LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097704.D
Acq On : 15 Aug 2017 21:25
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-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-BF081517.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	2.310	35	38	44	rVB	20645	30441	1.40%	0.158%
2	4.963	486	489	496	rVB	39297	38556	1.77%	0.200%
3	5.375	555	559	564	rVB	592032	500190	23.00%	2.597%
4	6.398	729	733	739	rVB	652687	535175	24.60%	2.779%
5	6.545	754	758	761	rBV	575659	517306	23.78%	2.686%
6	6.781	794	798	802	rBV	1289104	1056317	48.56%	5.485%
7	6.934	821	824	828	rVB	425977	369523	16.99%	1.919%
8	7.340	889	893	896	rBV	371375	286231	13.16%	1.486%
9	8.063	1012	1016	1020	rBV	1552003	1386214	63.73%	7.197%
10	9.139	1195	1199	1204	rVB	687246	520195	23.91%	2.701%
11	9.228	1209	1214	1218	rBV	47525	47071	2.16%	0.244%
12	9.304	1223	1227	1231	rVB2	25359	33470	1.54%	0.174%
13	9.534	1263	1266	1271	rBV	183962	171815	7.90%	0.892%
14	9.757	1302	1304	1308	rVB	86067	69166	3.18%	0.359%
15	9.822	1309	1315	1318	rVV	1484451	1431116	65.79%	7.431%
16	10.257	1386	1389	1392	rVB	136793	109007	5.01%	0.566%
17	10.480	1423	1427	1429	rBV	55974	61696	2.84%	0.320%
18	10.598	1444	1447	1451	rVB	359910	288702	13.27%	1.499%
19	10.733	1467	1470	1478	rBV	175326	210787	9.69%	1.094%
20	11.051	1522	1524	1530	rVB5	21385	32070	1.47%	0.167%
21	11.180	1543	1546	1548	rBV	202670	155264	7.14%	0.806%
22	11.210	1548	1551	1557	rVB	73066	78285	3.60%	0.406%
23	11.298	1562	1566	1569	rBV	1424704	1254210	57.66%	6.512%
24	11.533	1602	1606	1608	rBV3	33150	38045	1.75%	0.198%
25	11.604	1615	1618	1621	rBV	134745	121811	5.60%	0.632%
26	11.704	1632	1635	1639	rVB	1264103	1072970	49.33%	5.571%
27	11.833	1654	1657	1661	rBV2	81810	79328	3.65%	0.412%
28	12.016	1683	1688	1694	rVB2	129369	139399	6.41%	0.724%
29	12.392	1748	1752	1754	rBV	2295343	2164037	99.49%	11.236%
30	12.416	1754	1756	1759	rVB	2843484	2175190	100.00%	11.294%
31	12.498	1767	1770	1773	rBV	778224	632236	29.07%	3.283%
32	12.545	1773	1778	1783	rVV2	160302	215536	9.91%	1.119%
33	12.622	1789	1791	1797	rVB5	40622	46872	2.15%	0.243%
34	12.722	1804	1808	1814	rBV2	274470	295707	13.59%	1.535%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-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-BF081517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.774	1814	1817	1819	rVV	85026	70357	3.23%	0.365%
36	12.798	1819	1821	1823	rVB2	57664	44424	2.04%	0.231%
37	12.886	1832	1836	1839	rBV	388878	338823	15.58%	1.759%
38	12.998	1850	1855	1857	rBV4	33657	45558	2.09%	0.237%
39	13.057	1862	1865	1867	rBV2	58024	57422	2.64%	0.298%
40	13.145	1875	1880	1883	rBV2	72209	113278	5.21%	0.588%
41	13.227	1891	1894	1895	rBV	63920	67080	3.08%	0.348%
42	13.280	1901	1903	1909	rVB5	55669	63190	2.91%	0.328%
43	13.327	1909	1911	1917	rBV6	46990	52899	2.43%	0.275%
44	13.427	1925	1928	1931	rVB	203634	173242	7.96%	0.899%
45	13.651	1962	1966	1968	rBV4	44691	59455	2.73%	0.309%
46	13.892	2004	2007	2010	rBV	61981	60578	2.78%	0.315%
47	13.933	2010	2014	2018	rBV	1086805	930407	42.77%	4.831%
48	14.116	2043	2045	2049	rBV	42921	39650	1.82%	0.206%
49	14.421	2095	2097	2102	rVB	39793	34434	1.58%	0.179%
50	14.727	2146	2149	2153	rBV2	62454	84174	3.87%	0.437%
51	15.363	2253	2257	2263	rVB	673880	861050	39.59%	4.471%

