LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099926.D
Acq On : 28 Oct 2017 19:22
Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

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-BF102317.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	5.004	493	496	514	rBV	139377	213644	14.48%	1.313%
2	5.410	562	565	588	rBV	1244330	1390744	94.26%	8.544%
3	6.428	735	738	757	rBV	1260319	1409399	95.52%	8.659%
4	6.557	757	760	772	rVB	1633544	1469034	99.56%	9.025%
5	6.787	796	799	809	rBV	604237	549193	37.22%	3.374%
6	6.940	821	825	841	rBV	1297360	1151892	78.07%	7.077%
7	7.357	892	896	908	rBV	881323	854635	57.92%	5.251%
8	8.069	1013	1017	1034	rVB	825966	751557	50.94%	4.617%
9	8.628	1109	1112	1121	rBV	42185	40673	2.76%	0.250%
10	9.139	1195	1199	1202	rBV	1831440	1475464	100.00%	9.065%
11	9.469	1251	1255	1257	rBV	150813	132109	8.95%	0.812%
12	9.539	1263	1267	1277	rVB	274985	226697	15.36%	1.393%
13	9.786	1305	1309	1311	rBV	55906	45069	3.05%	0.277%
14	9.822	1311	1315	1325	rVB	945831	790618	53.58%	4.857%
15	10.533	1433	1436	1442	rBV	154620	126988	8.61%	0.780%
16	10.616	1447	1450	1461	rBV	740264	662426	44.90%	4.070%
17	11.310	1565	1568	1572	rBV	673383	649185	44.00%	3.988%
18	11.686	1629	1632	1636	rBV	103944	86065	5.83%	0.529%
19	11.827	1652	1656	1663	rBV3	48970	58640	3.97%	0.360%
20	12.374	1745	1749	1751	rBV	196519	174516	11.83%	1.072%
21	12.392	1751	1752	1761	rVB	140790	124285	8.42%	0.764%
22	12.480	1764	1767	1769	rVB	57843	41424	2.81%	0.254%
23	12.533	1772	1776	1779	rBV	48265	42477	2.88%	0.261%
24	12.763	1810	1815	1823	rVB	37908	44183	2.99%	0.271%
25	12.892	1833	1837	1841	rBV	1119112	935200	63.38%	5.746%
26	13.092	1868	1871	1876	rVB4	15747	21432	1.45%	0.132%
27	13.657	1963	1967	1970	rBV	381509	299872	20.32%	1.842%
28	13.774	1983	1987	1994	rBV2	100251	110443	7.49%	0.679%
29	13.916	2008	2011	2015	rVB	42713	31075	2.11%	0.191%
30	13.963	2015	2019	2022	rVV	560982	514582	34.88%	3.161%
31	13.986	2022	2023	2028	rVB	22993	19591	1.33%	0.120%
32	14.321	2074	2080	2083	rBV7	11778	28416	1.93%	0.175%
33	14.404	2090	2094	2101	rBV3	25065	43596	2.95%	0.268%
34	14.698	2141	2144	2148	rBV	21049	21717	1.47%	0.133%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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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-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.021	2193	2199	2202	rBV2	84394	125411	8.50%	0.770%
36	15.051	2202	2204	2209	rVB4	21102	26816	1.82%	0.165%
37	15.304	2244	2247	2255	rBV	13685	19875	1.35%	0.122%
38	15.386	2255	2261	2264	rVV2	70104	113440	7.69%	0.697%
39	15.421	2264	2267	2277	rVB	416525	535559	36.30%	3.290%
40	15.804	2328	2332	2338	rVB	116264	167354	11.34%	1.028%
41	15.863	2338	2342	2349	rVB9	12485	23041	1.56%	0.142%
42	16.292	2409	2415	2422	rBV	101841	179750	12.18%	1.104%
43	16.857	2504	2511	2518	rBV	81988	167791	11.37%	1.031%
44	17.362	2592	2597	2604	rBV6	20307	46939	3.18%	0.288%
45	17.527	2618	2625	2632	rVB3	63767	142385	9.65%	0.875%
46	18.321	2753	2760	2776	rVB4	35255	127662	8.65%	0.784%
47	19.268	2913	2921	2928	rBV6	22056	64103	4.34%	0.394%

Sum of corrected areas: 16276967

LSC Report - Integrated Chromatogram

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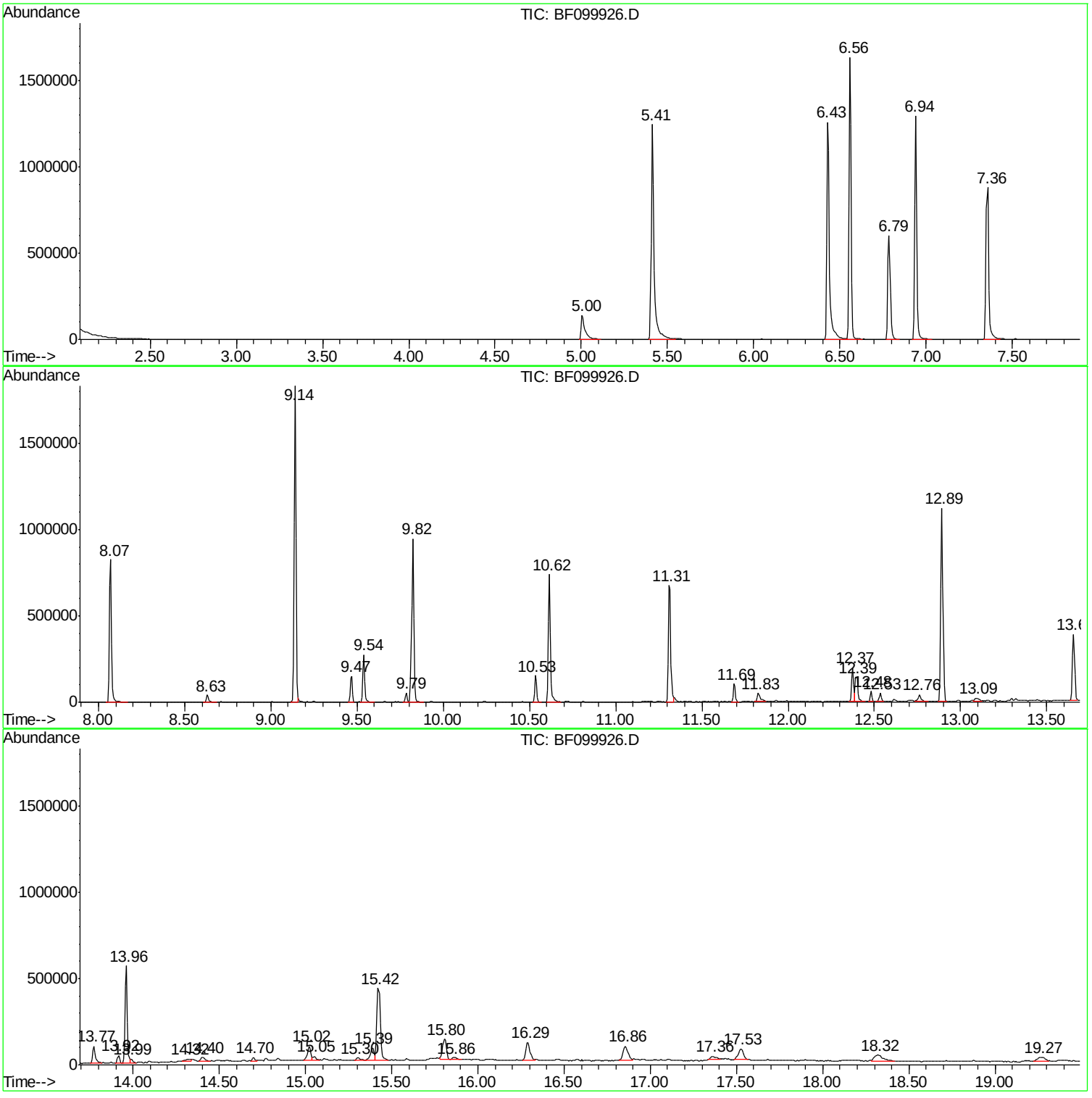
Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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\BF102817\
Data File : BF099926.D
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Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

