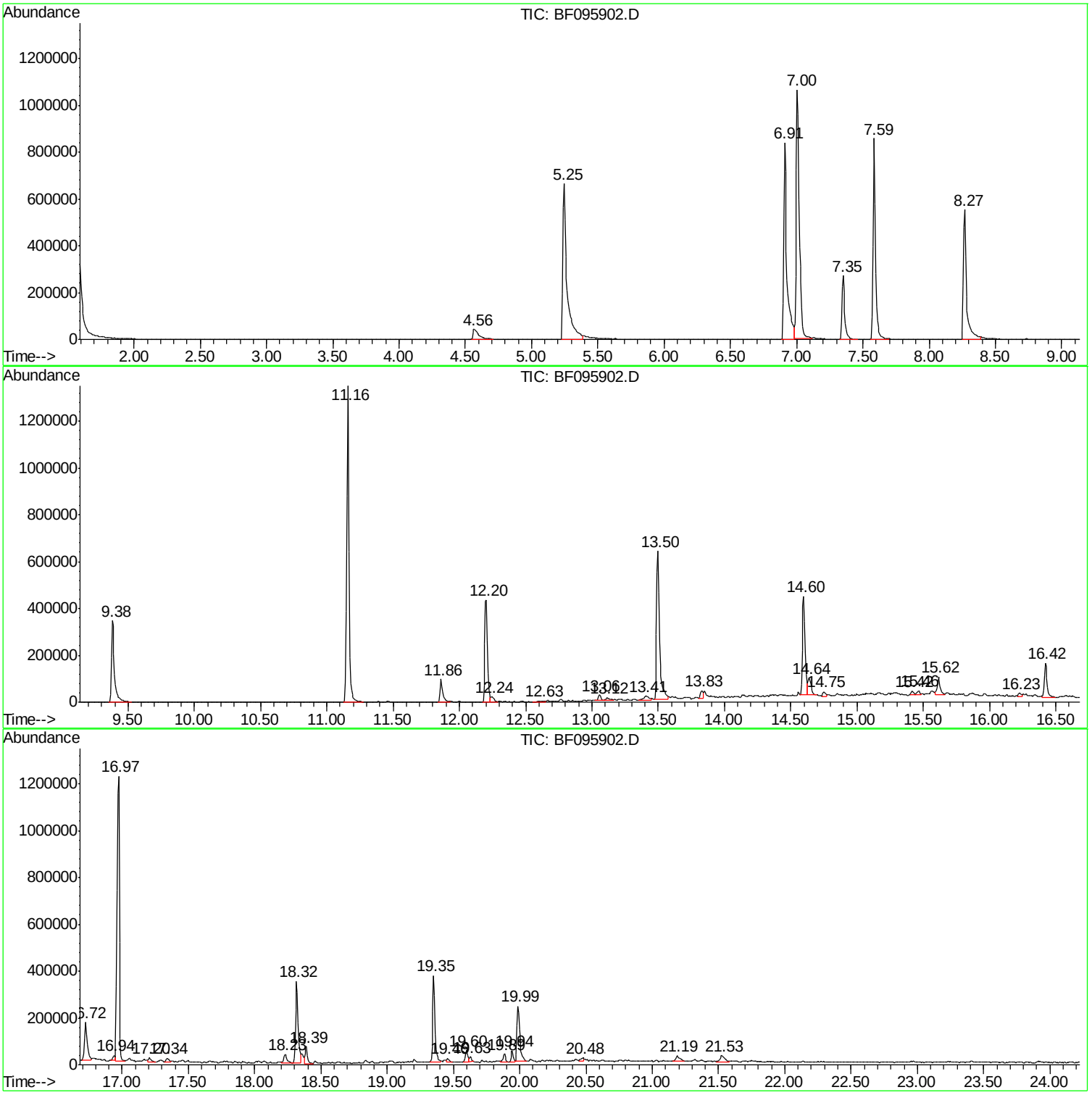
ClientSampleId : RO-VNJ217

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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Data File : BF095902.D
Acq On : 13 Jun 2017 19:39
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Instrument : BNA_F
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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