Sum of corrected areas: 19259959

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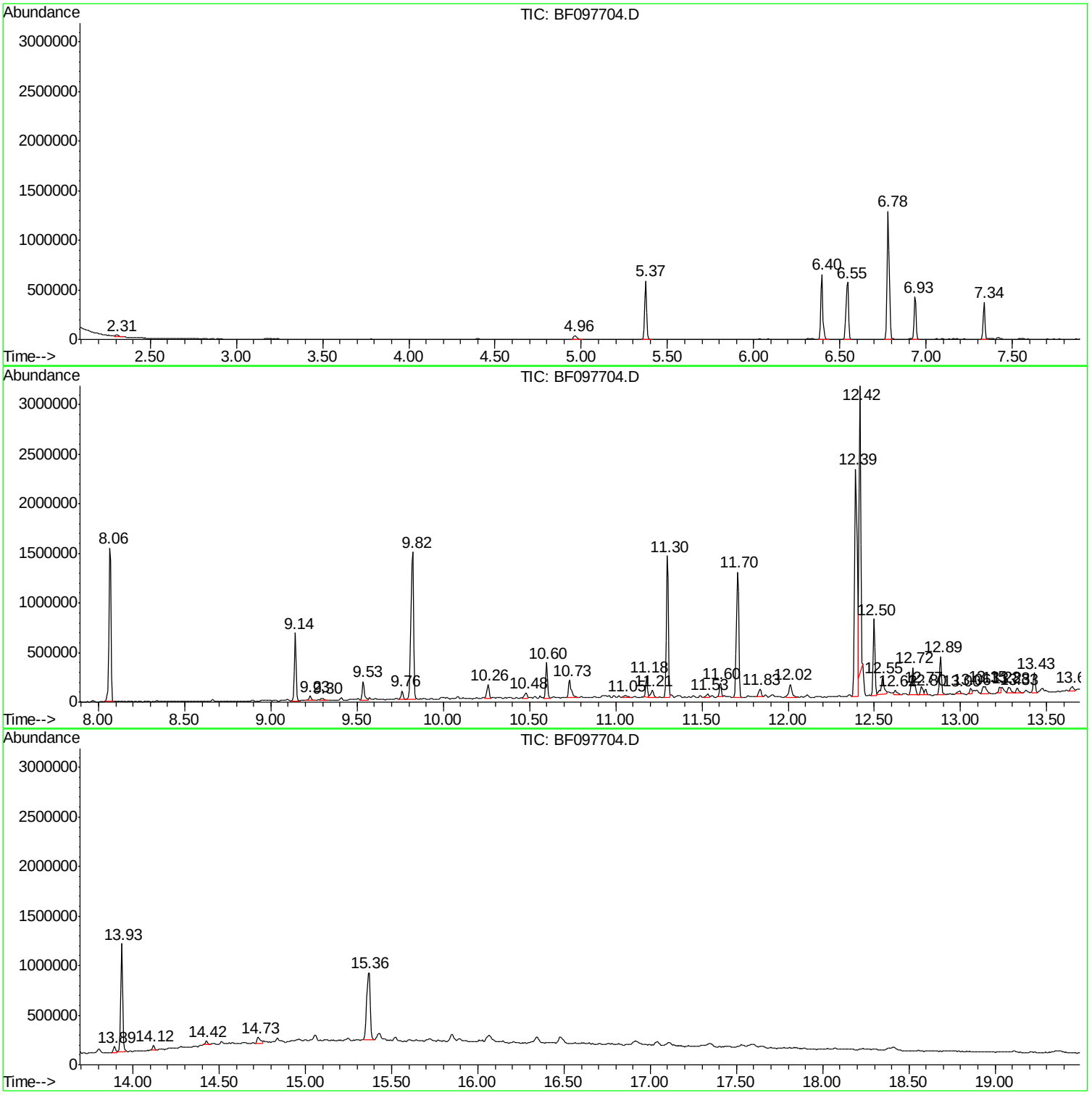
BNA_F
ClientSampleId :
NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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Operator : SJ/JU
Sample : I4700-01 10X
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
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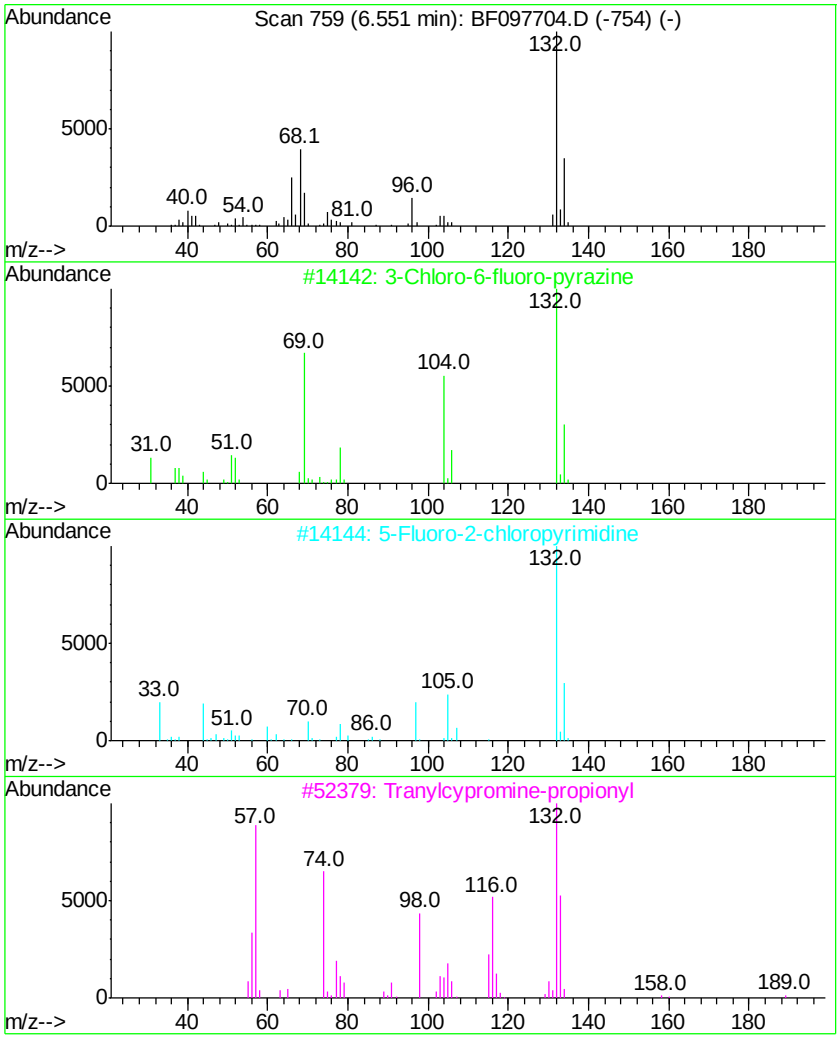
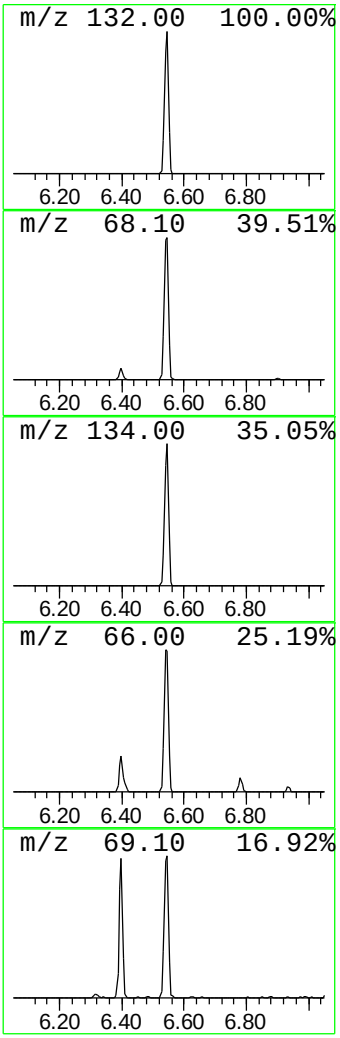
Peak Number 1 unknown6.55 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	9.79 ng	517306	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Aminoindole	132	C8H8N2	005192-03-0	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097704.D
Acq On : 15 Aug 2017 21:25
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
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Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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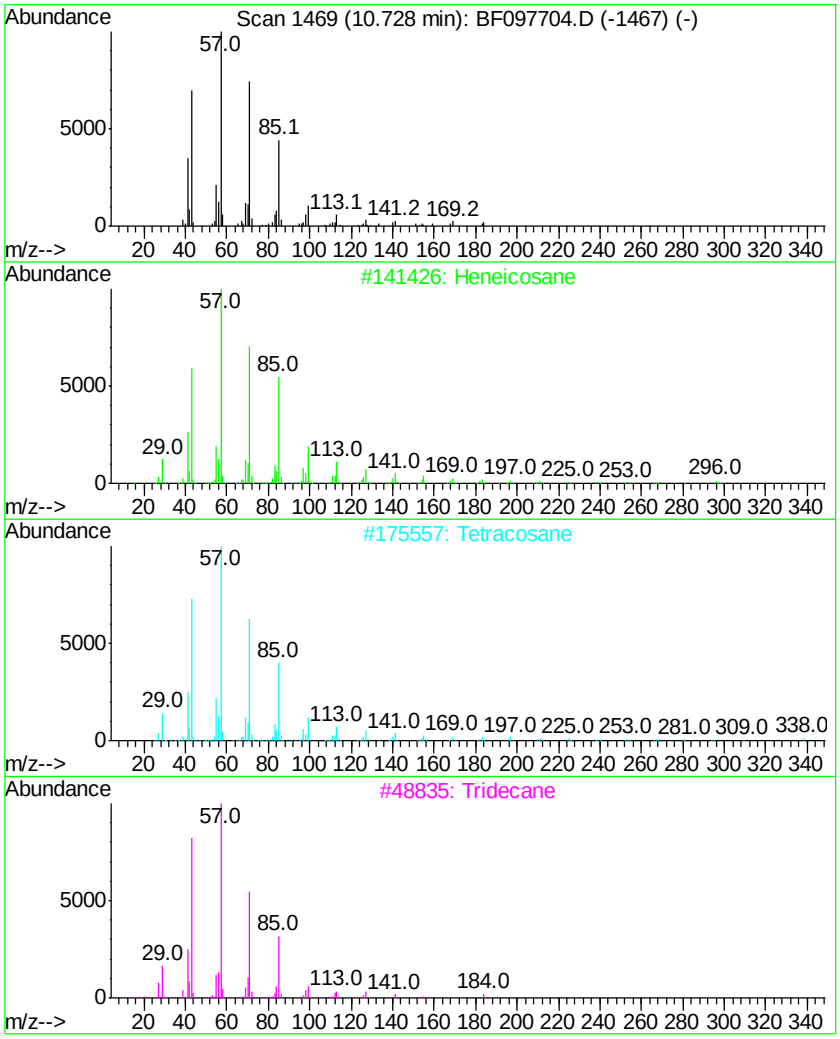
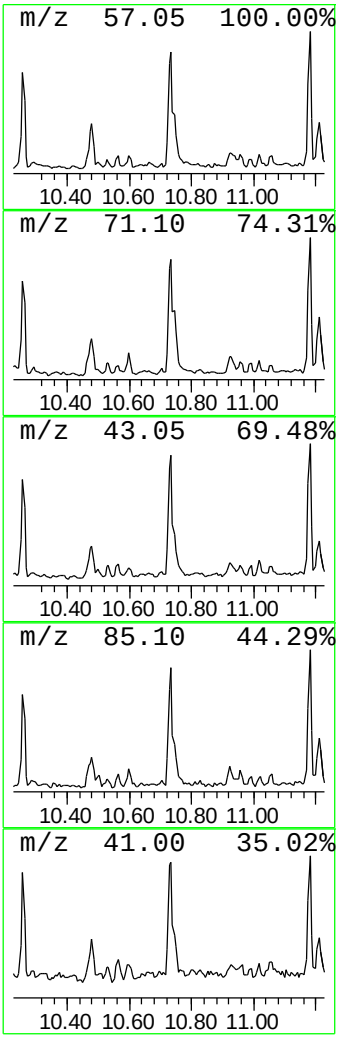
Peak Number 3 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	3.36 ng	210787	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90





