LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096287.D
Acq On : 29 Jun 2017 13:08
Operator : SJ/MA
Sample : I3906-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

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-BF062717.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	4.334	376	382	386	rBV	70543	84011	2.58%	0.266%
2	4.963	485	489	495	rVB	654957	777853	23.89%	2.466%
3	5.387	556	561	564	rVB	3148056	3256087	100.00%	10.322%
4	6.357	721	726	728	rBV	29876	37738	1.16%	0.120%
5	6.398	728	733	736	rBV	3202178	3247044	99.72%	10.294%
6	6.540	752	757	760	rBV	3374551	3136932	96.34%	9.944%
7	6.769	792	796	800	rBV	1224698	1016157	31.21%	3.221%
8	6.928	819	823	826	rVB	2701054	2316920	71.16%	7.345%
9	7.328	885	891	894	rBV	2221059	1971887	60.56%	6.251%
10	7.422	902	907	911	rVB	70364	75140	2.31%	0.238%
11	7.757	958	964	966	rBV	81809	98998	3.04%	0.314%
12	8.051	1010	1014	1017	rBV	1637882	1343108	41.25%	4.258%
13	9.128	1192	1197	1200	rBV	3286166	2949948	90.60%	9.352%
14	9.222	1207	1213	1216	rBV4	48269	53377	1.64%	0.169%
15	9.522	1259	1264	1267	rBV	1251249	1048141	32.19%	3.323%
16	9.751	1300	1303	1307	rVB	59635	51655	1.59%	0.164%
17	9.804	1307	1312	1316	rBV2	1409167	1232523	37.85%	3.907%
18	10.245	1385	1387	1390	rVB	97849	82731	2.54%	0.262%
19	10.469	1421	1425	1428	rBV	47542	51299	1.58%	0.163%
20	10.586	1441	1445	1448	rBV	1653510	1445105	44.38%	4.581%
21	10.722	1464	1468	1469	rBV	135732	121560	3.73%	0.385%
22	11.169	1541	1544	1546	rBV	112365	95761	2.94%	0.304%
23	11.198	1546	1549	1554	rVB	62029	65122	2.00%	0.206%
24	11.280	1560	1563	1566	rBV	1041070	950298	29.19%	3.013%
25	11.357	1571	1576	1579	rVB6	25204	39688	1.22%	0.126%
26	11.516	1600	1603	1606	rBV4	42894	42009	1.29%	0.133%
27	11.592	1613	1616	1619	rBV	95965	81216	2.49%	0.257%
28	11.692	1630	1633	1637	rVB2	86157	83613	2.57%	0.265%
29	11.816	1651	1654	1658	rBV2	277385	259294	7.96%	0.822%
30	11.892	1664	1667	1670	rBV3	29853	35844	1.10%	0.114%
31	11.998	1682	1685	1693	rVB	95434	94520	2.90%	0.300%
32	12.216	1719	1722	1726	rBV6	21630	35920	1.10%	0.114%
33	12.333	1740	1742	1745	rBV3	35093	33720	1.04%	0.107%
34	12.374	1745	1749	1750	rBV	240637	212236	6.52%	0.673%

LSC Area Percent Report

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Acq On : 29 Jun 2017 13:08
Operator : SJ/MA
Sample : I3906-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

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-BF062717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.392	1750	1752	1756	rVB	243931	220024	6.76%	0.698%
36	12.486	1765	1768	1772	rBV3	52278	74671	2.29%	0.237%
37	12.604	1785	1788	1791	rBV2	135636	151264	4.65%	0.480%
38	12.757	1812	1814	1817	rVB	72632	60268	1.85%	0.191%
39	12.868	1829	1833	1836	rBV	2227072	1959209	60.17%	6.211%
40	13.116	1872	1875	1878	rVB	115771	100997	3.10%	0.320%
41	13.457	1930	1933	1937	rBV	136082	143188	4.40%	0.454%
42	13.768	1983	1986	1995	rBV2	291801	434193	13.33%	1.376%
43	13.915	2007	2011	2014	rBV	924462	824594	25.32%	2.614%
44	14.098	2040	2042	2046	rVB	137913	135083	4.15%	0.428%
45	14.404	2092	2094	2097	rBV	209627	188883	5.80%	0.599%
46	14.704	2143	2145	2148	rBV	160231	186973	5.74%	0.593%
47	15.345	2250	2254	2258	rVB	509701	637594	19.58%	2.021%