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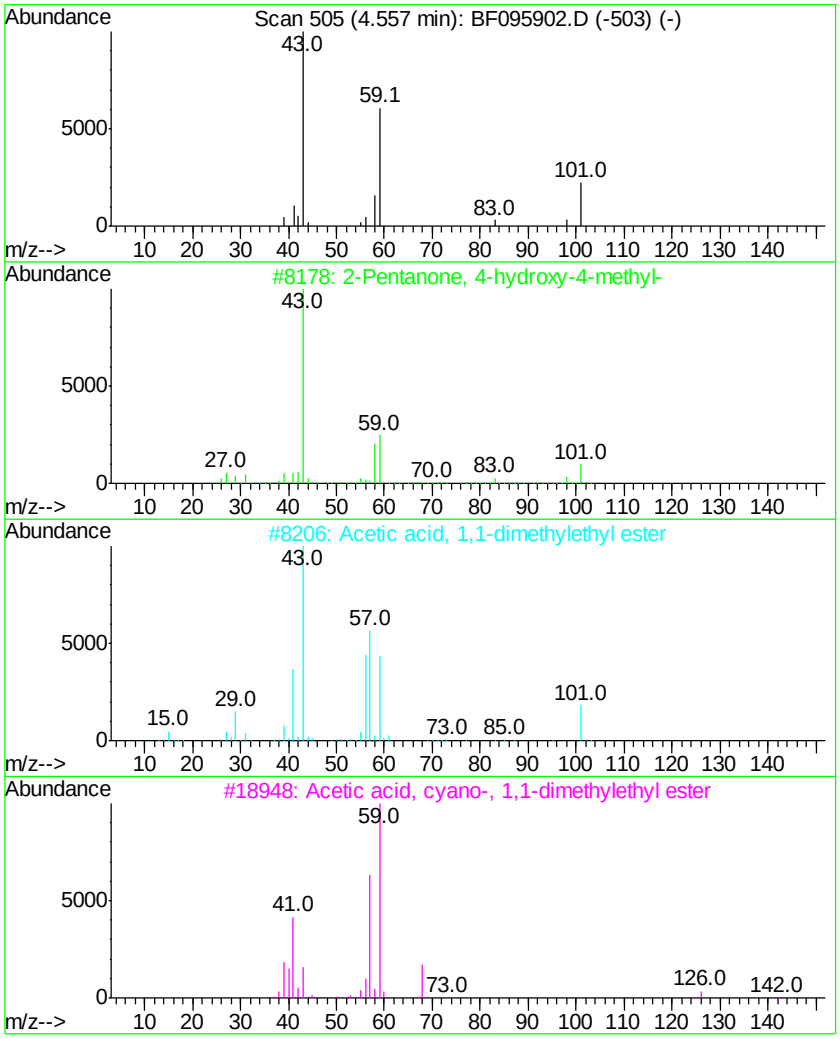
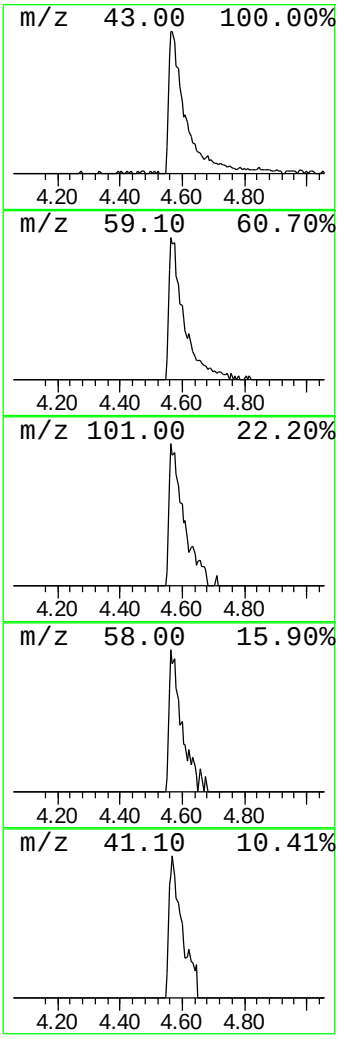
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	7.37 ng	141804	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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Instrument : BNA_F
ClientSampleId : RO-VNJ217