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Data File : BF097704.D
Acq On : 15 Aug 2017 21:25
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
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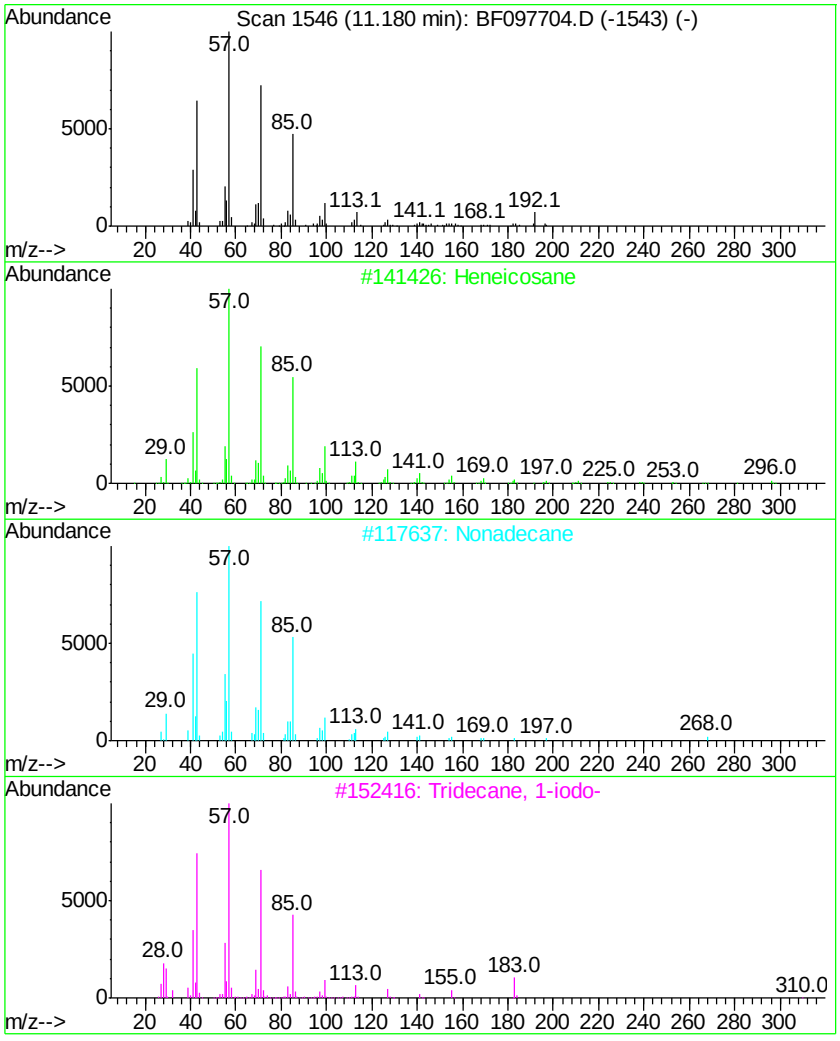
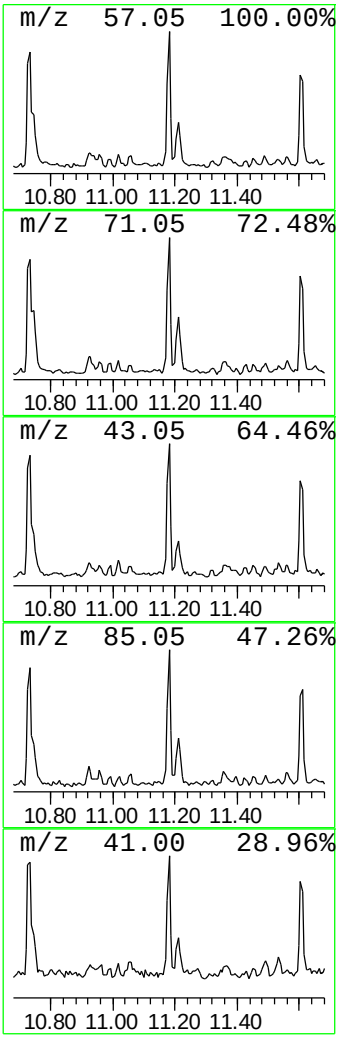
Peak Number 4 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	2.48 ng	155264	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Nonadecane	268	C19H40	000629-92-5	87
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4	Hexacosane	366	C26H54	000630-01-3	64
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64