Sum of corrected areas: 31544396

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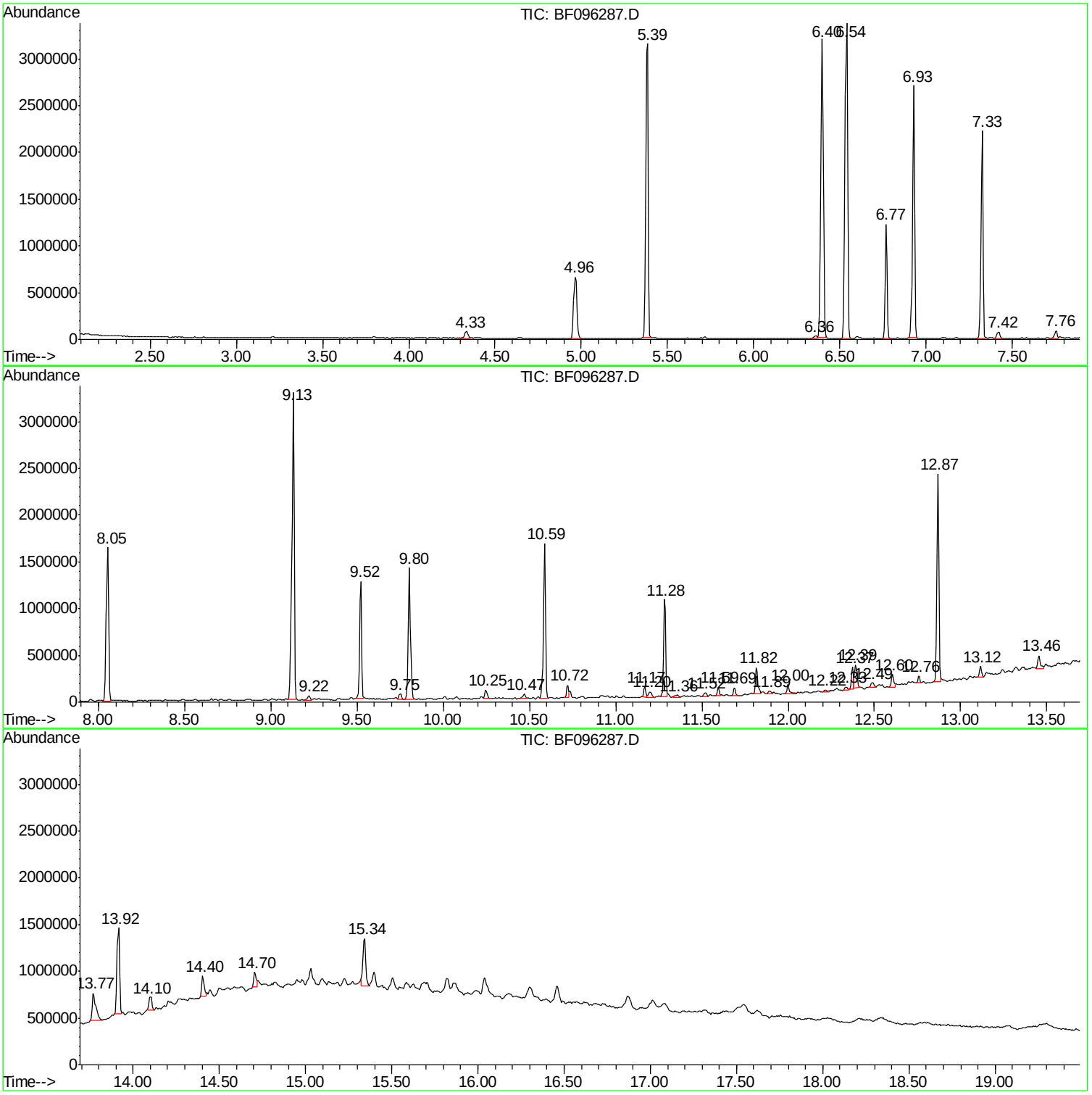
Instrument :
BNA_F
ClientSampleId :
EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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 : BF096287.D
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Operator : SJ/MA
Sample : I3906-04
Misc :
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Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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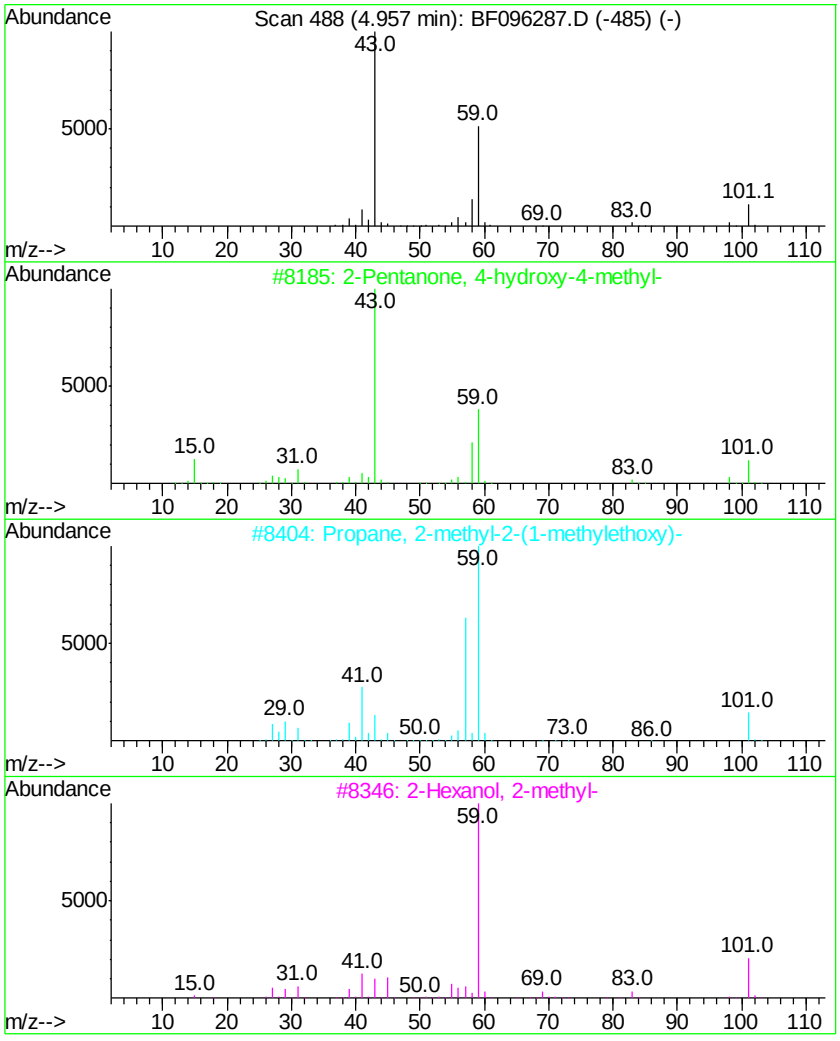
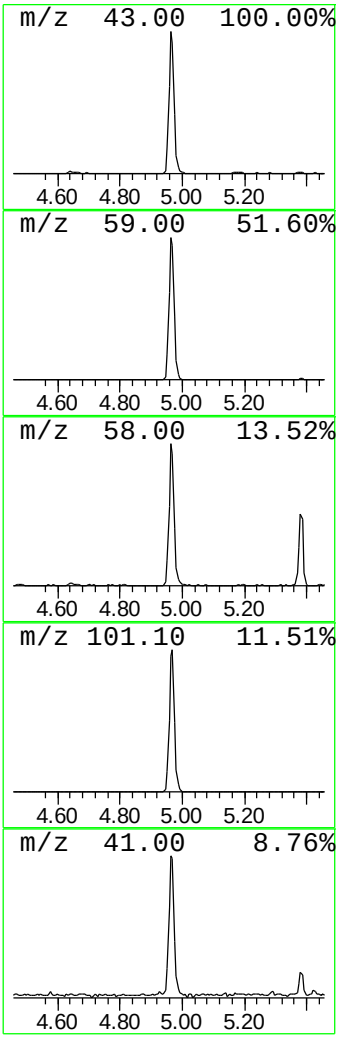
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	15.31 ng	777853	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

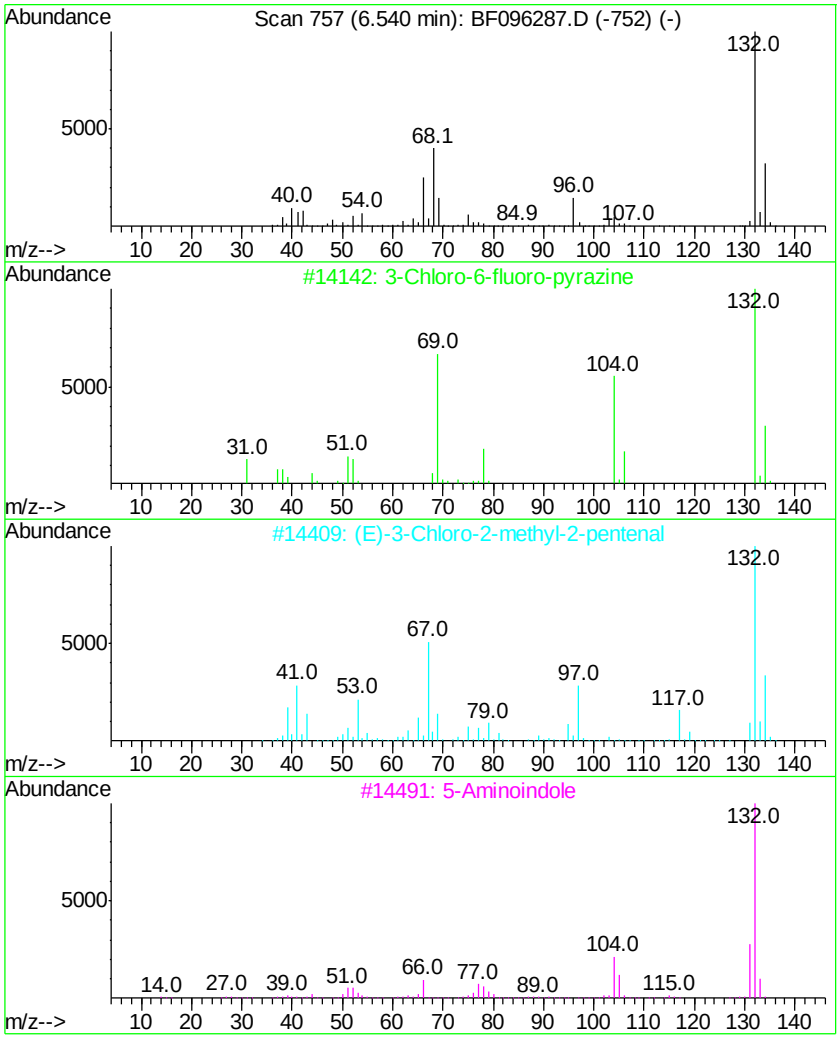
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

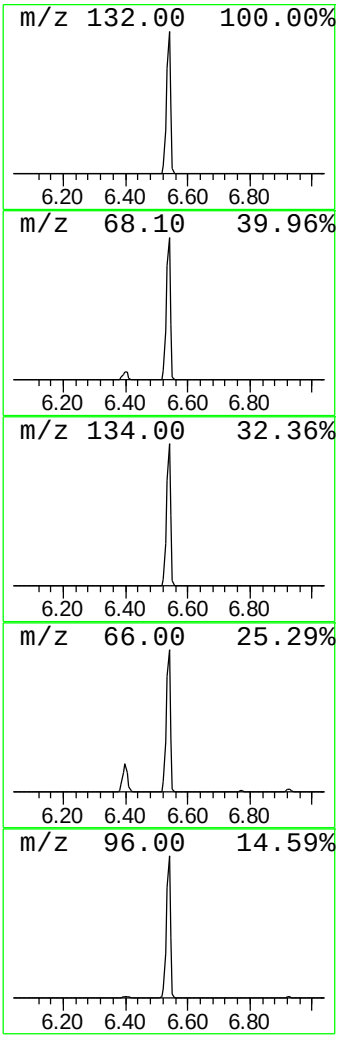
****

Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	61.74 ng	3136930	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Acq On : 29 Jun 2017 13:08
Operator : SJ/MA
Sample : I3906-04
Misc :
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Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