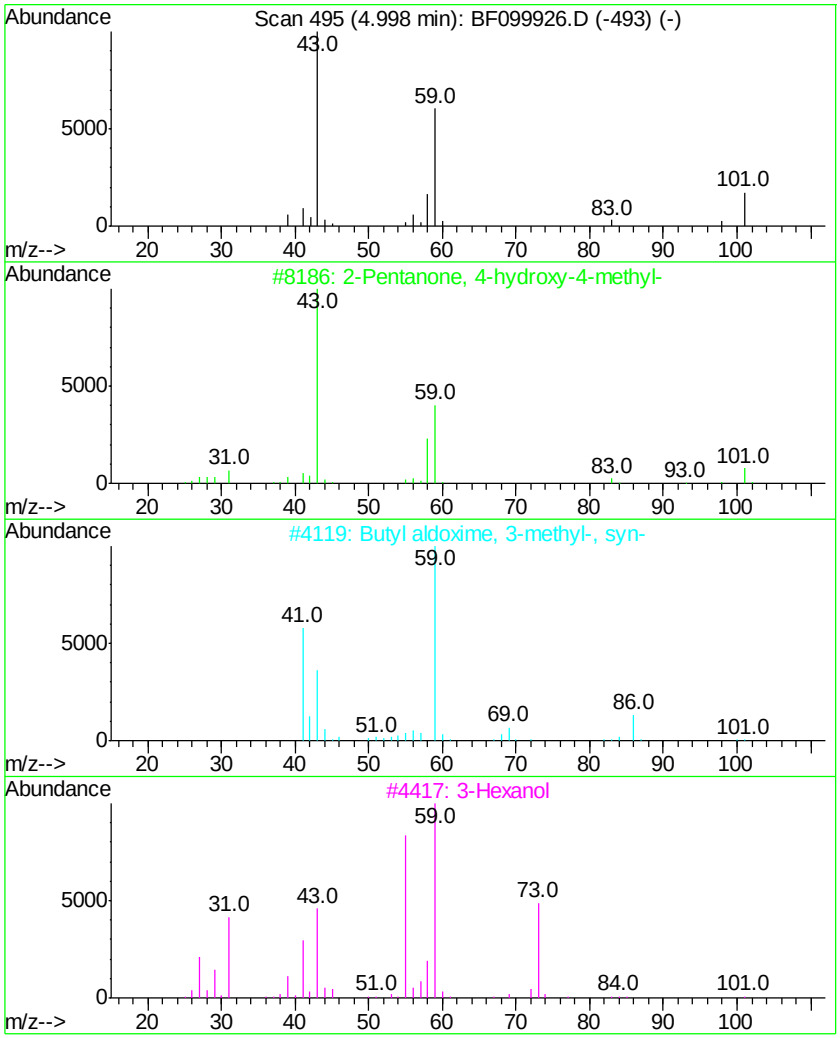
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

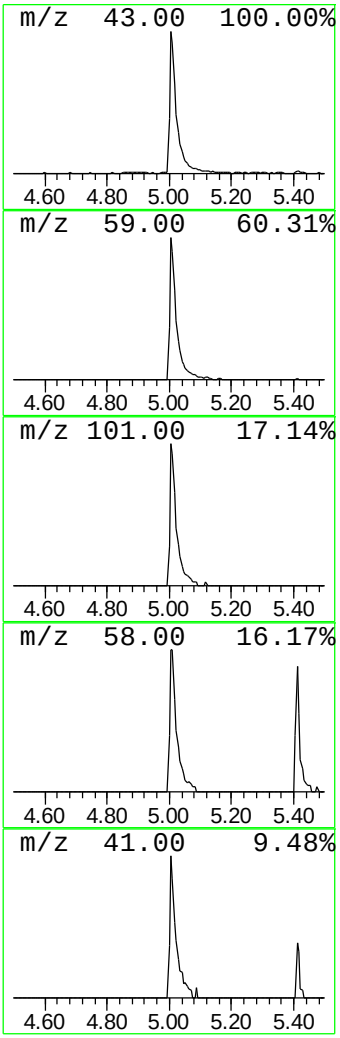
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	7.78 ng	213644	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	38
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : I6146-01
Misc :
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Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

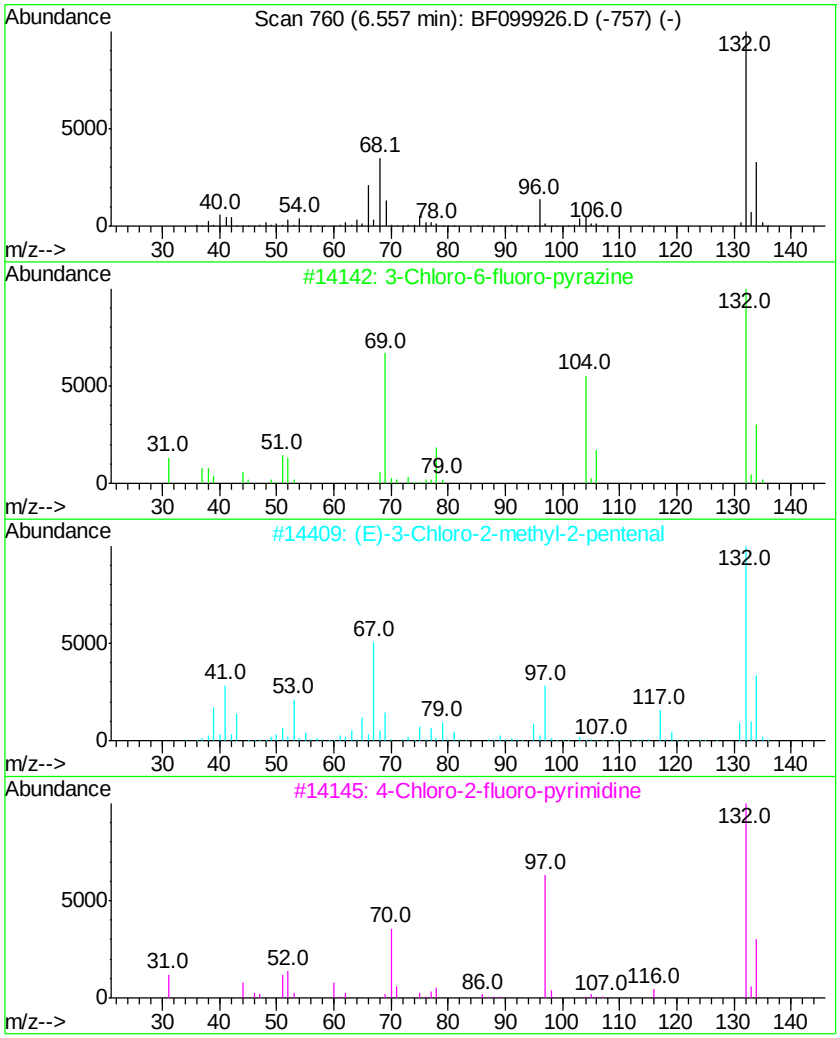
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

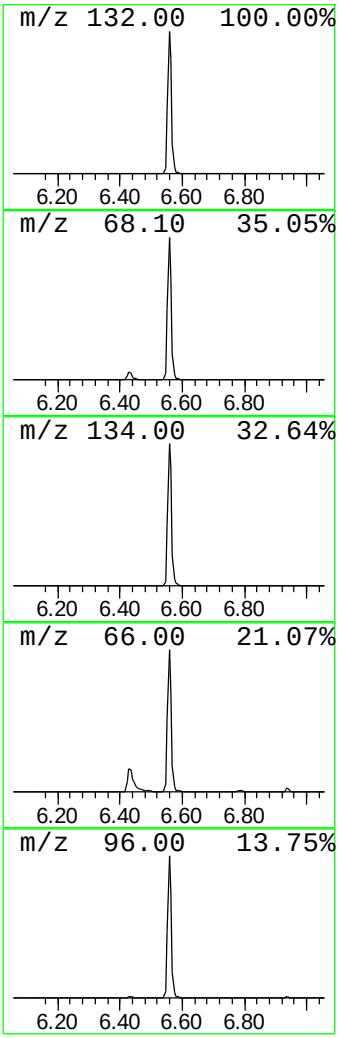
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	53.50 ng	1469030	1,4-Dichlorobenzene-d4	6.79