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

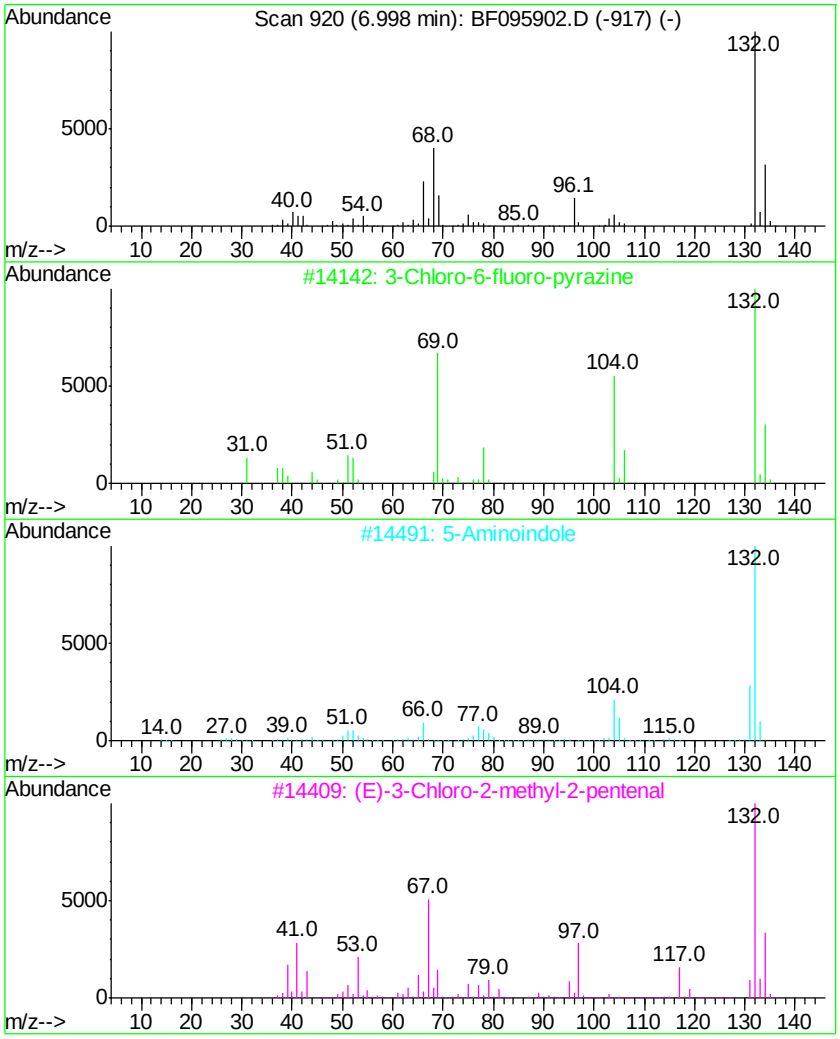
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

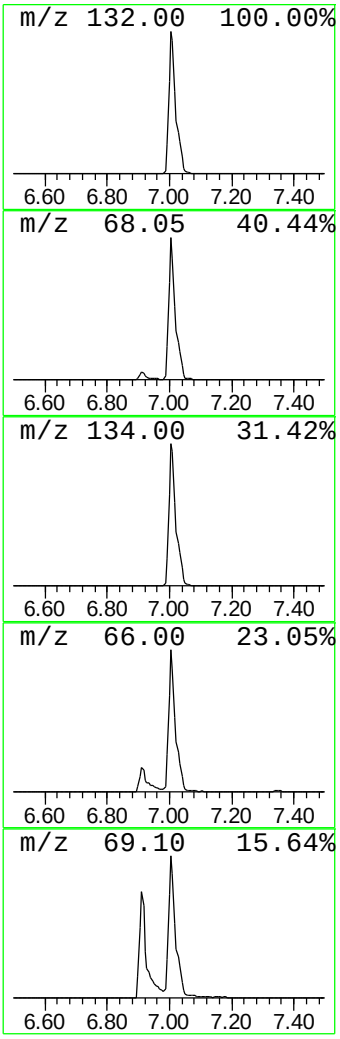
****

Peak Number 2 unknown7.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	90.01 ng	1731030	1,4-Dichlorobenzene-d4	7.35

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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061317\
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Acq On : 13 Jun 2017 19:39
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Sample : I3643-01
Misc :
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Instrument : BNA_F
ClientSampleId : RO-VNJ217