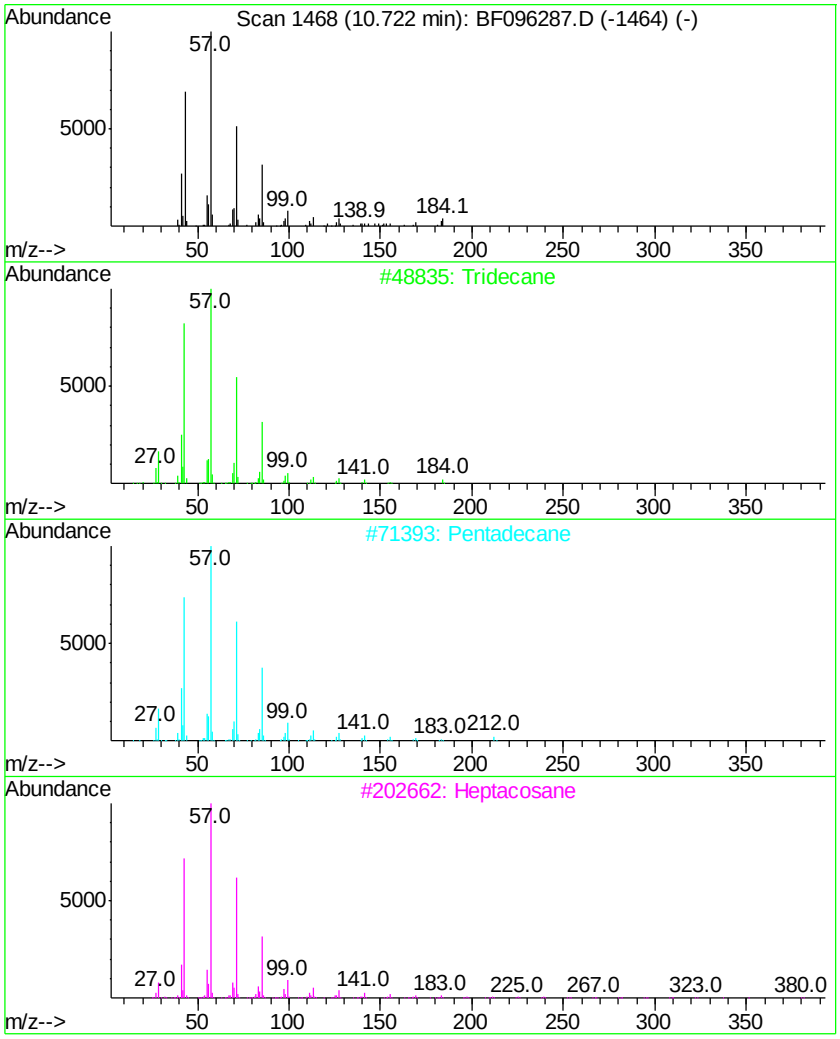
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

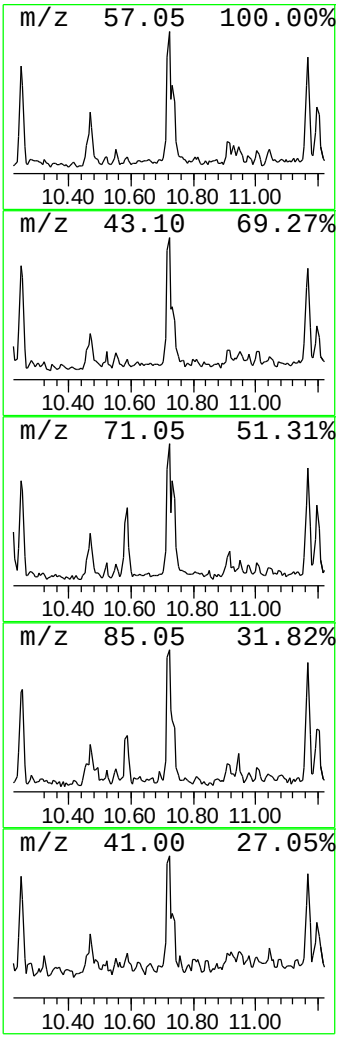
****

Peak Number 4 Tridecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.56 ng	121560	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Heptacosane	380	C27H56	000593-49-7	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Octacosane	394	C28H58	000630-02-4	80





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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TIC Library : C:\DATABASE\NIST11.L
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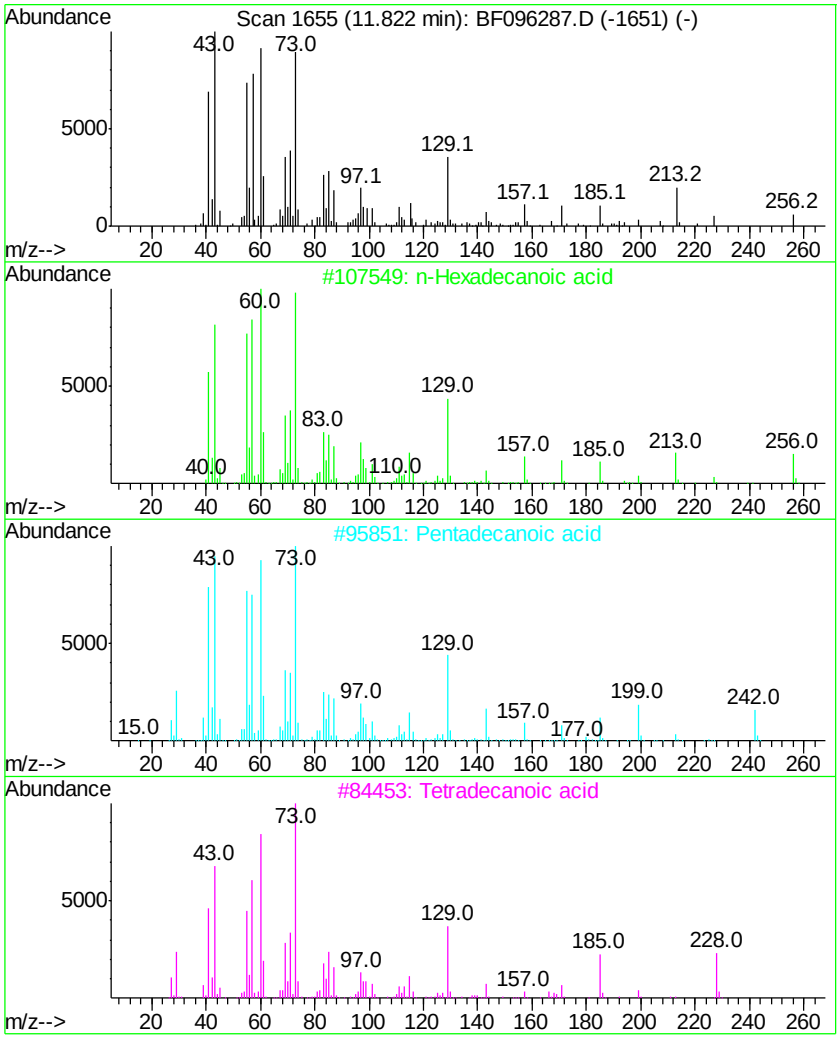
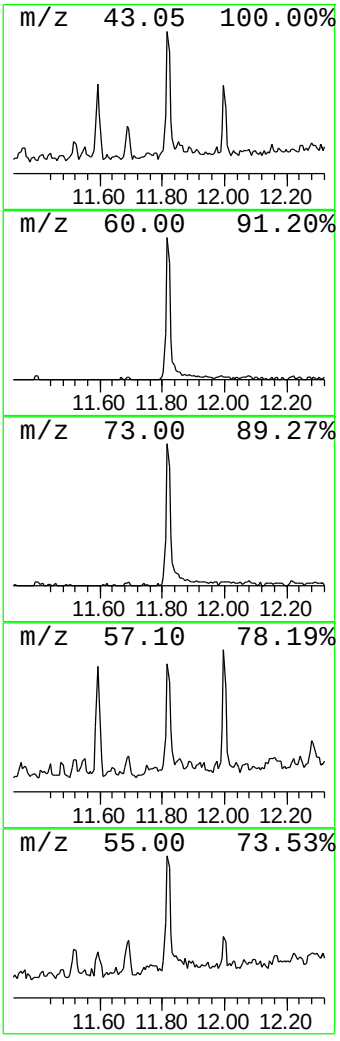
Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	5.46 ng	259294	Phenanthrene-d10	11.28