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	35
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Sample : I6146-01
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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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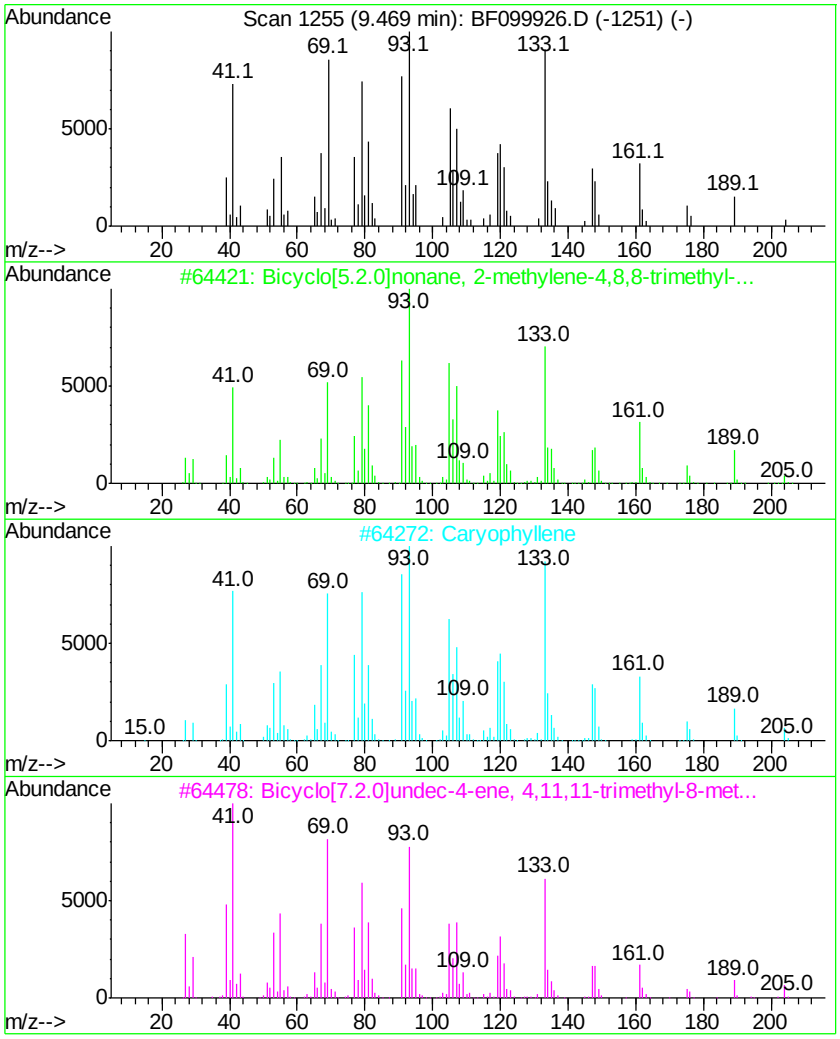
TIC Integration Parameters: LSCINT.P

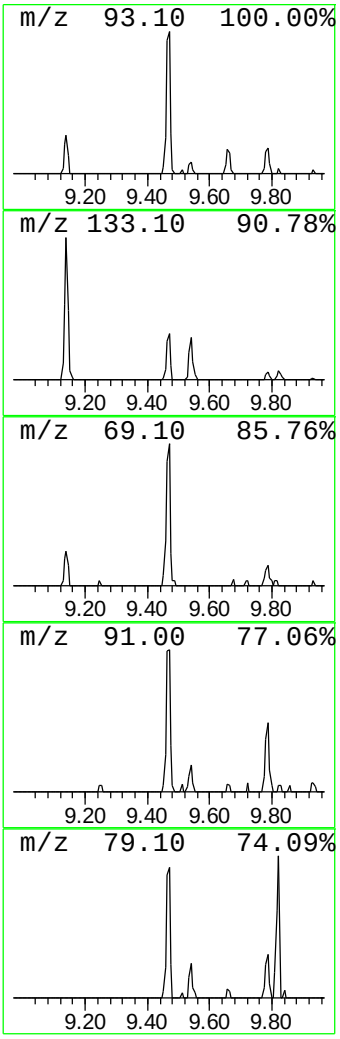
****

Peak Number 4 Bicyclo[5.2.0]nonane, 2-met... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.47	3.34 ng	132109	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	95
2	Caryophyllene	204	C15H24	000087-44-5	94
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	62
5	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	50





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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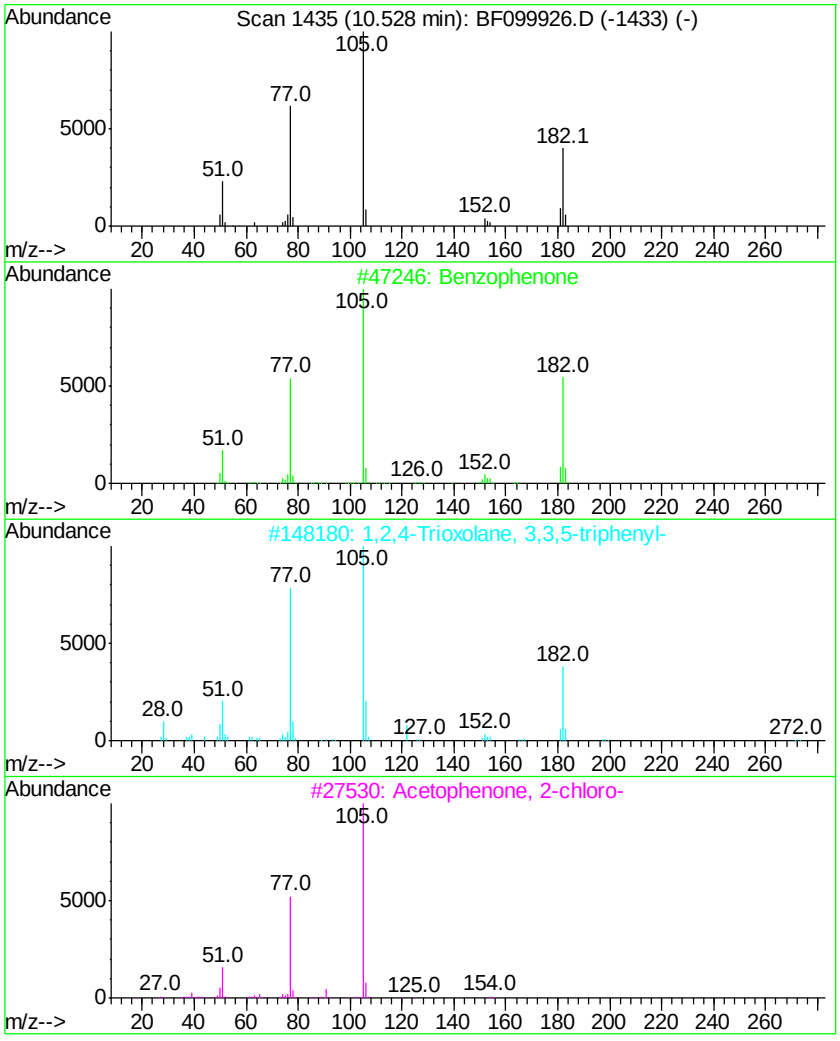
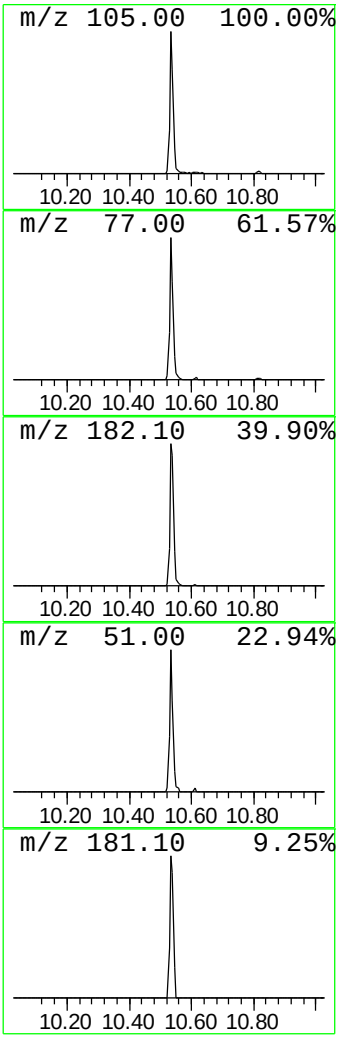
Peak Number 5 Benzophenone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	3.21 ng	126988	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43
5	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	43