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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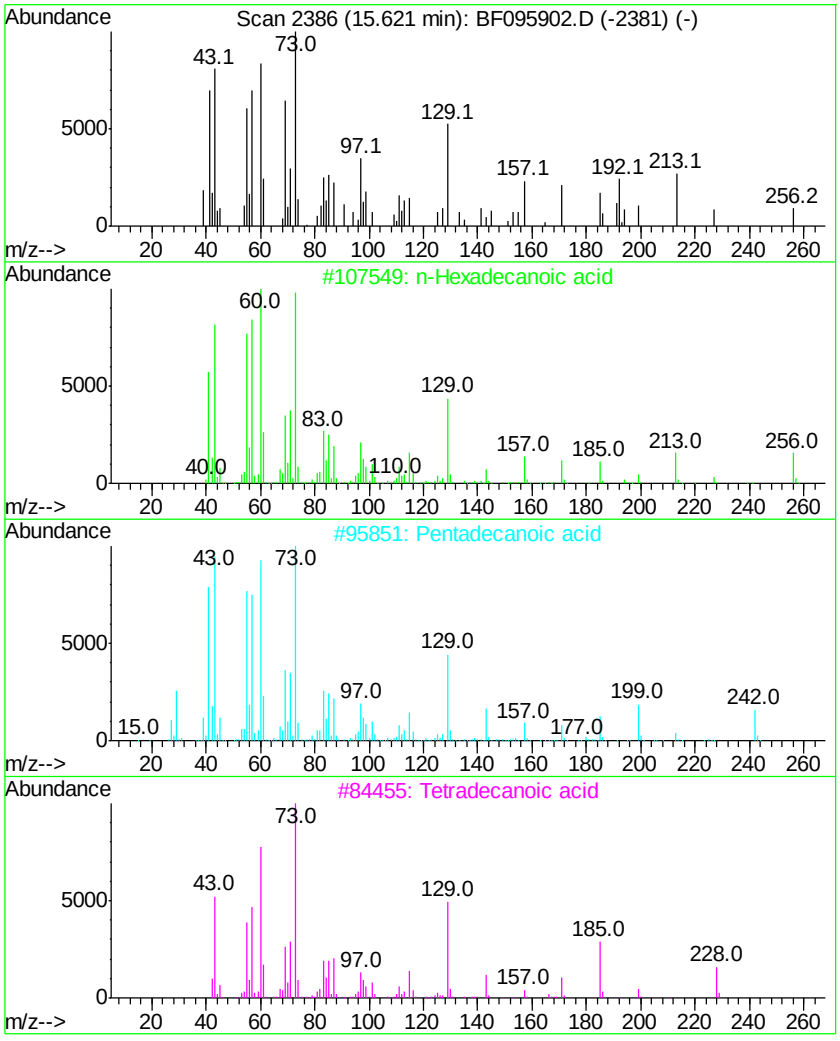
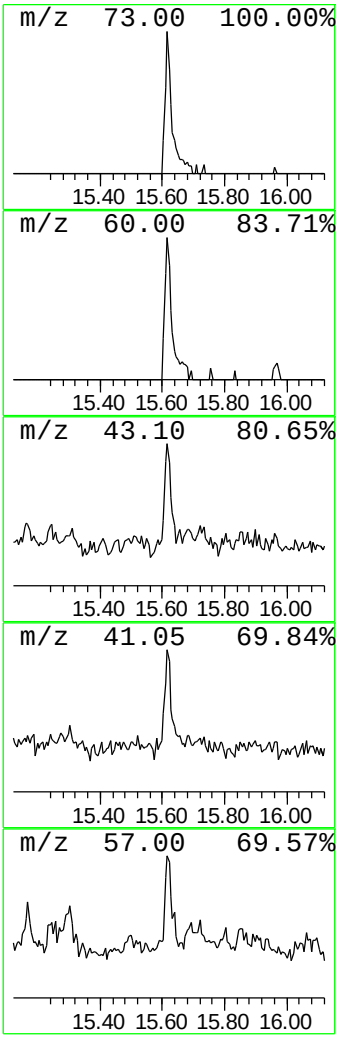
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	3.53 ng	106025	Phenanthrene-d10	14.60

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	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	50