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	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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Sample : I3906-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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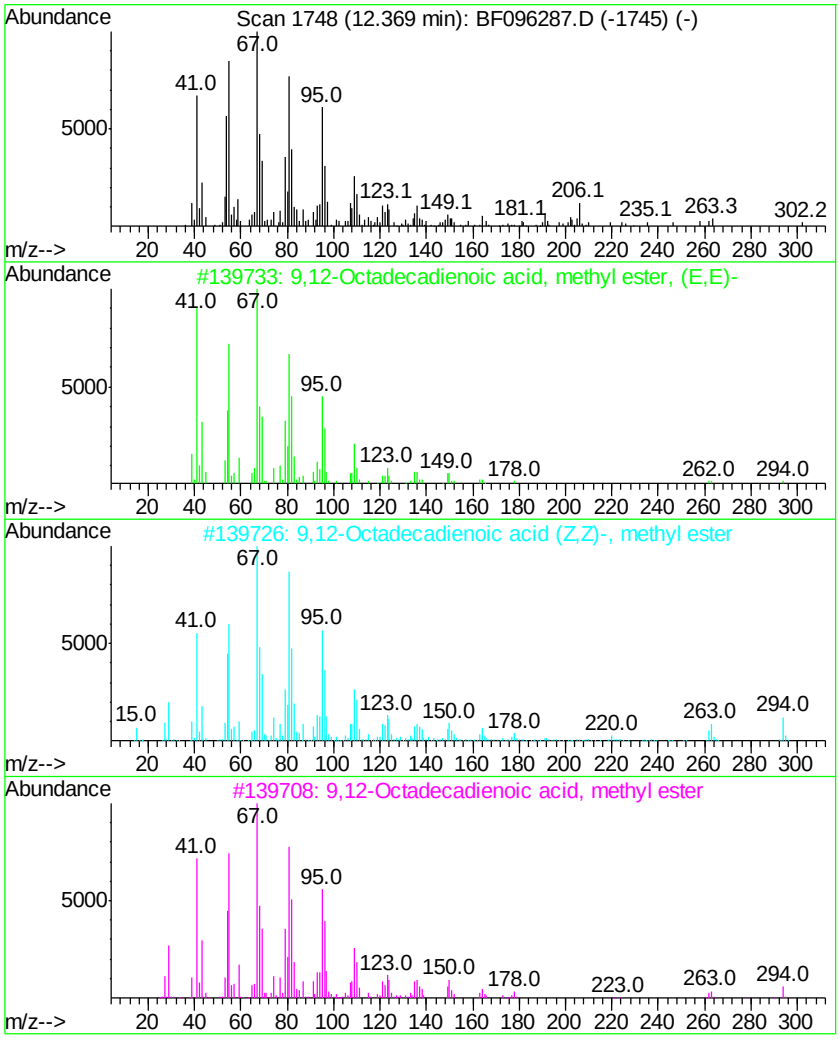
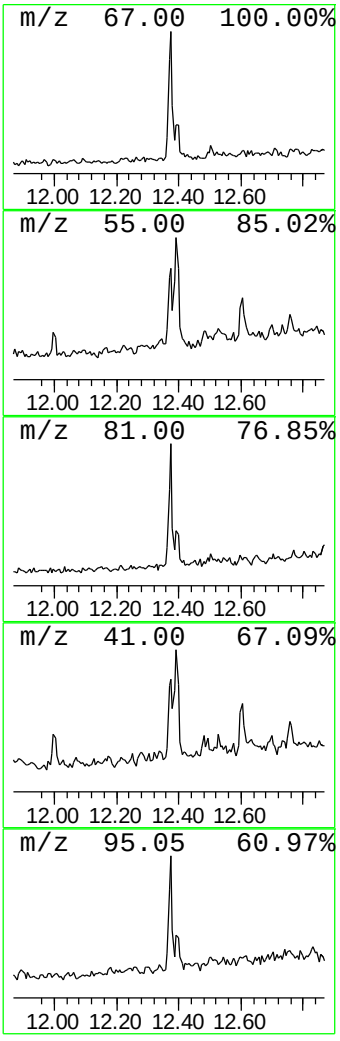
Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	4.47 ng	212236	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	95
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	94
4	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	87
5	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	87





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Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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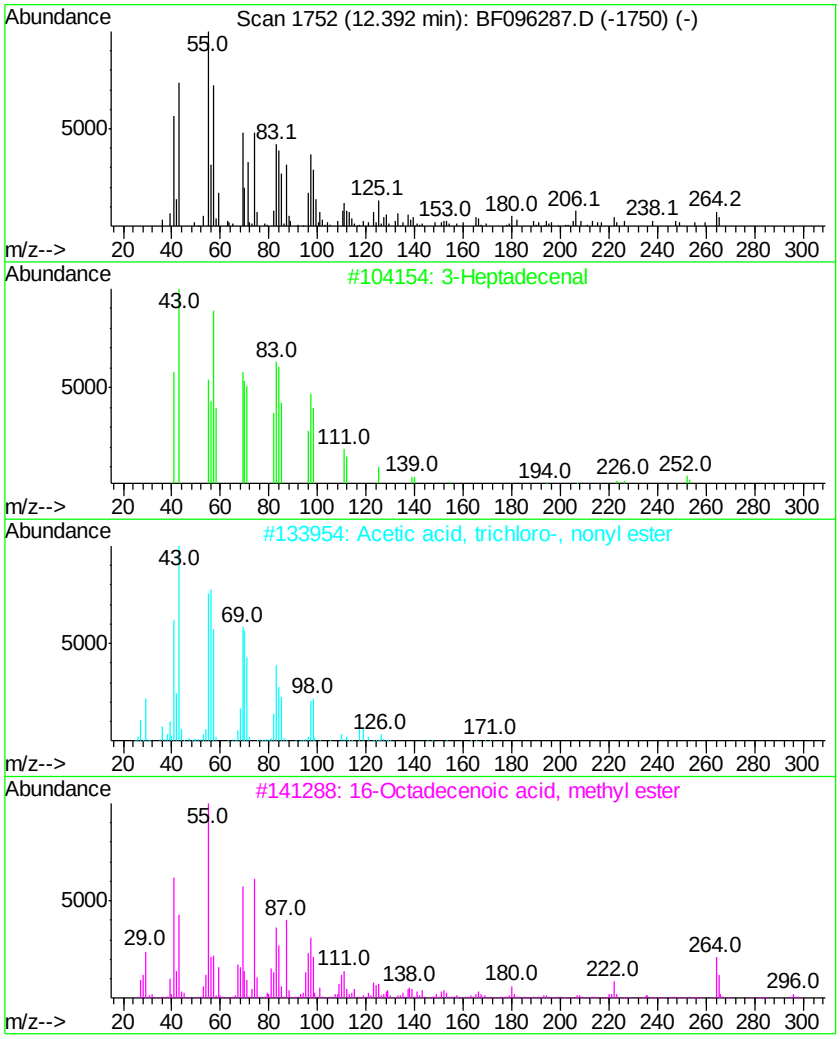
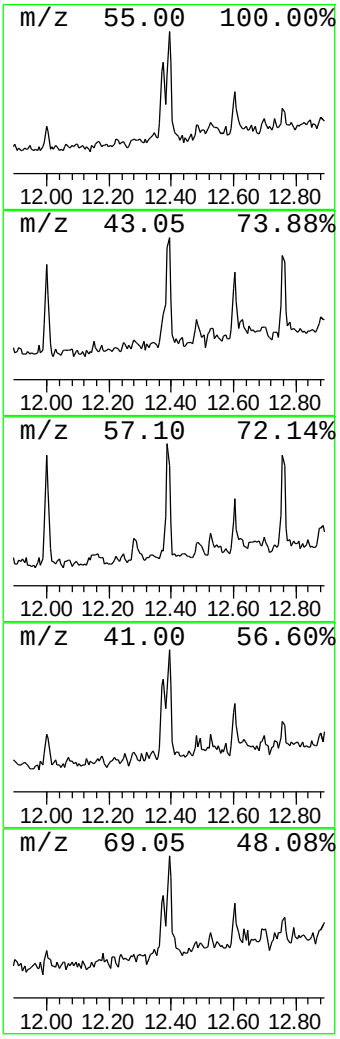
Peak Number 8 3-Heptadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	4.63 ng	220024	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptadecenal	252	C17H32O	1000143-48-7	52
2	Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	47
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	47
4	Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	35
5	17-Pentatriacontene	491	C35H70	006971-40-0	35