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Sample : I4700-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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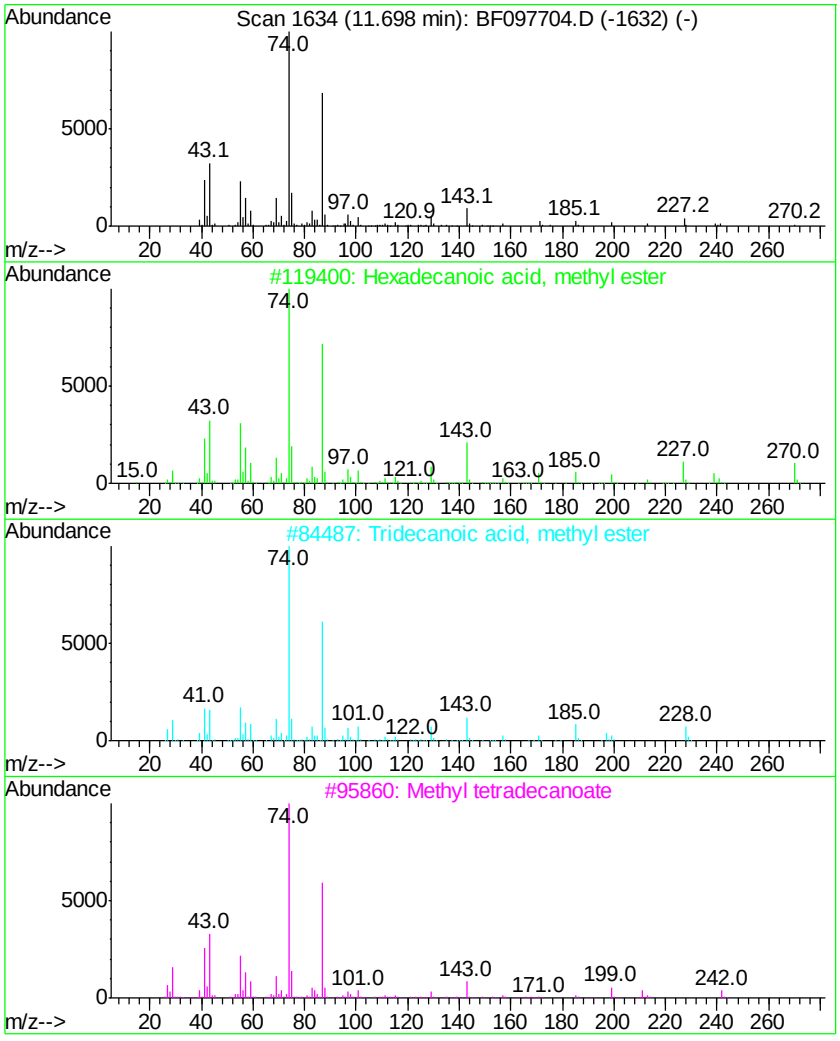
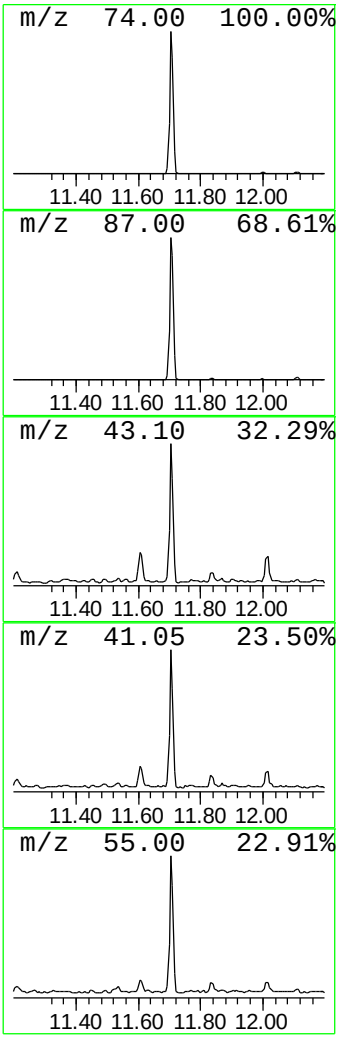
Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	17.11 ng	1072970	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	90
5	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	90





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Sample : I4700-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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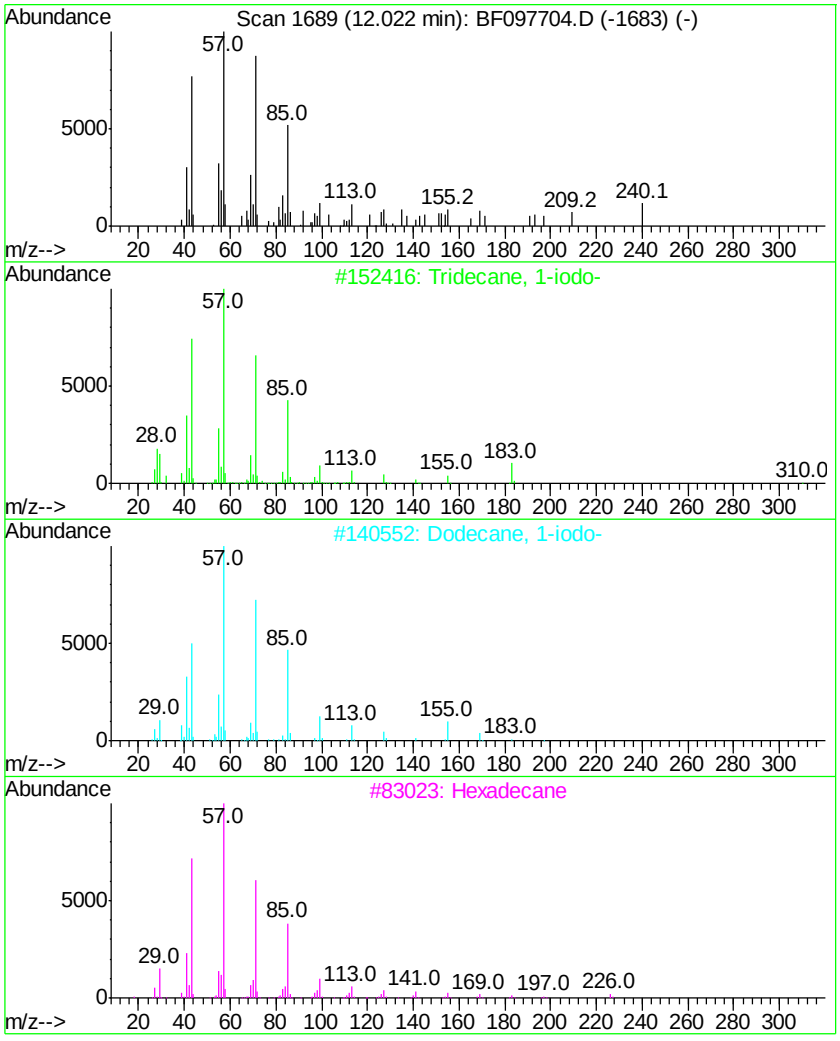
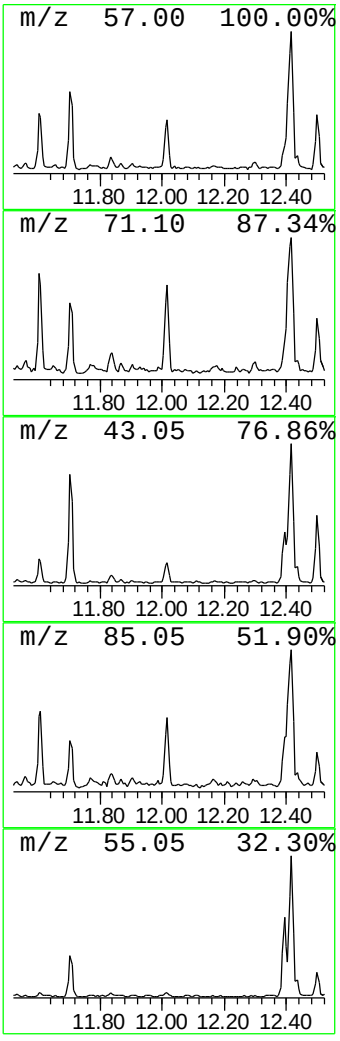
Peak Number 6 Tridecane, 1-iodo- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.22 ng	139399	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	90
3	Hexadecane	226	C16H34	000544-76-3	87
4	Tetradecane	198	C14H30	000629-59-4	87
5	Eicosane	282	C20H42	000112-95-8	87