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Sample : I6146-01
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Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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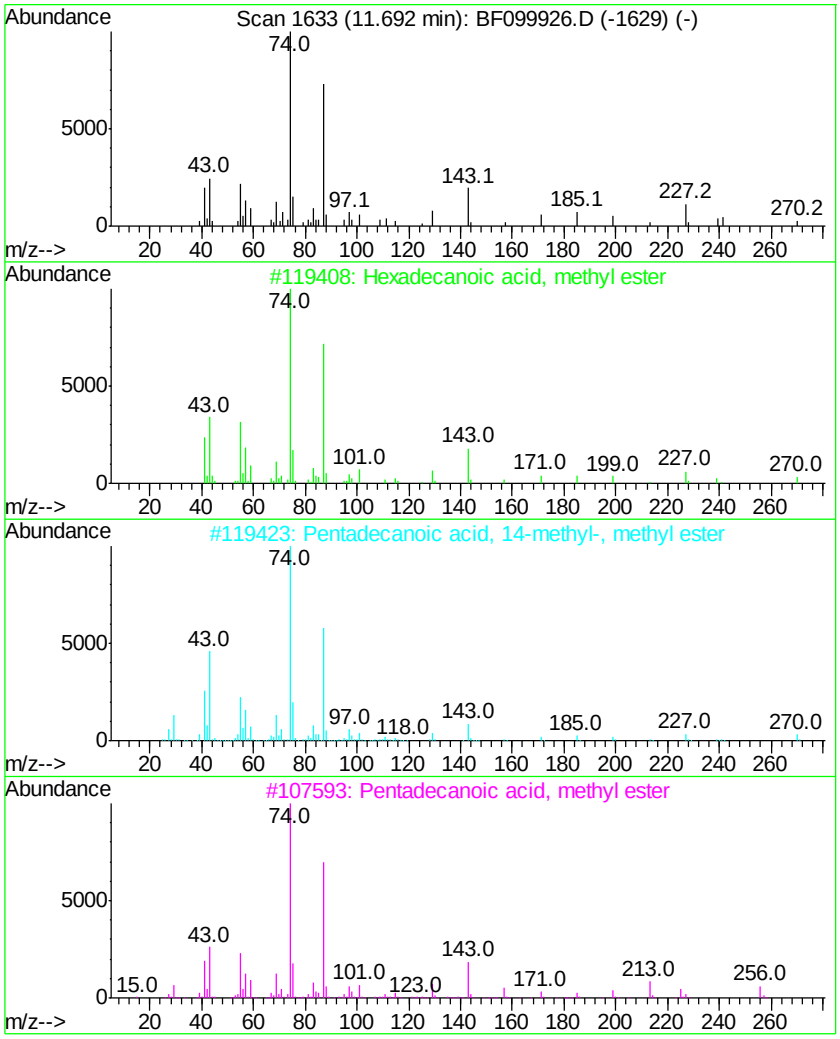
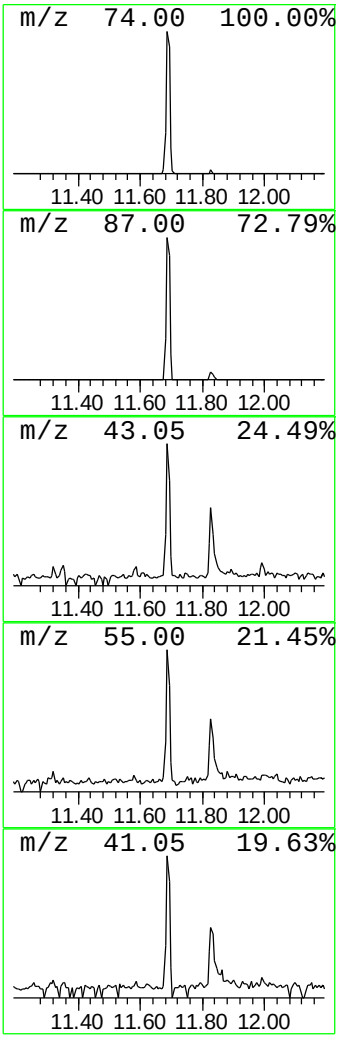
Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.65 ng	86065	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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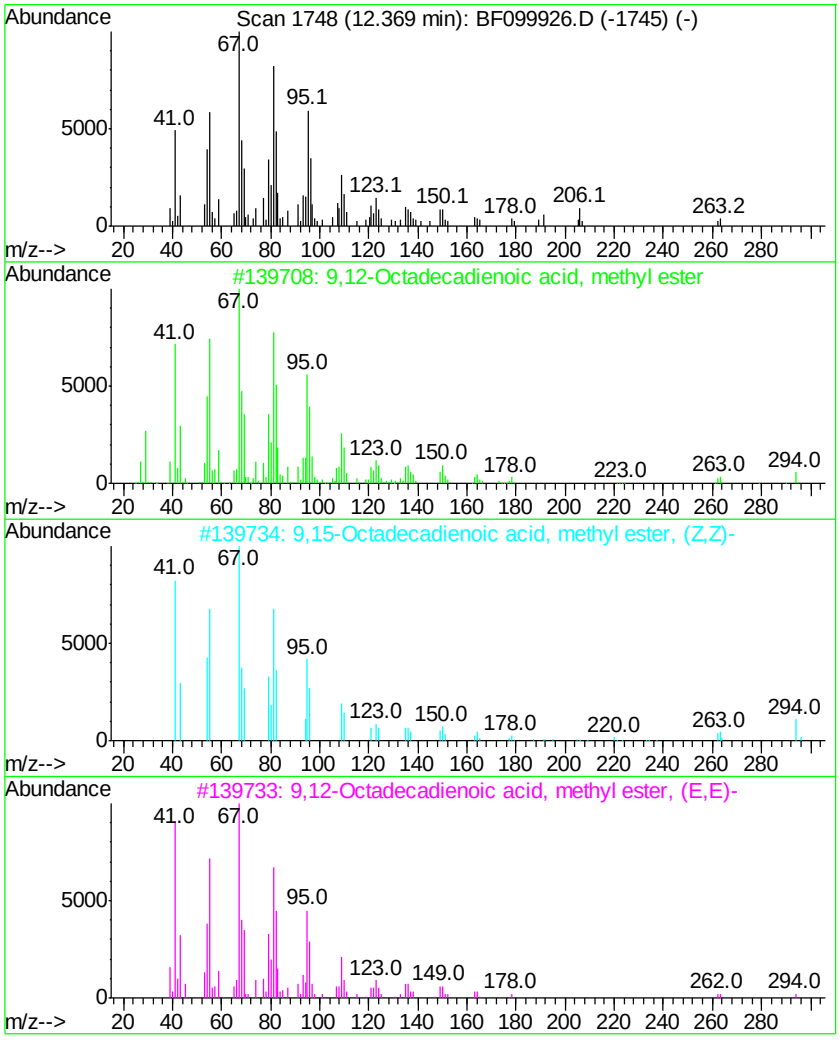
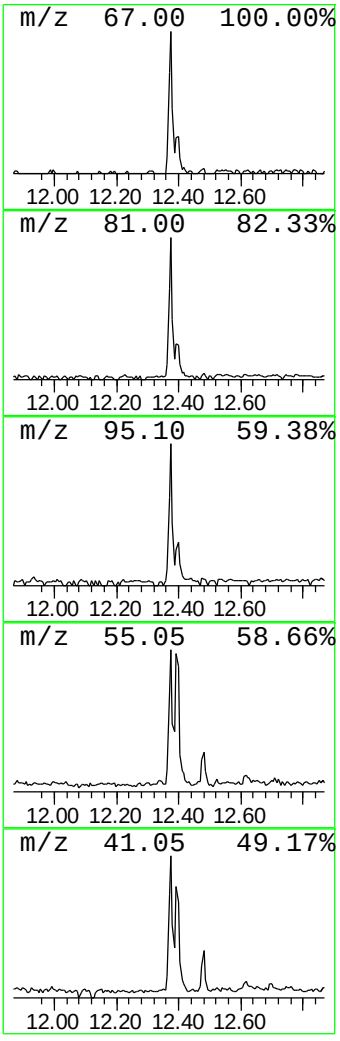
Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	5.38 ng	174516	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	98
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
5	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	93