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TIC Library : C:\DATABASE\NIST11.L
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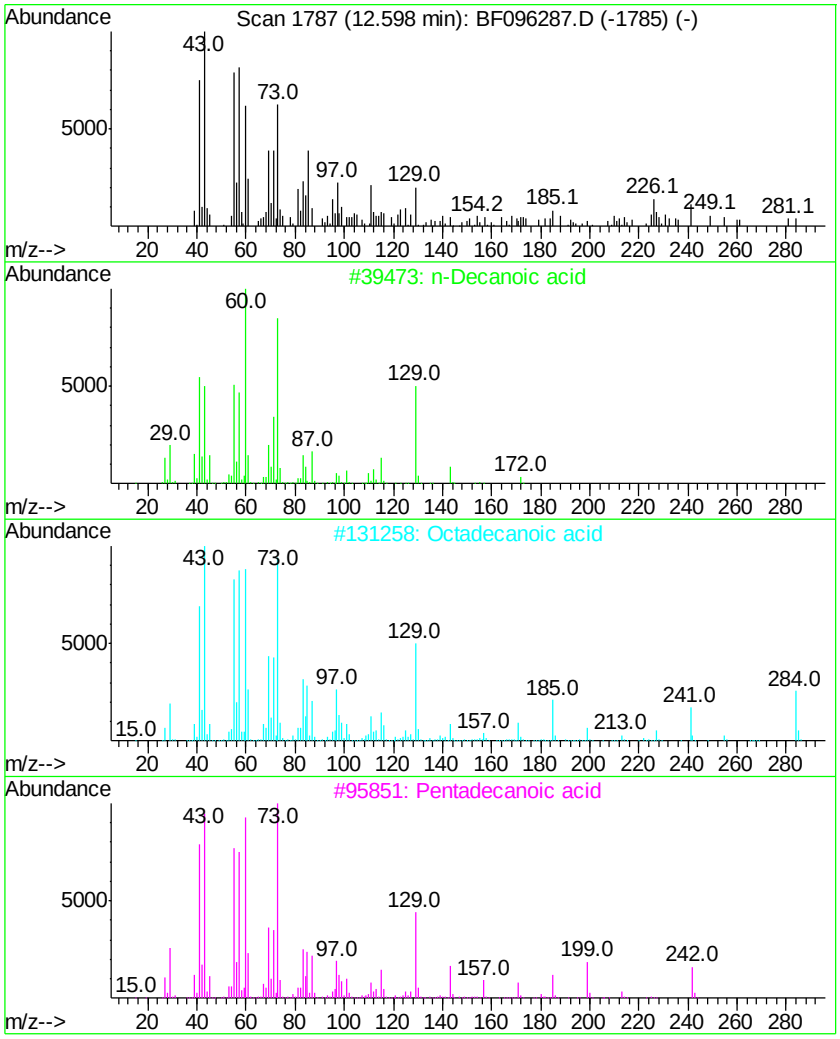
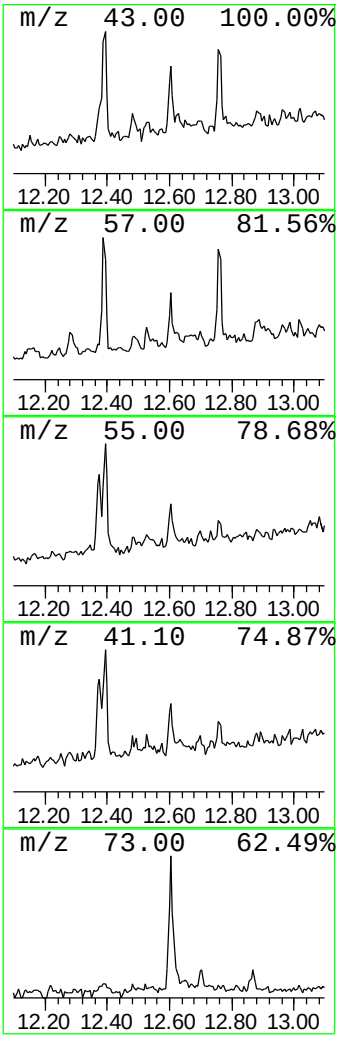
****

Peak Number 9 n-Decanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	3.67 ng	151264	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	86
2	Octadecanoic acid	284	C18H36O2	000057-11-4	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	52
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	42





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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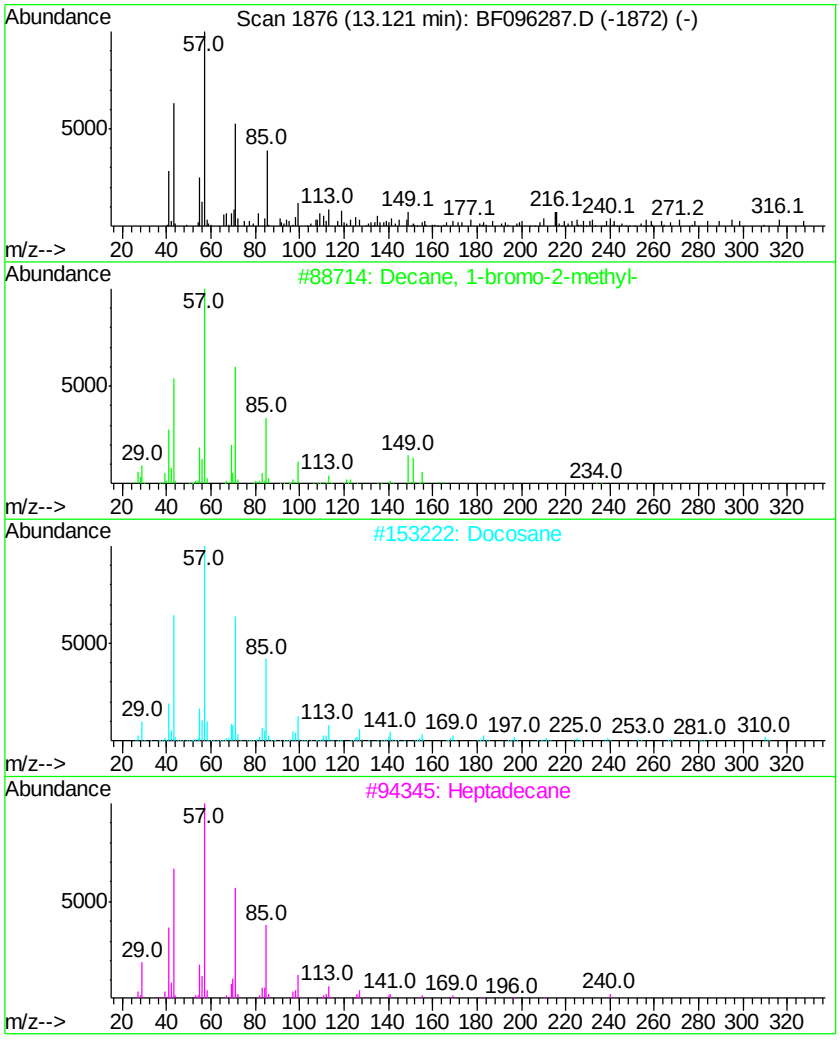
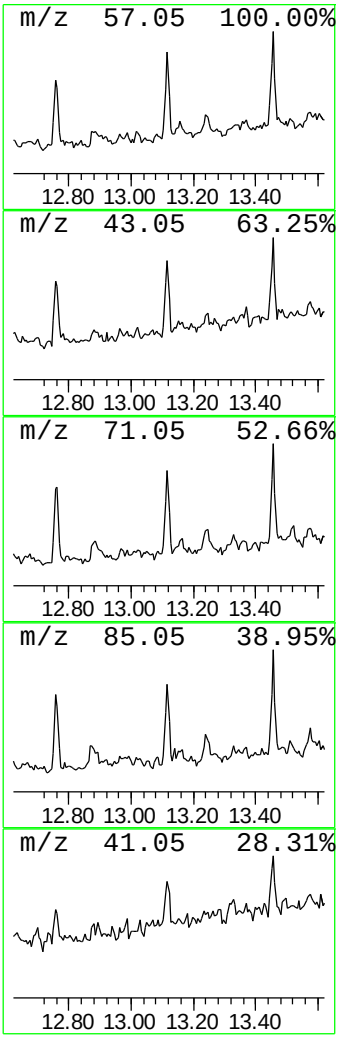
Peak Number 10 Decane, 1-bromo-2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	2.45 ng	100997	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	81
2	Docosane	310	C22H46	000629-97-0	74
3	Heptadecane	240	C17H36	000629-78-7	72
4	Octacosane	394	C28H58	000630-02-4	72
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	72