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Sample : I3643-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-VNJ217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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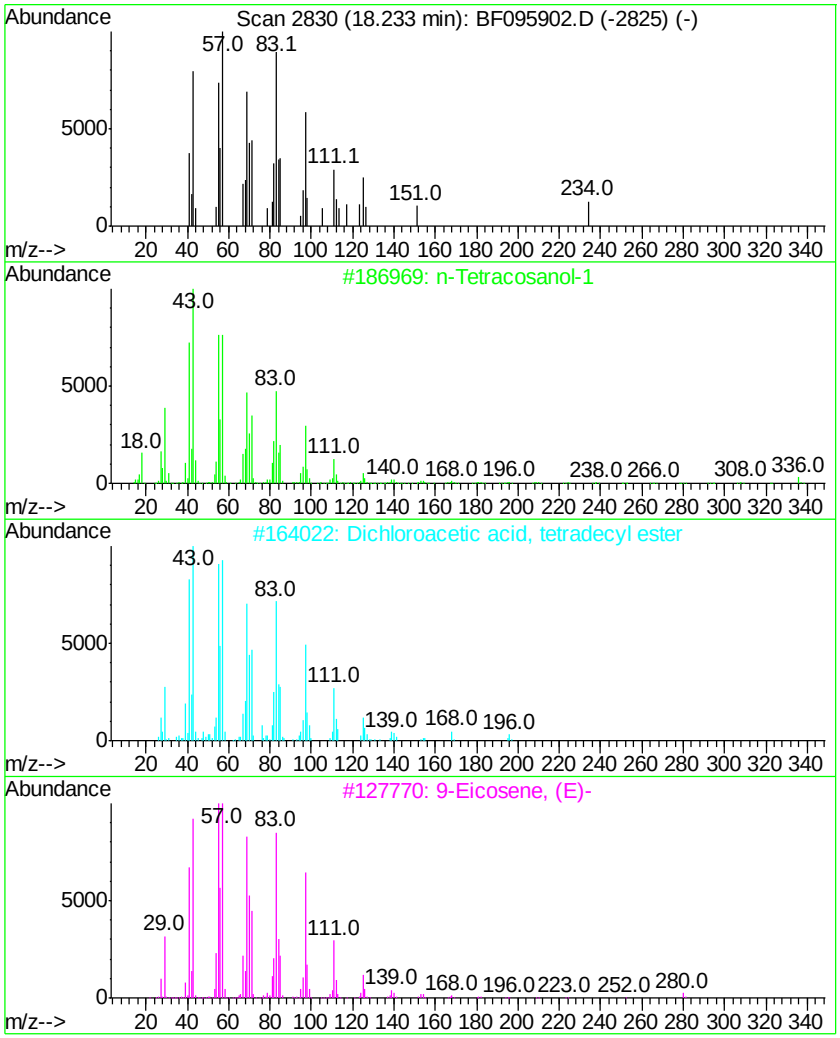
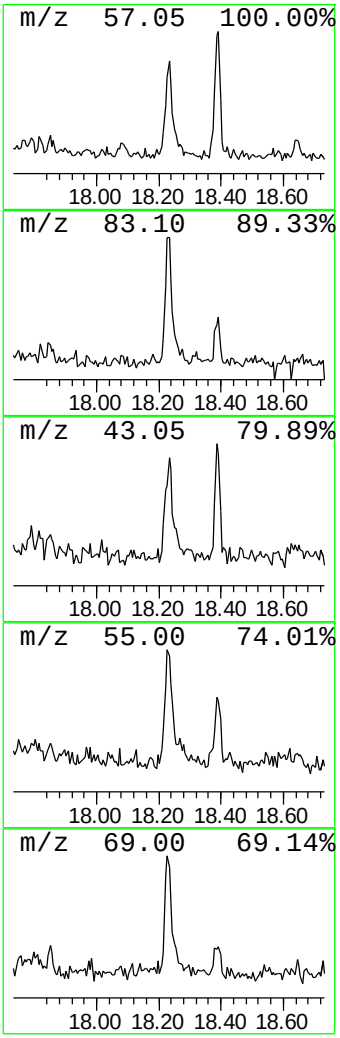
Peak Number 5 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.23	2.64 ng	63638	Chrysene-d12	18.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	90
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	87
4	1-Hexadecanol	242	C16H34O	036653-82-4	83
5	Behenic alcohol	326	C22H46O	000661-19-8	83