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Misc :
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Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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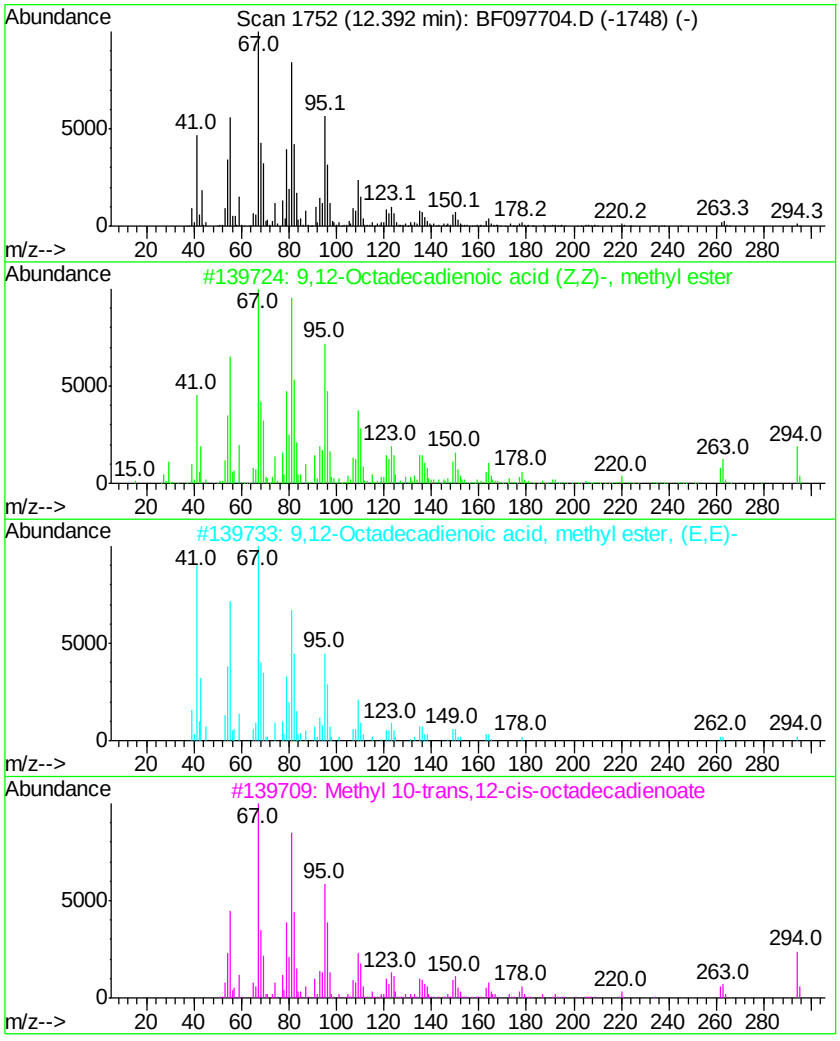
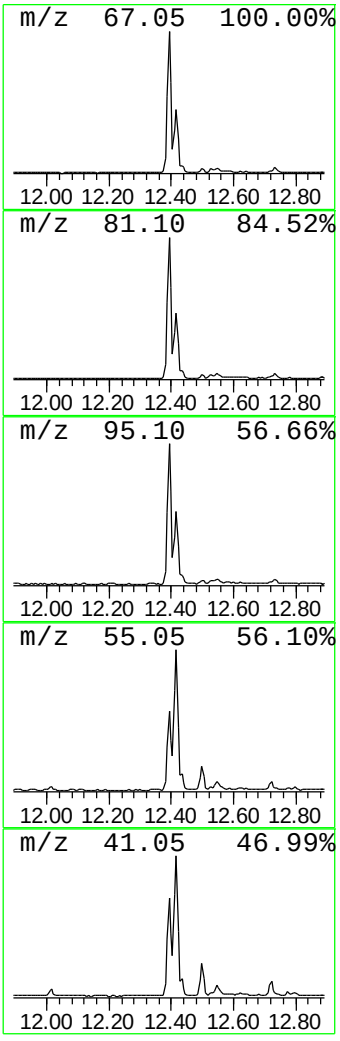
Peak Number 7 9,12-Octadecadienoic acid (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	34.51 ng	2164040	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98
5	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95





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Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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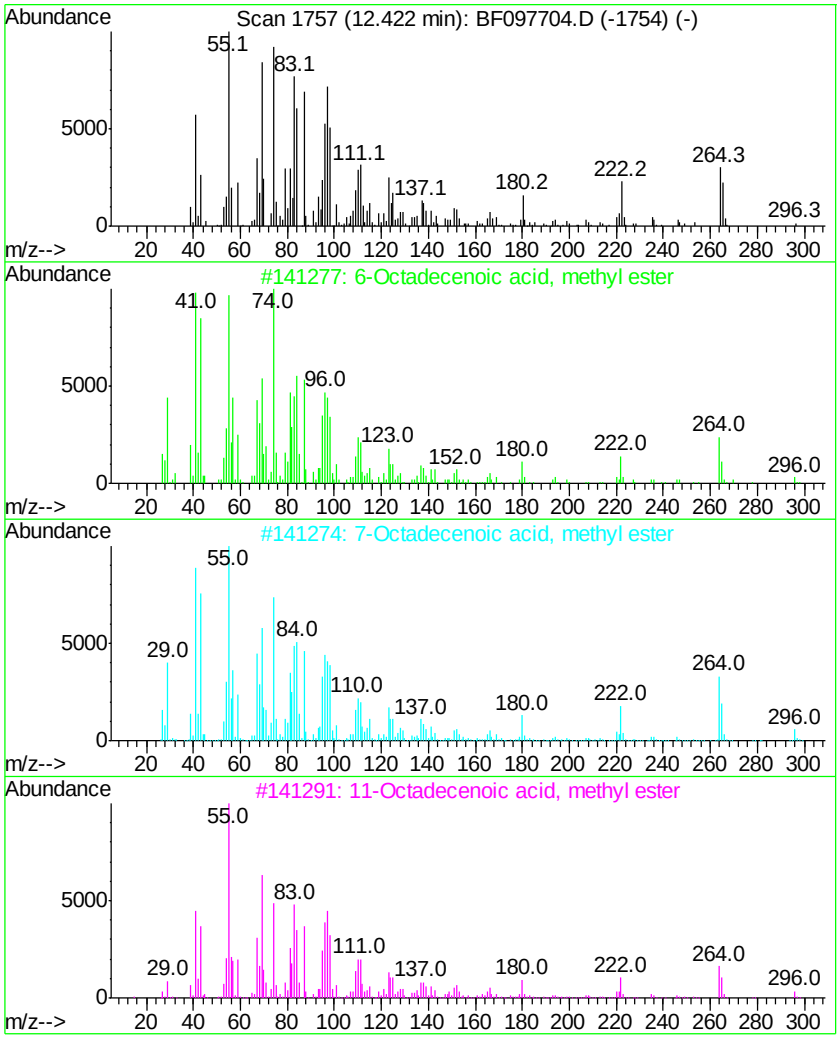
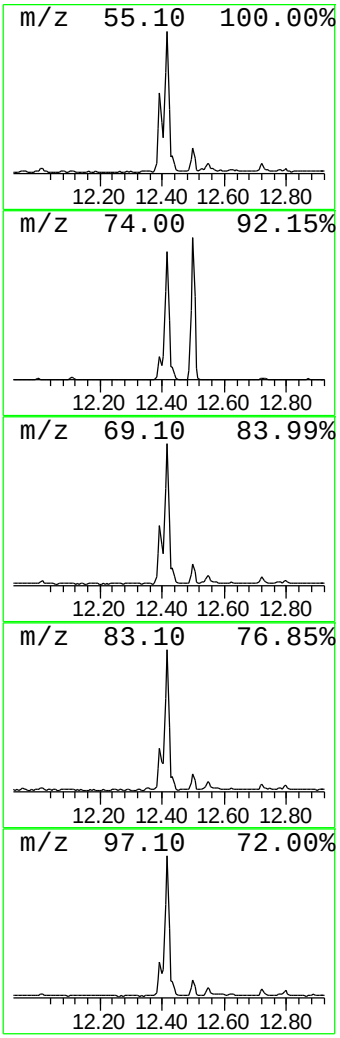
Peak Number 8 6-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	34.69 ng	2175190	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
2	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	96
3	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	96
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	96
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081517\
Data File : BF097704.D
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Operator : SJ/JU
Sample : I4700-01 10X
Misc :
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Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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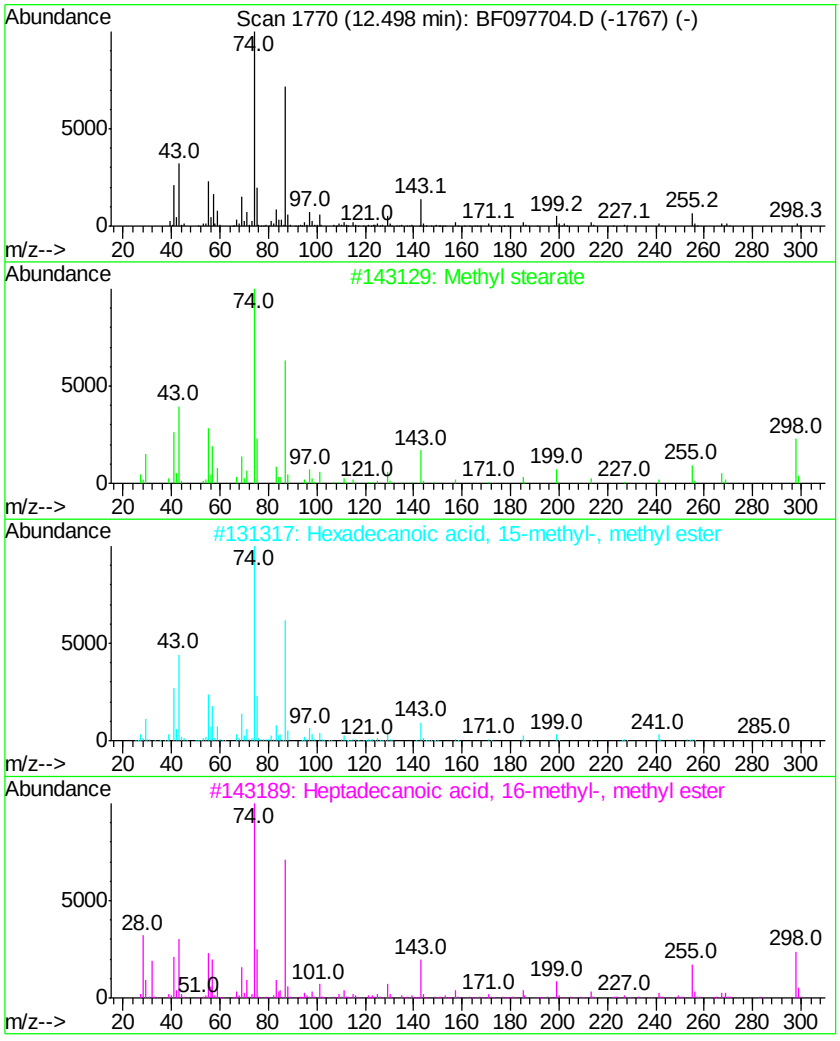
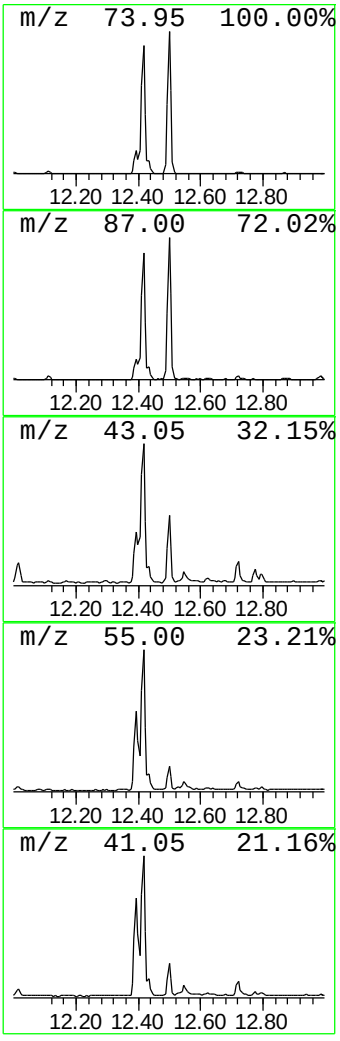
Peak Number 9 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	10.08 ng	632236	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	91
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91