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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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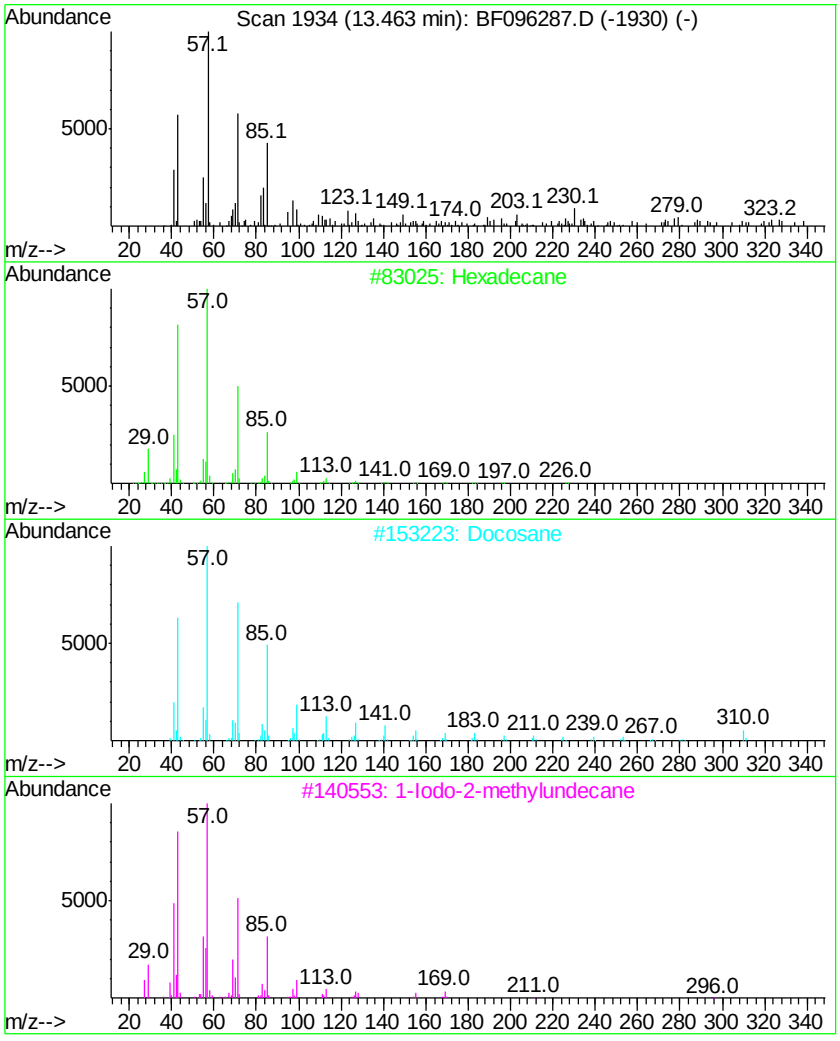
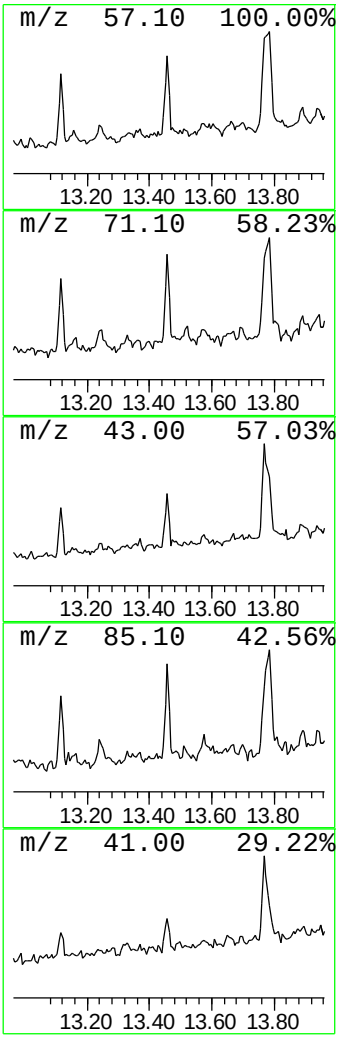
Peak Number 11 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	3.47 ng	143188	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Docosane	310	C22H46	000629-97-0	87
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	80
5	Tricosane	324	C23H48	000638-67-5	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096287.D
Acq On : 29 Jun 2017 13:08
Operator : SJ/MA
Sample : I3906-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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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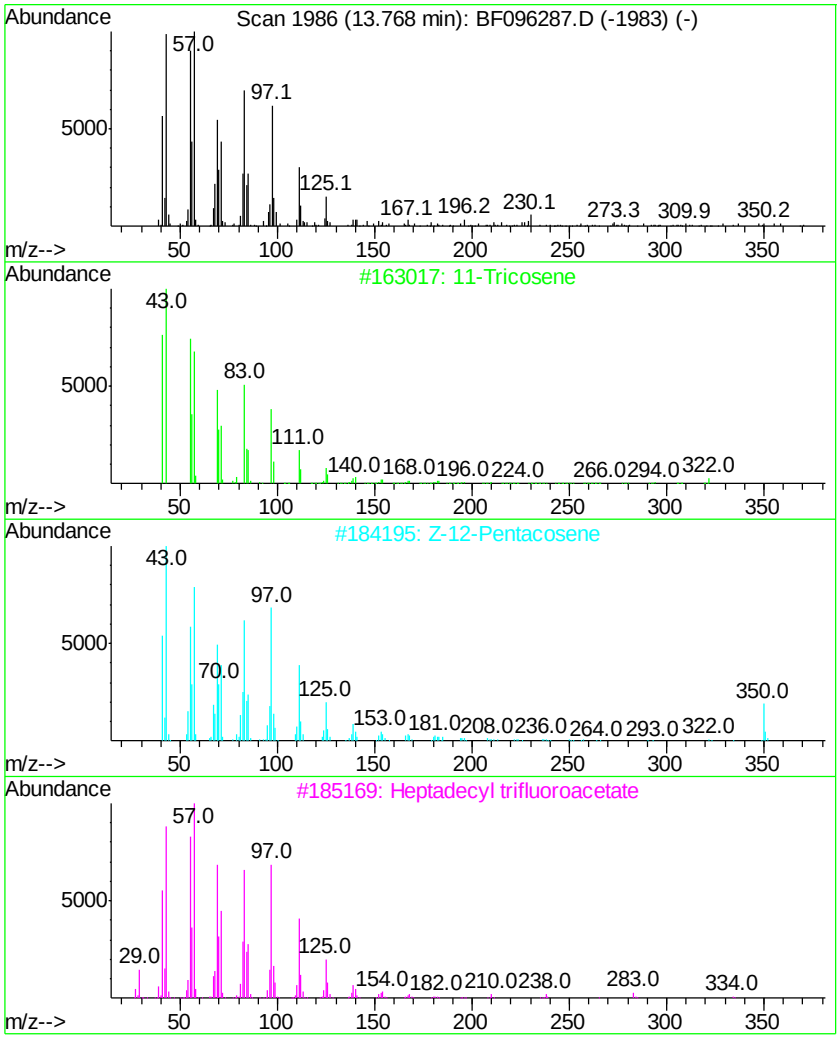
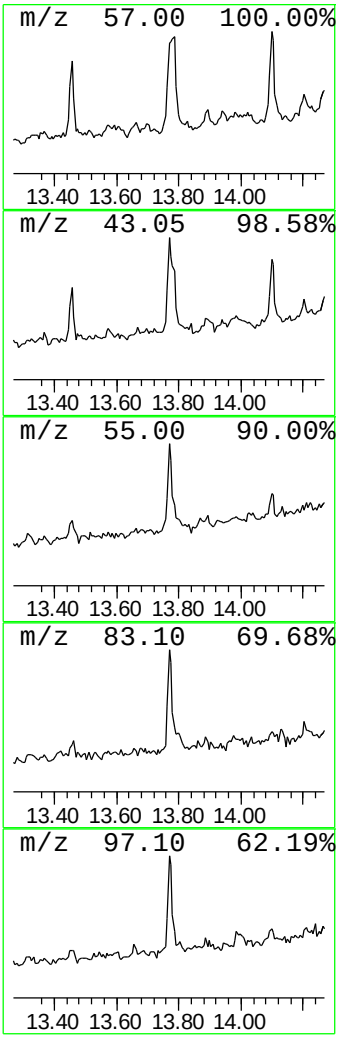
Peak Number 12 11-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	10.53 ng	434193	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	95
2	Z-12-Pentacosene	350	C25H50	1000131-09-4	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	Cycloeicosane	280	C20H40	000296-56-0	91
5	10-Heneicosene (c,t)	294	C21H42	095008-11-0	91