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-VNJ217

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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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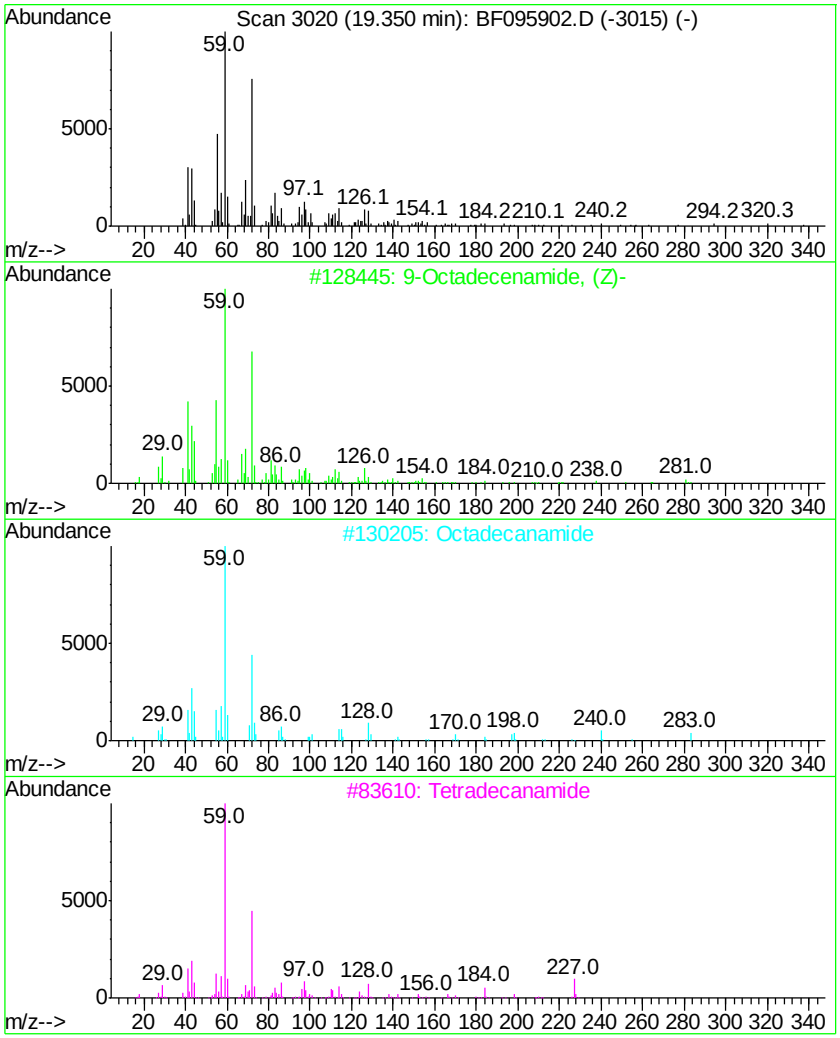
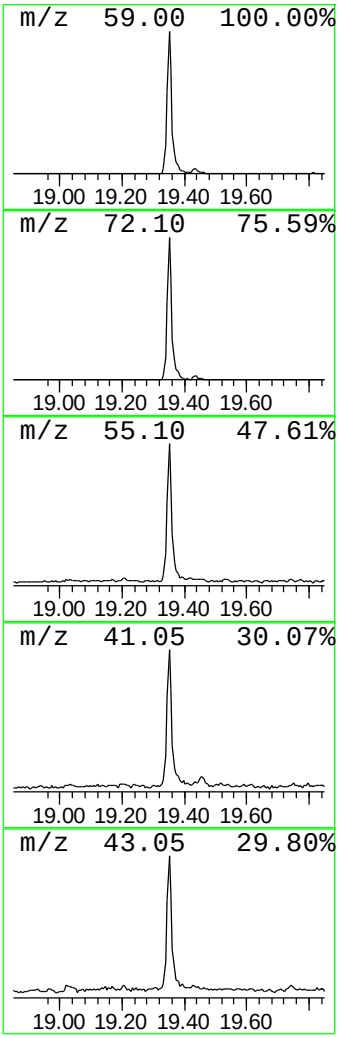
Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	24.64 ng	424318	Perylene-d12	19.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Octadecanamide	283	C18H37NO	000124-26-5	53
3	Tetradecanamide	227	C14H29NO	000638-58-4	50
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50
5	Dodecanamide	199	C12H25NO	001120-16-7	47





Tentatively Identified Compound (LSC) summary

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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...	4.56	7.4	ng	141804	1	7.35	384627	20.0
unknown7.00	7.00	90.0	ng	1731030	1	7.35	384627	20.0
n-Hexadecanoic acid	15.62	3.5	ng	106025	4	14.60	600464	20.0
n-Tetracosanol-1	18.23	2.6	ng	63638	5	18.32	482830	20.0
9-Octadecenamide,...	19.35	24.6	ng	424318	6	19.99	344358	20.0