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Data File : BF097704.D
Acq On : 15 Aug 2017 21:25
Operator : SJ/JU
Sample : I4700-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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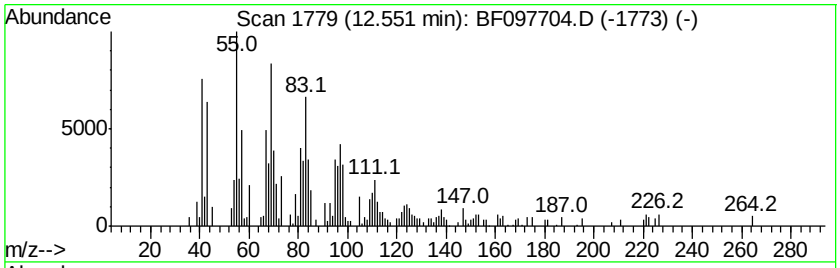
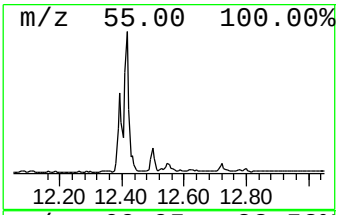
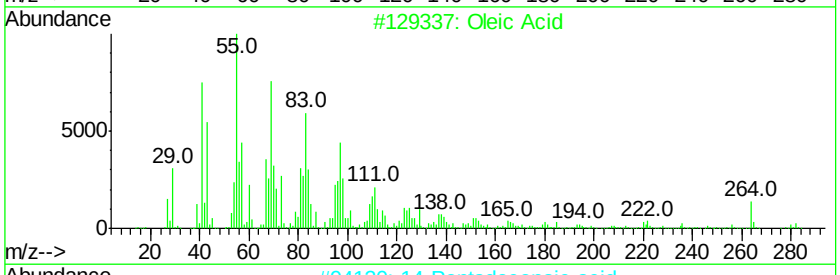
Peak Number 10 Oleic Acid Concentration Rank 9

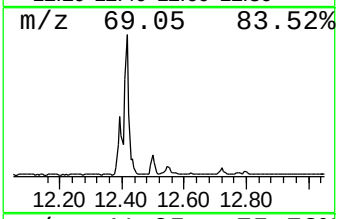
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	3.44 ng	215536	Phenanthrene-d10	11.30

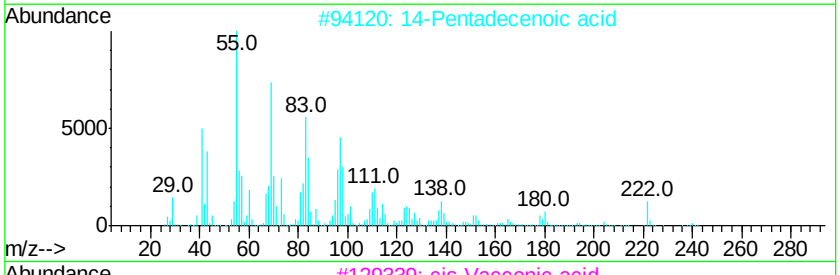
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	81
2	14-Pentadecenoic acid	240	C15H28O2	017351-34-7	72
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	60
4	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	58
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	53