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Acq On : 29 Jun 2017 13:08
Operator : SJ/MA
Sample : I3906-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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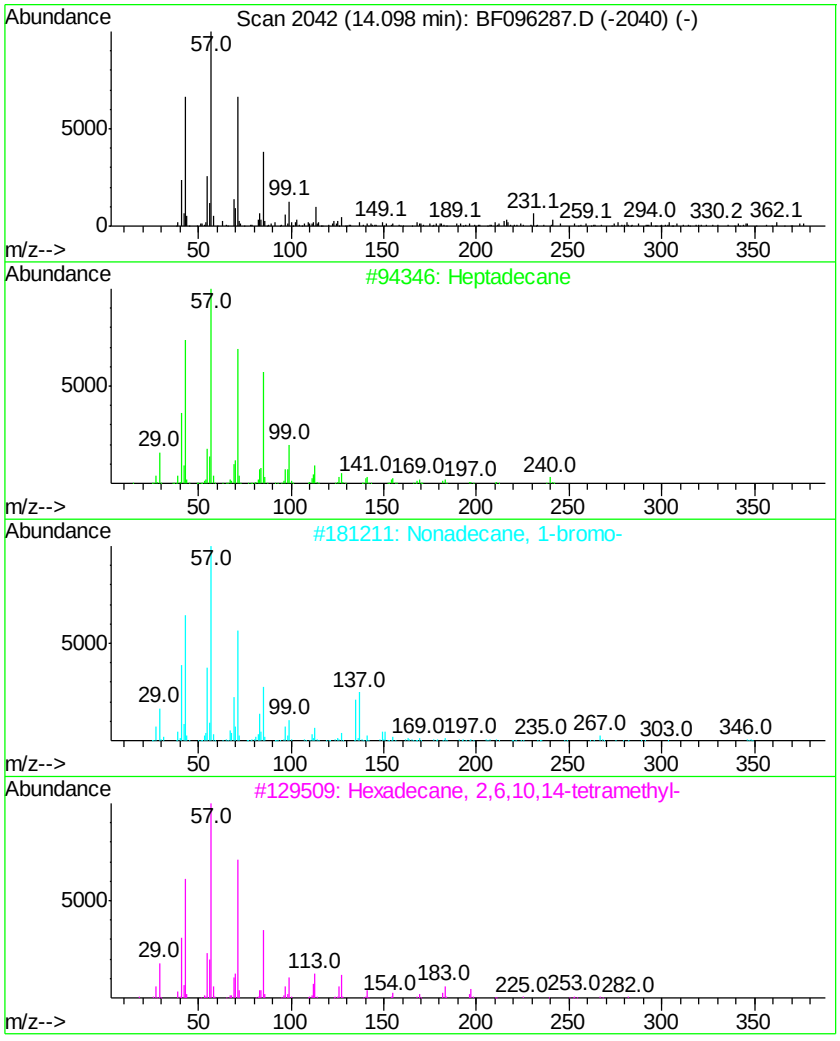
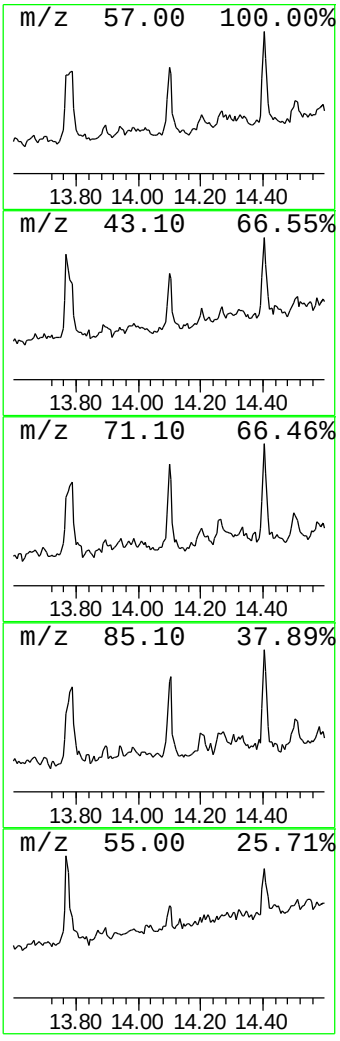
Peak Number 13 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	3.28 ng	135083	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Nonadecane, 1-bromo-	346	C19H39Br	004434-66-6	86
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	83
5	Heneicosane	296	C21H44	000629-94-7	80