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

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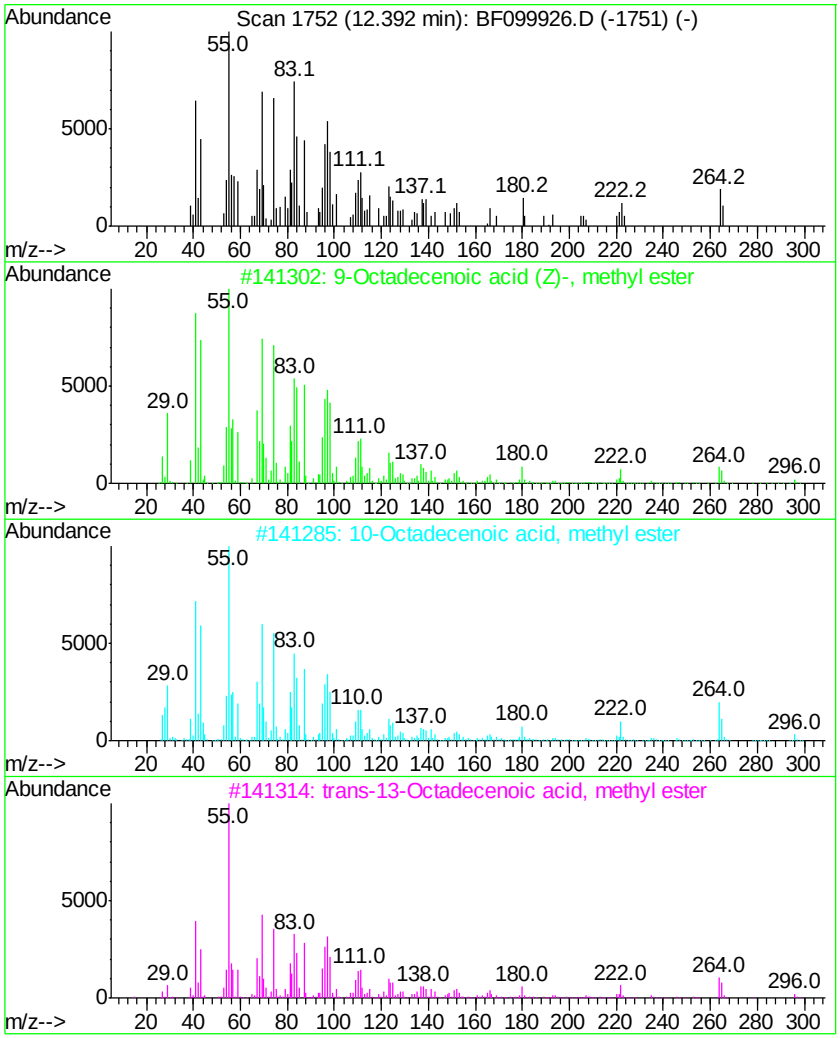
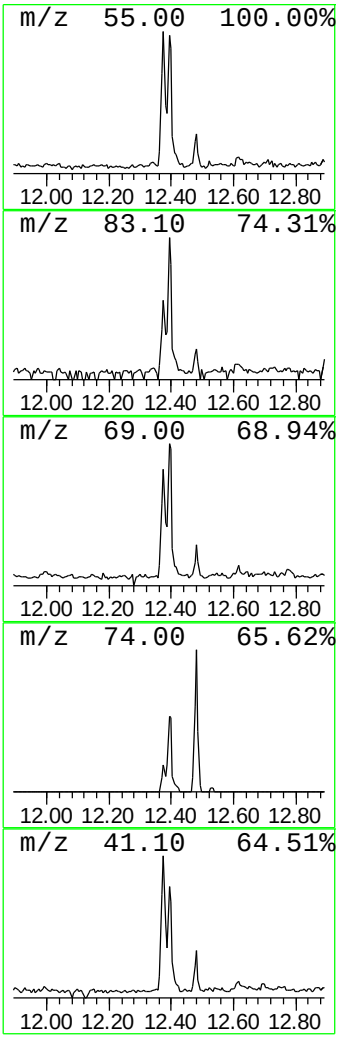
Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	3.83 ng	124285	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	83
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	76
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	74
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	70





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099926.D
Acq On : 28 Oct 2017 19:22
Operator : SJ/JU
Sample : I6146-01
Misc :
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Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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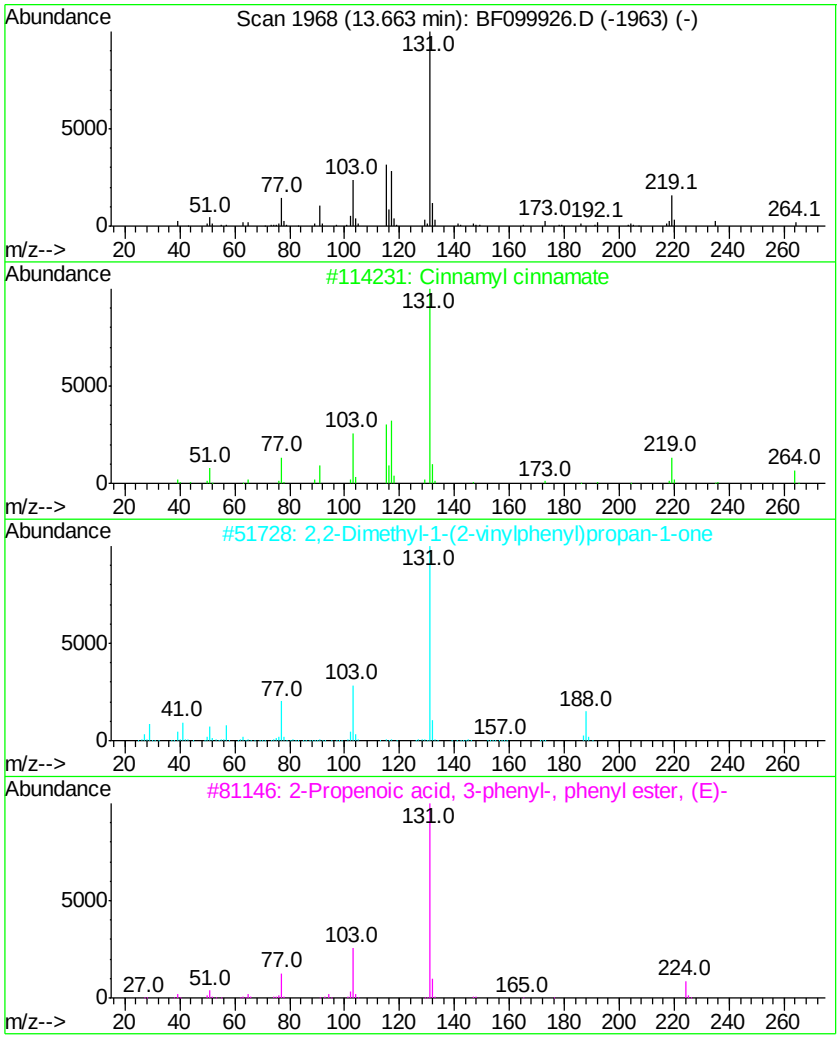
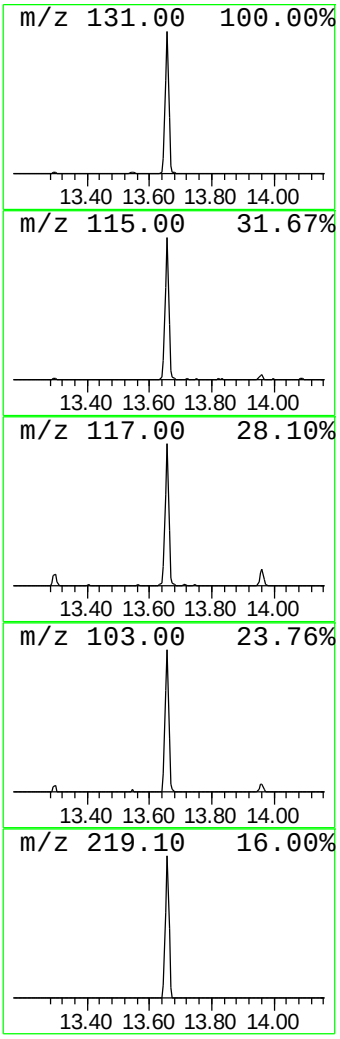
Peak Number 9 Cinnamyl cinnamate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	11.66 ng	299872	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	49
3	2-Propenoic acid, 3-phenyl-, phe...	224	C15H12O2	025695-77-6	47
4	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	47
5	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47