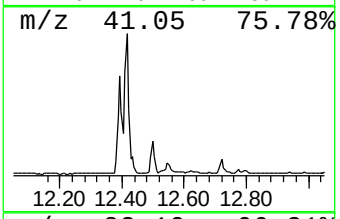


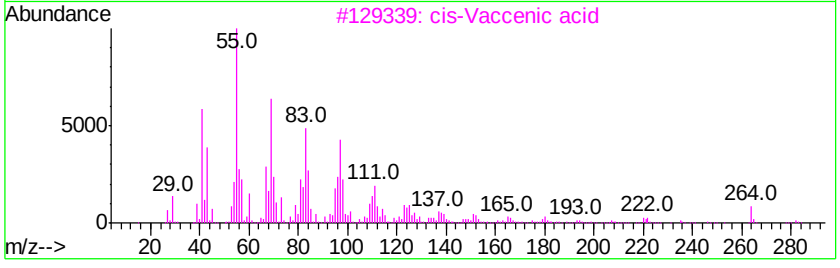


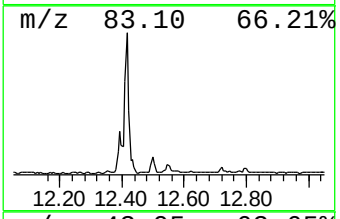


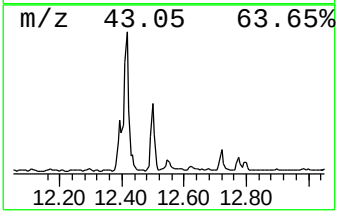












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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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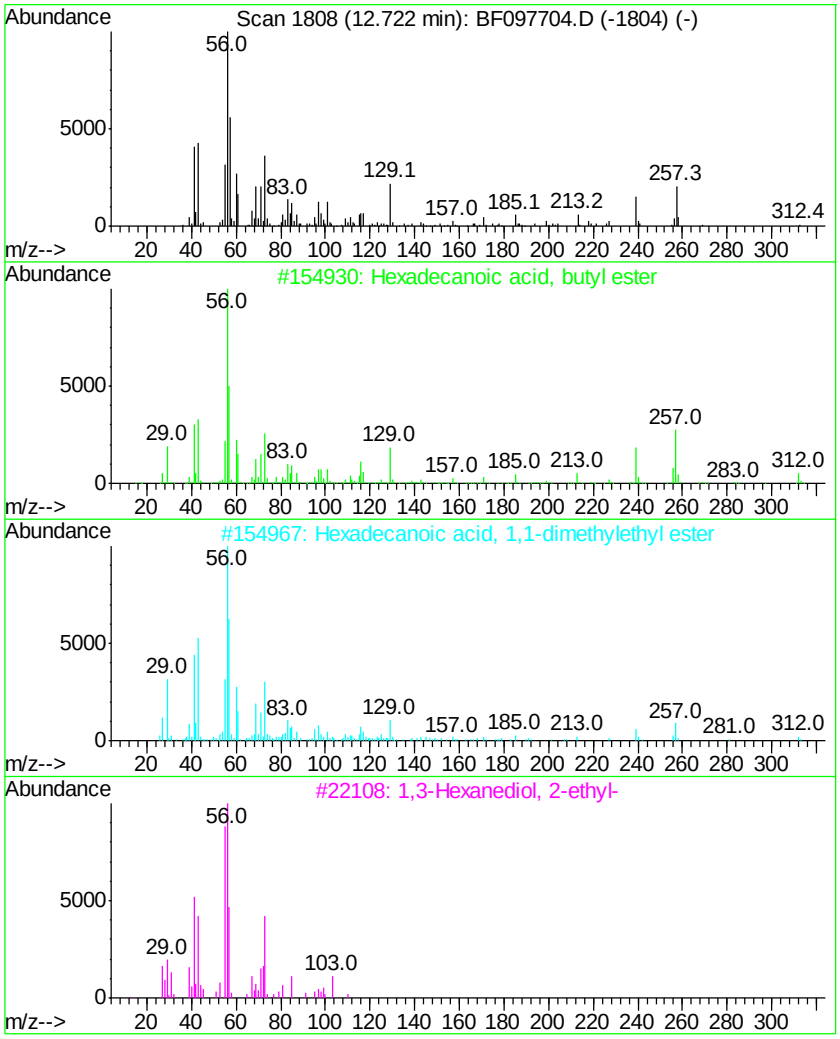
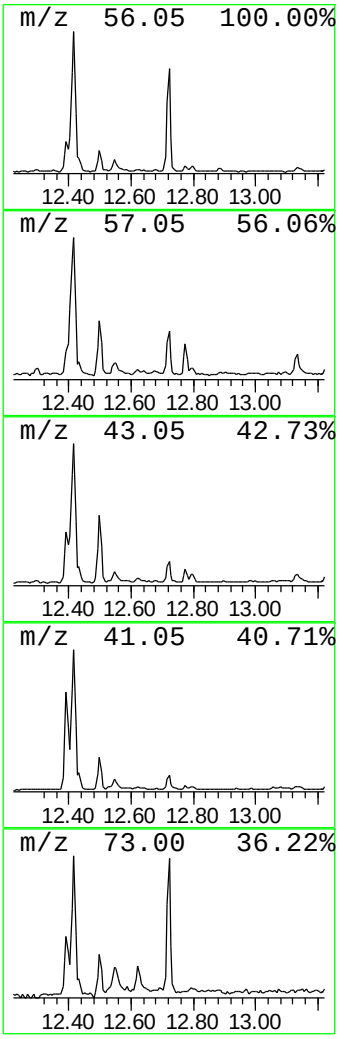
Peak Number 11 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	6.36 ng	295707	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
3	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : NB-01-080917-A

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

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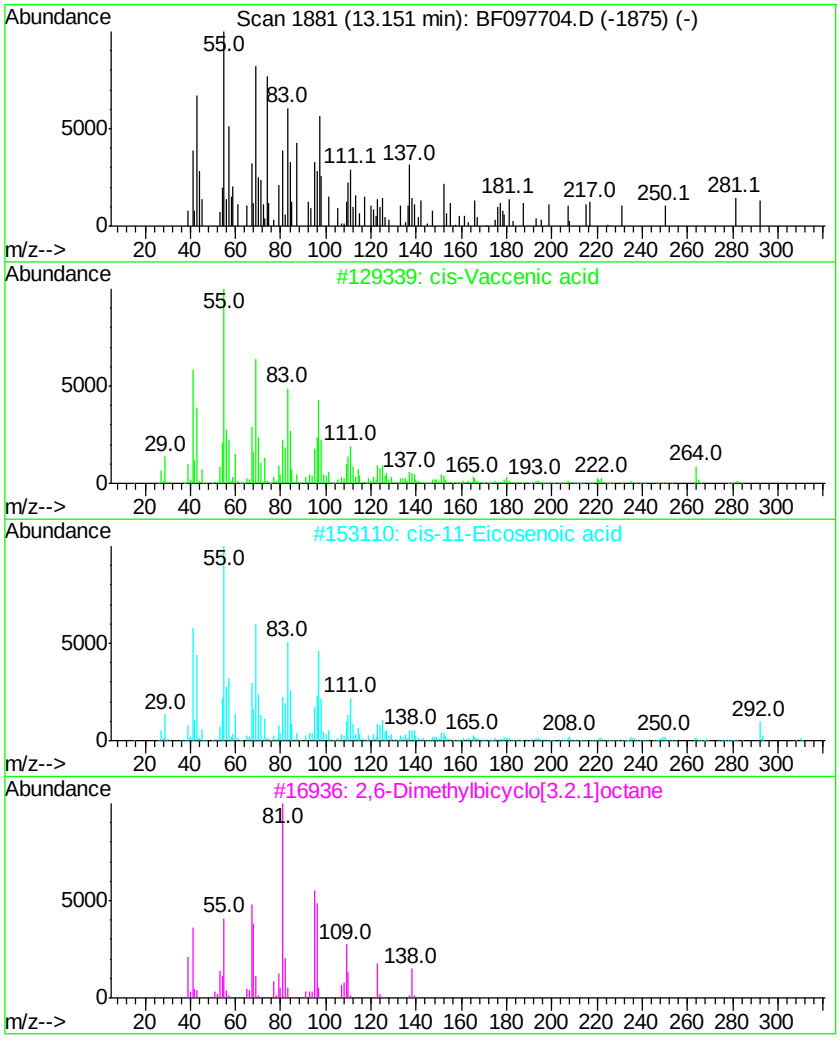
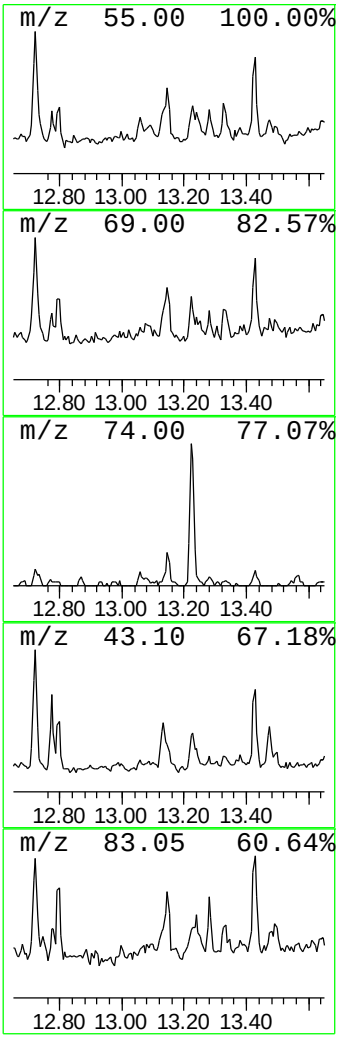
Peak Number 12 cis-Vaccenic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.15	2.44 ng	113278	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	68
2	cis-11-Eicosenoic acid	310	C20H38O2	005561-99-9	64
3	2,6-Dimethylbicyclo[3.2.1]octane	138	C10H18	1000215-28-2	53
4	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	53
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	52