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Data File : BF096287.D
Acq On : 29 Jun 2017 13:08
Operator : SJ/MA
Sample : I3906-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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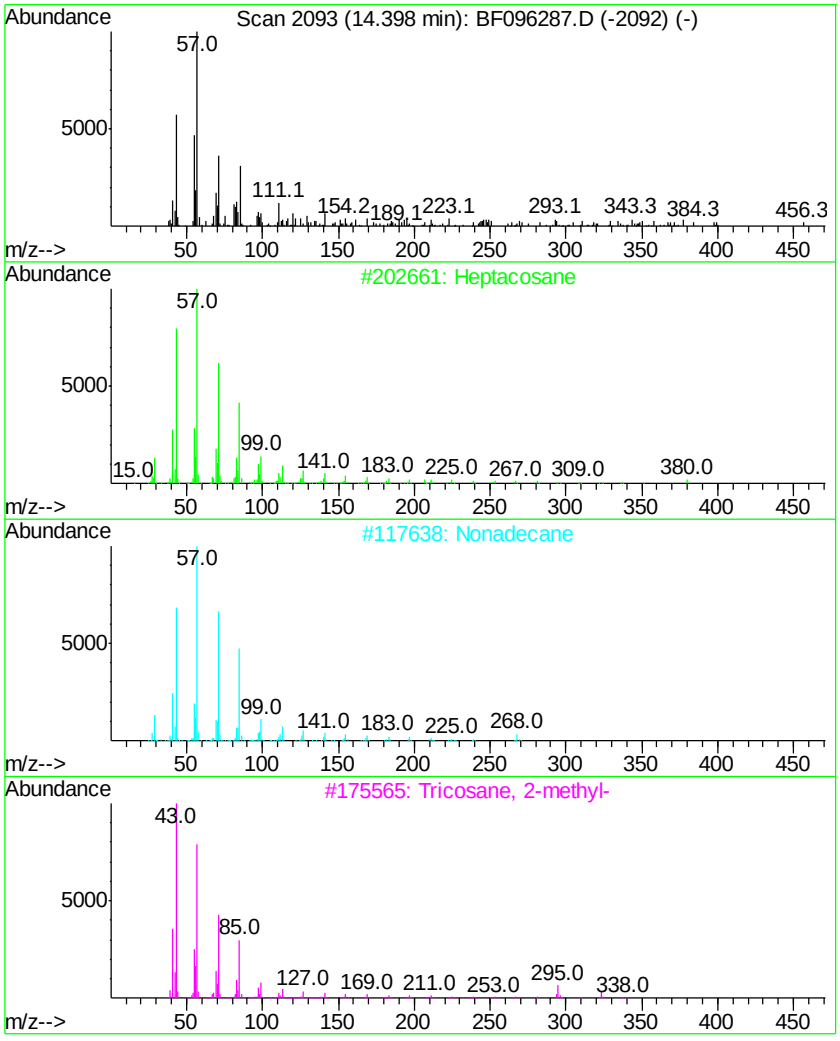
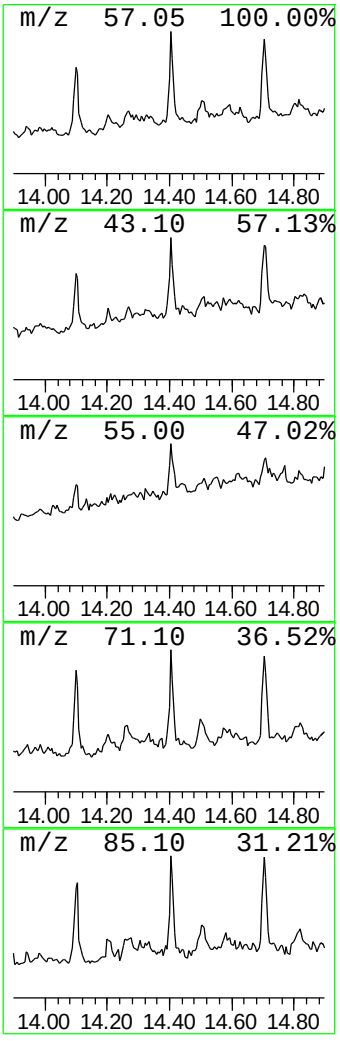
Peak Number 14 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	4.58 ng	188883	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	97
2	Nonadecane	268	C19H40	000629-92-5	93
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
4	Tetracosane	338	C24H50	000646-31-1	89
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	89





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096287.D
Acq On : 29 Jun 2017 13:08
Operator : SJ/MA
Sample : I3906-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-02-062317-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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TIC Library : C:\DATABASE\NIST11.L
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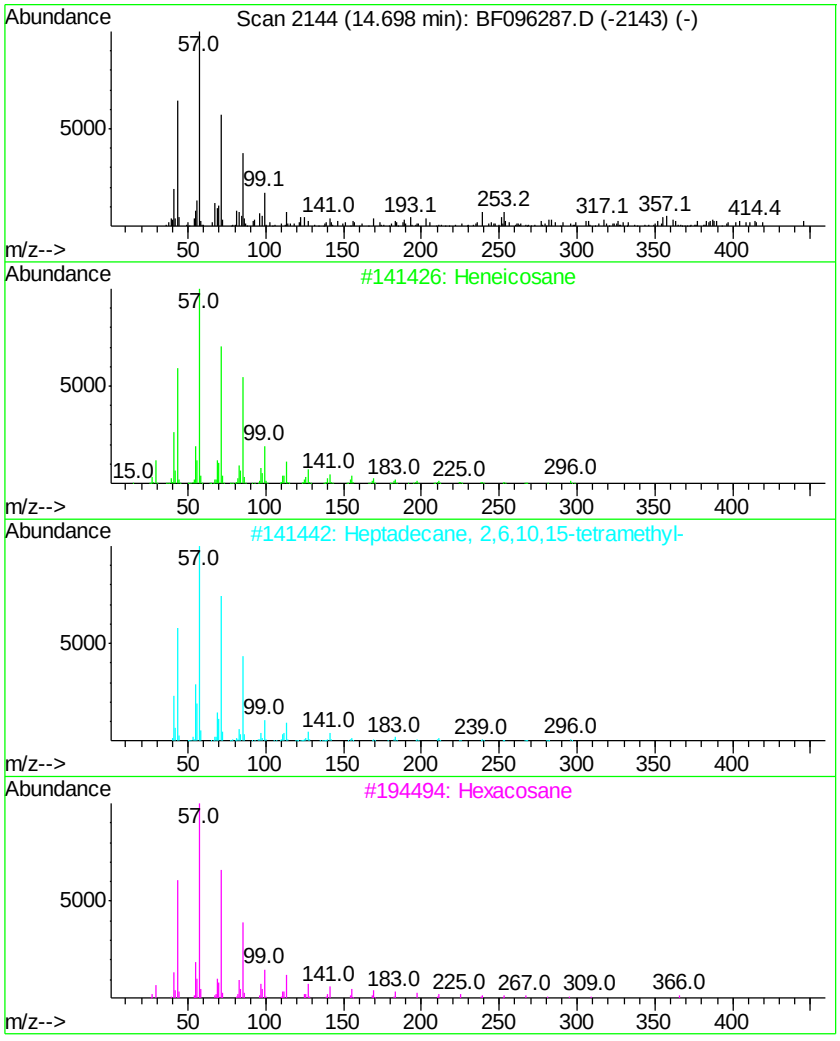
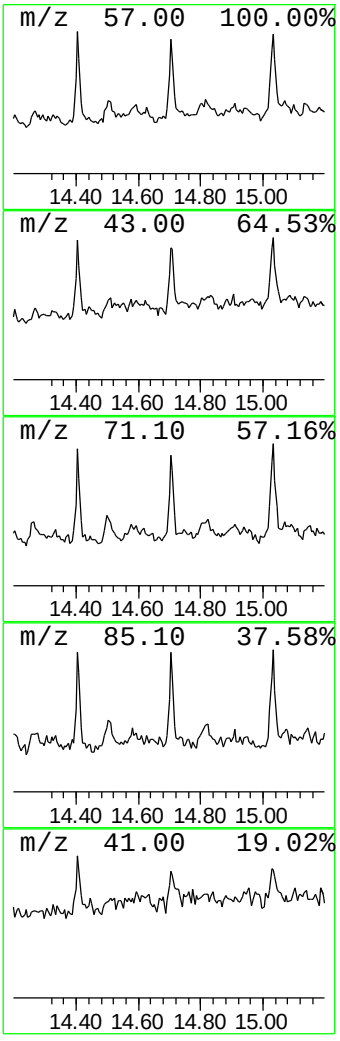
Peak Number 15 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	5.86 ng	186973	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	96
3	Hexacosane	366	C26H54	000630-01-3	91
4	Docosane	310	C22H46	000629-97-0	91
5	Octadecane	254	C18H38	000593-45-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062917\
Data File : BF096287.D
Acq On : 29 Jun 2017 13:08
Operator : SJ/MA
Sample : I3906-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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...	4.96	15.3	ng	777853	1	6.77	1016160	20.0
unknown6.54	6.54	61.7	ng	3136930	1	6.77	1016160	20.0
Tridecane	10.72	2.6	ng	121560	4	11.28	950298	20.0
n-Hexadecanoic acid	11.82	5.5	ng	259294	4	11.28	950298	20.0
9,12-Octadecadien...	12.37	4.5	ng	212236	4	11.28	950298	20.0
3-Heptadecenal	12.39	4.6	ng	220024	4	11.28	950298	20.0
n-Decanoic acid	12.60	3.7	ng	151264	5	13.92	824594	20.0
Decane, 1-bromo-2...	13.12	2.5	ng	100997	5	13.92	824594	20.0
Hexadecane	13.46	3.5	ng	143188	5	13.92	824594	20.0
11-Tricosene	13.77	10.5	ng	434193	5	13.92	824594	20.0
Heptadecane	14.10	3.3	ng	135083	5	13.92	824594	20.0
Heptacosane	14.40	4.6	ng	188883	5	13.92	824594	20.0
Heneicosane	14.70	5.9	ng	186973	6	15.34	637594	20.0