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Data File : BF099926.D
Acq On : 28 Oct 2017 19:22
Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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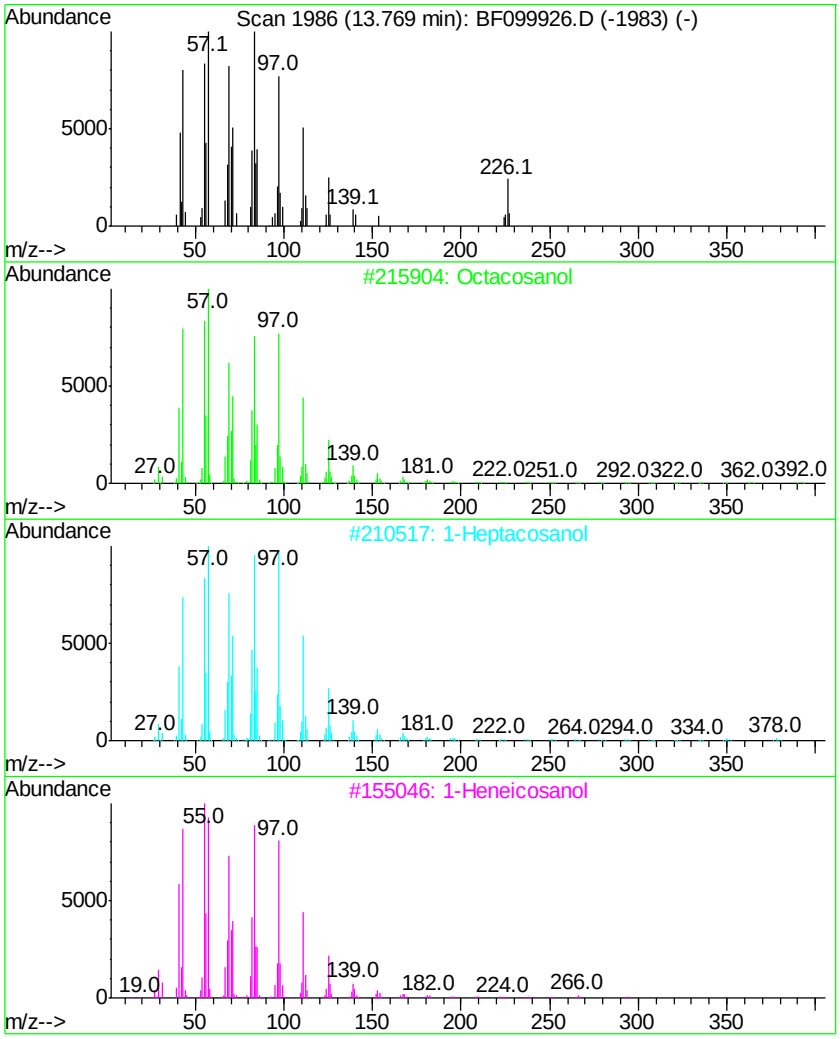
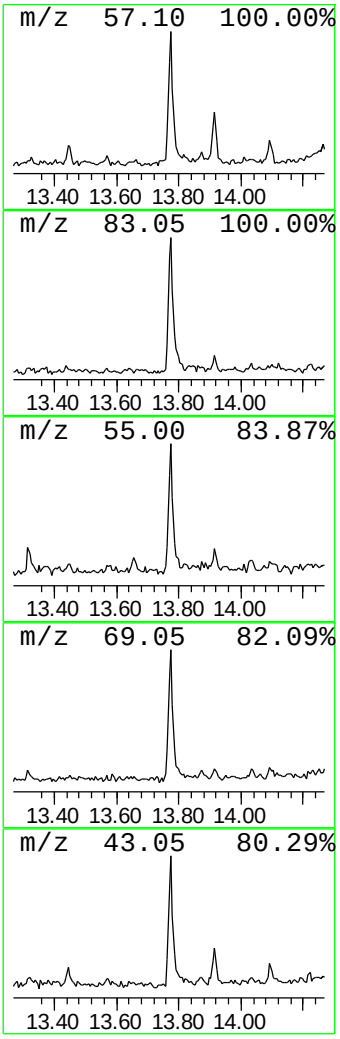
Peak Number 10 Octacosanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	4.29 ng	110443	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	93
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	1-Nonadecene	266	C19H38	018435-45-5	90
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





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Acq On : 28 Oct 2017 19:22
Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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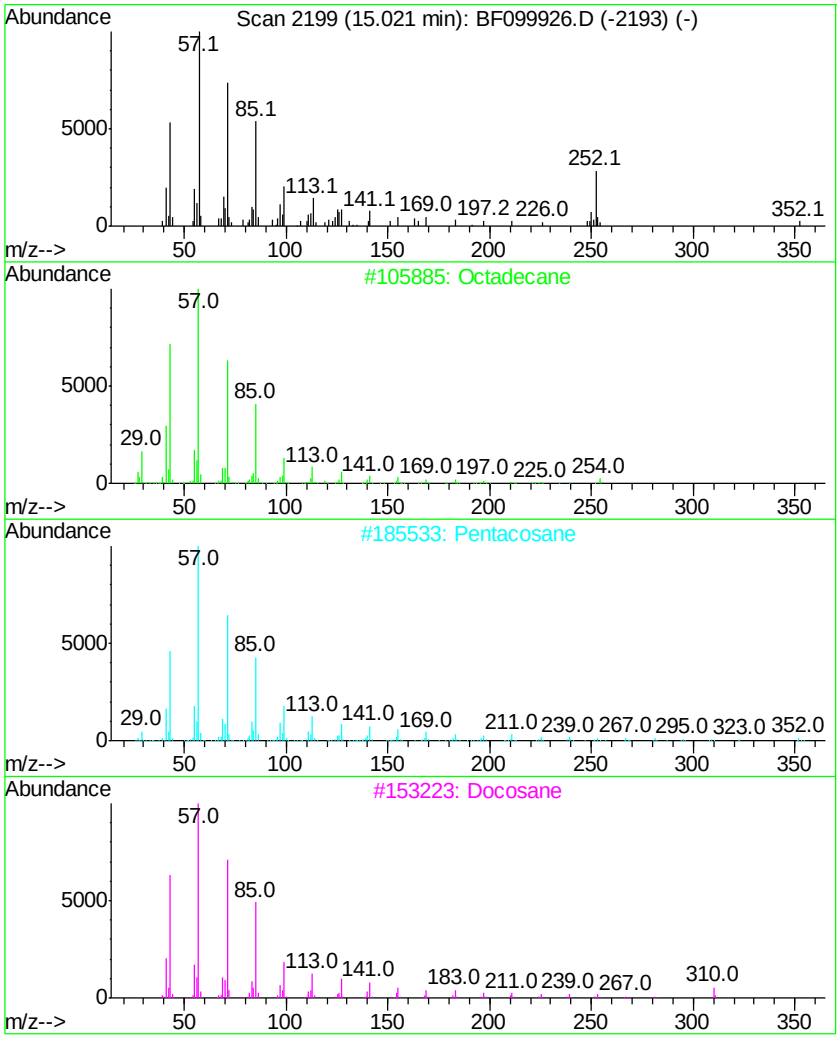
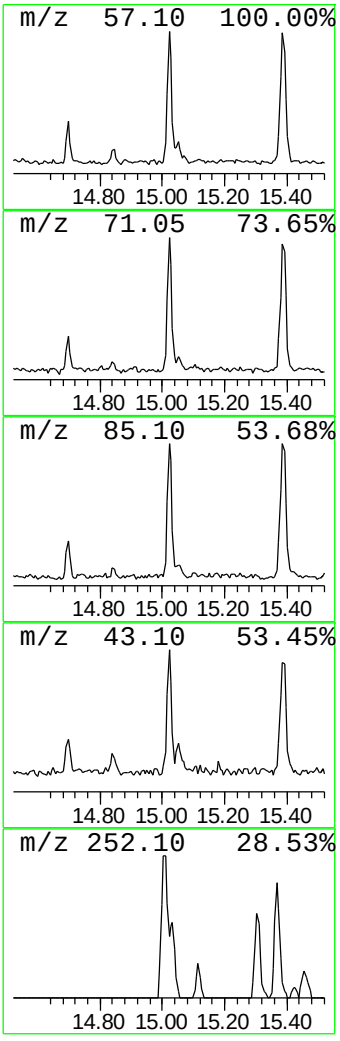
Peak Number 11 Octadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	4.68 ng	125411	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Pentacosane	352	C25H52	000629-99-2	94
3	Docosane	310	C22H46	000629-97-0	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Heneicosane	296	C21H44	000629-94-7	87