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Sample : I4700-01 10X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-01-080917-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Integration Parameters: LSCINT.P

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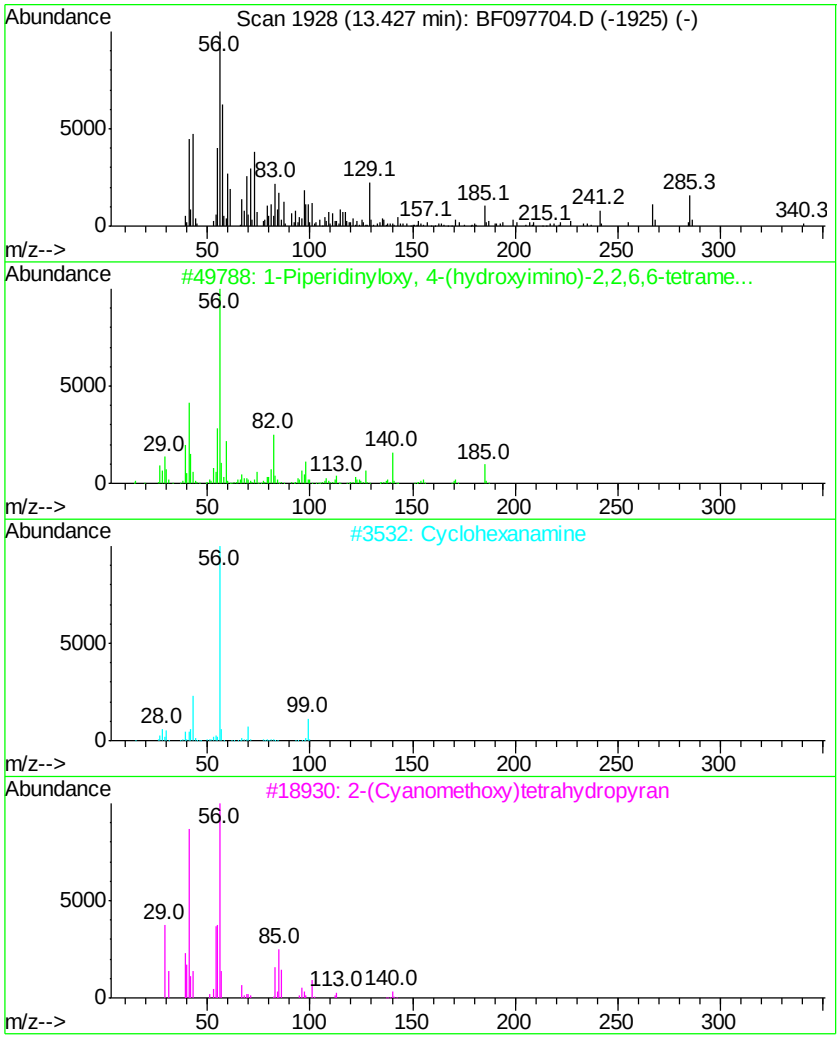
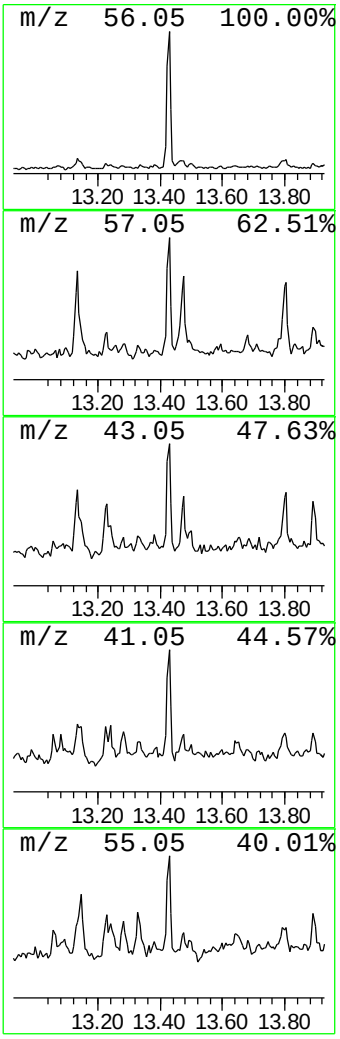
Peak Number 13 unknown13.43 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	3.72 ng	173242	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Piperidinyloxy, 4-(hydroxyimin...	185	C9H17N2O2	003229-75-2	38
2	Cyclohexanamine	99	C6H13N	000108-91-8	35
3	2-(Cyanomethoxy)tetrahydropyran	141	C7H11NO2	017521-49-2	35
4	5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1000376-27-1	35
5	2-Butyl-1-decene	196	C14H28	051655-65-3	35





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.55	6.55	9.8	ng	517306	1	6.78	1056320	20.0
Heneicosane	10.73	3.4	ng	210787	4	11.30	1254210	20.0
Nonadecane	11.18	2.5	ng	155264	4	11.30	1254210	20.0
Hexadecanoic acid...	11.70	17.1	ng	1072970	4	11.30	1254210	20.0
Tridecane, 1-iodo-	12.02	2.2	ng	139399	4	11.30	1254210	20.0
9,12-Octadecadien...	12.39	34.5	ng	2164040	4	11.30	1254210	20.0
6-Octadecenoic ac...	12.42	34.7	ng	2175190	4	11.30	1254210	20.0
Methyl stearate	12.50	10.1	ng	632236	4	11.30	1254210	20.0
Oleic Acid	12.55	3.4	ng	215536	4	11.30	1254210	20.0
Hexadecanoic acid...	12.72	6.4	ng	295707	5	13.93	930407	20.0
cis-Vaccenic acid	13.15	2.4	ng	113278	5	13.93	930407	20.0
unknown13.43	13.43	3.7	ng	173242	5	13.93	930407	20.0