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Acq On : 28 Oct 2017 19:22
Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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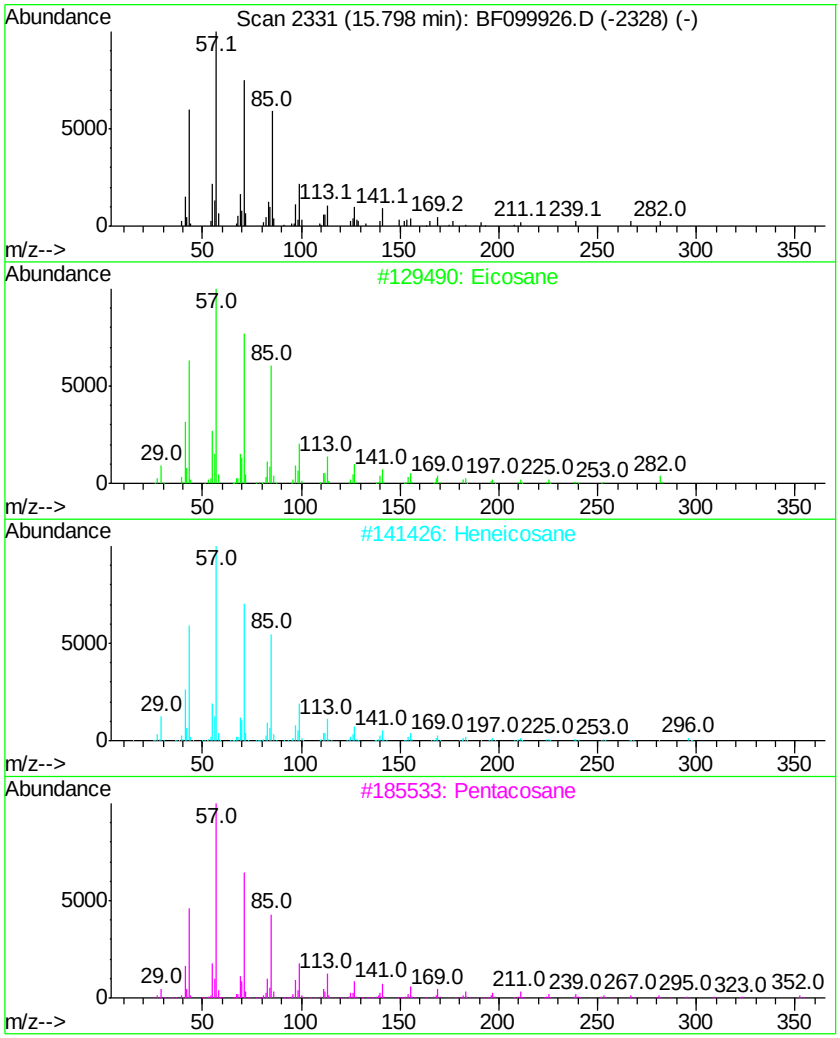
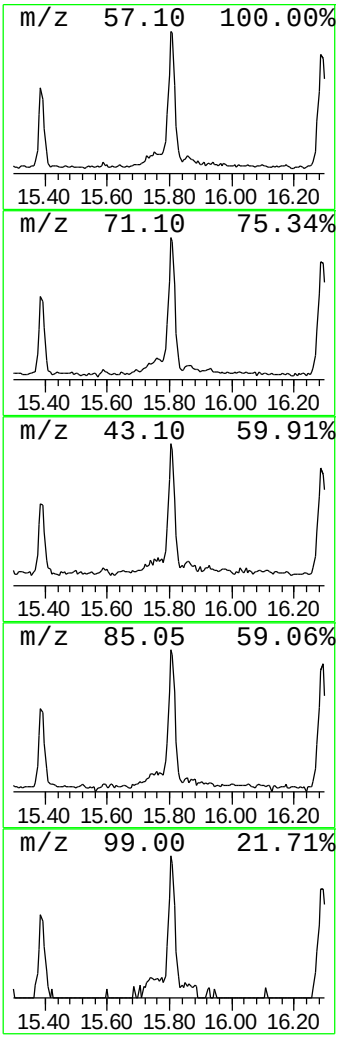
Peak Number 12 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	6.25 ng	167354	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heneicosane	296	C21H44	000629-94-7	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Triacontane	422	C30H62	000638-68-6	91





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Acq On : 28 Oct 2017 19:22
Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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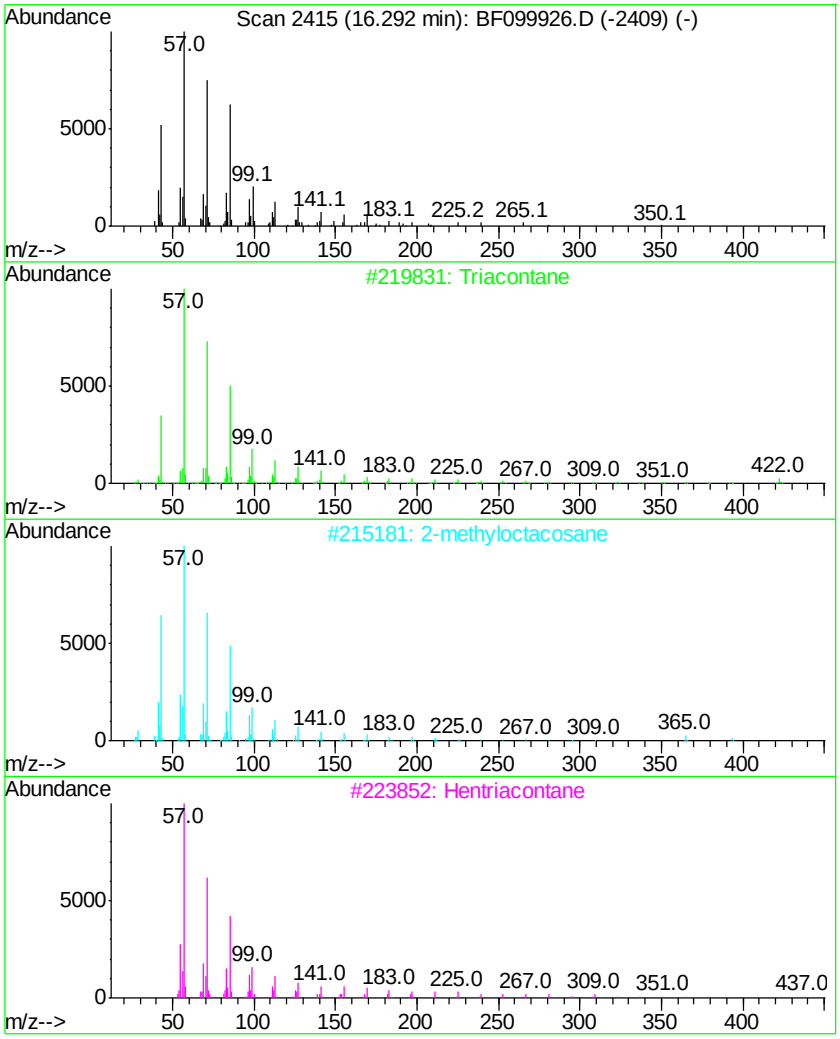
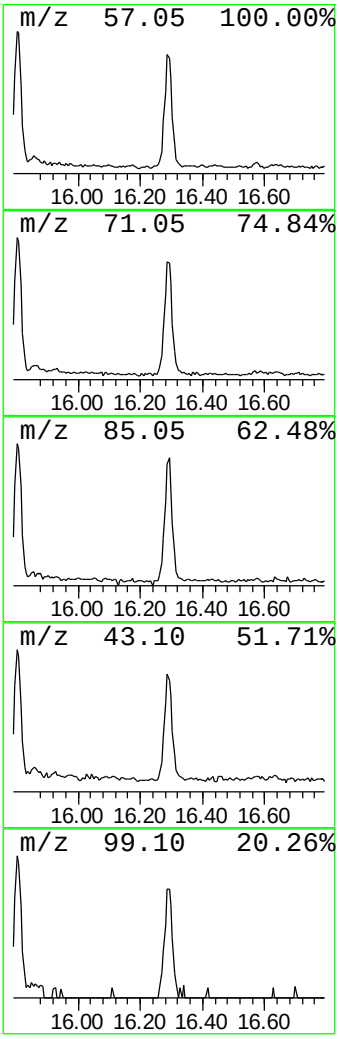
Peak Number 13 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	6.71 ng	179750	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	91





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Data File : BF099926.D
Acq On : 28 Oct 2017 19:22
Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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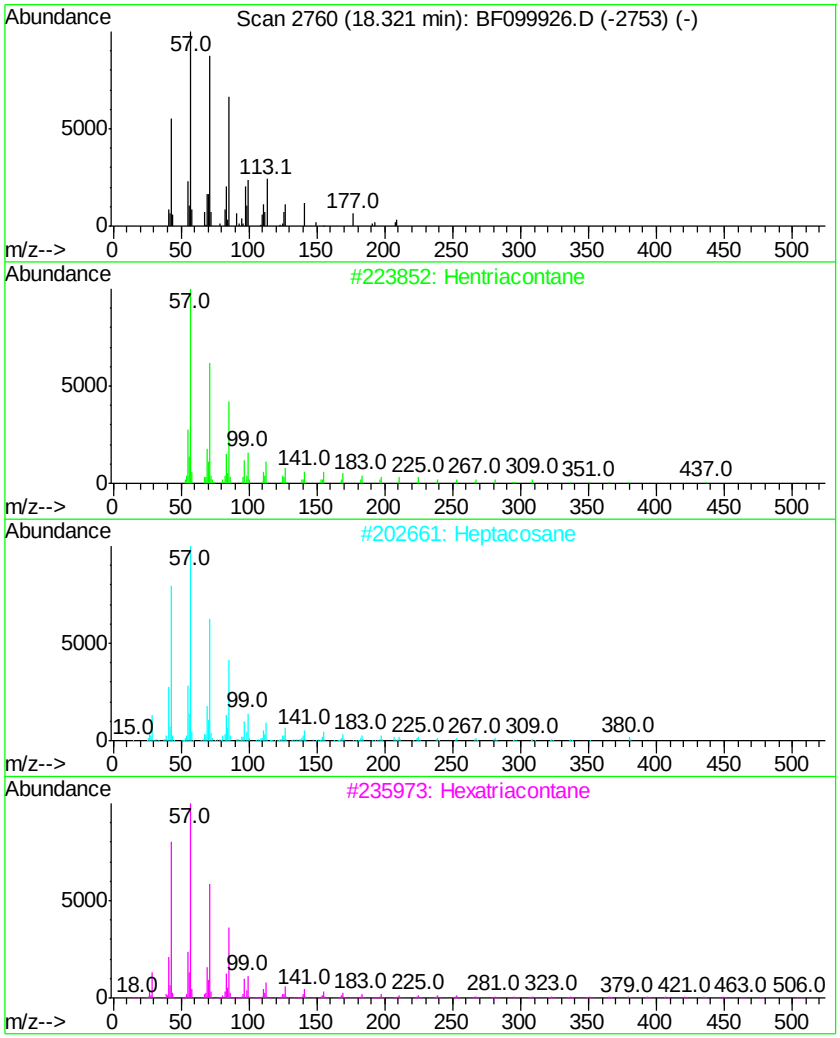
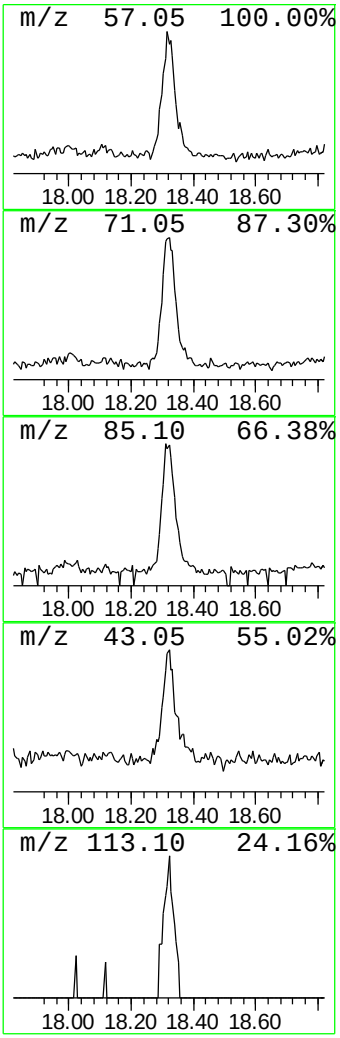
Peak Number 16 Hentriacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	4.77 ng	127662	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	90
2	Heptacosane	380	C27H56	000593-49-7	83
3	Hexatriacontane	507	C36H74	000630-06-8	83
4	Hexacosane	366	C26H54	000630-01-3	78
5	Octacosane	394	C28H58	000630-02-4	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099926.D
Acq On : 28 Oct 2017 19:22
Operator : SJ/JU
Sample : I6146-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AU-06-102517-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	5.00	7.8	ng	213644	1	6.79	549193	20.0
unknown6.56	6.56	53.5	ng	1469030	1	6.79	549193	20.0
Bicyclo[5.2.0]non...	9.47	3.3	ng	132109	3	9.82	790618	20.0
Benzophenone	10.53	3.2	ng	126988	3	9.82	790618	20.0
Hexadecanoic acid...	11.69	2.6	ng	86065	4	11.31	649185	20.0
9,12-Octadecadien...	12.37	5.4	ng	174516	4	11.31	649185	20.0
9-Octadecenoic ac...	12.39	3.8	ng	124285	4	11.31	649185	20.0
Cinnamyl cinnamate	13.66	11.7	ng	299872	5	13.96	514582	20.0
Octacosanol	13.77	4.3	ng	110443	5	13.96	514582	20.0
Octadecane	15.02	4.7	ng	125411	6	15.42	535559	20.0
Eicosane	15.80	6.3	ng	167354	6	15.42	535559	20.0
Triacontane	16.29	6.7	ng	179750	6	15.42	535559	20.0
Hentriacontane	18.32	4.8	ng	127662	6	15.42	535559	20.0