LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071917\
Data File : BF096889.D
Acq On : 20 Jul 2017 00:12
Operator : SJ/JU
Sample : I4258-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-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-BF071317.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	4.751	466	470	481	rVB	148531	203880	9.59%	1.057%
2	5.193	541	545	559	rBV	2128923	2125139	100.00%	11.016%
3	6.240	718	723	737	rBV	2005056	2065150	97.18%	10.705%
4	6.357	739	743	747	rBV	1958985	1938369	91.21%	10.048%
5	6.587	779	782	786	rBV	802911	649126	30.55%	3.365%
6	6.745	805	809	812	rBV	1753165	1480911	69.69%	7.676%
7	7.151	873	878	881	rBV	1392253	1266258	59.58%	6.564%
8	7.869	996	1000	1004	rBV	1049591	935669	44.03%	4.850%
9	8.951	1179	1184	1187	rBV	2061819	1840074	86.59%	9.538%
10	9.045	1197	1200	1205	rVB	25891	22958	1.08%	0.119%
11	9.345	1247	1251	1254	rBV	275887	228886	10.77%	1.186%
12	9.575	1287	1290	1292	rVB	35234	30690	1.44%	0.159%
13	9.622	1292	1298	1301	rBV	913463	866101	40.76%	4.489%
14	10.069	1371	1374	1378	rVB	46543	39423	1.86%	0.204%
15	10.292	1407	1412	1414	rBV	22414	30109	1.42%	0.156%
16	10.404	1427	1431	1441	rVB	1005087	888381	41.80%	4.605%
17	10.539	1451	1454	1462	rBV	74933	94123	4.43%	0.488%
18	10.733	1485	1487	1491	rVB4	16372	21258	1.00%	0.110%
19	10.986	1527	1530	1533	rBV2	68897	59525	2.80%	0.309%
20	11.016	1533	1535	1539	rVB	41154	38992	1.83%	0.202%
21	11.098	1544	1549	1551	rBV	688406	624287	29.38%	3.236%
22	11.116	1551	1552	1556	rVB	33759	28063	1.32%	0.145%
23	11.416	1599	1603	1607	rBV2	77528	87790	4.13%	0.455%
24	11.457	1607	1610	1616	rVB8	15978	24274	1.14%	0.126%
25	11.510	1616	1619	1622	rBV3	34060	36422	1.71%	0.189%
26	11.575	1626	1630	1631	rBV4	19237	24501	1.15%	0.127%
27	11.704	1649	1652	1655	rBV4	35291	39272	1.85%	0.204%
28	11.816	1668	1671	1677	rVB2	86348	94554	4.45%	0.490%
29	11.980	1695	1699	1703	rBV6	21564	45457	2.14%	0.236%
30	12.145	1725	1727	1730	rBV	36721	40419	1.90%	0.210%
31	12.192	1732	1735	1736	rVV2	94156	100113	4.71%	0.519%
32	12.210	1736	1738	1740	rVB	130662	111314	5.24%	0.577%
33	12.304	1751	1754	1757	rBV	76669	81266	3.82%	0.421%
34	12.351	1760	1762	1767	rVB5	32677	39881	1.88%	0.207%

LSC Area Percent Report

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Sample : I4258-04
Misc :
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Instrument : BNA_F
ClientSampleId : OK-02-071817-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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.527	1789	1792	1794	rBV	55803	46265	2.18%	0.240%
36	12.574	1798	1800	1803	rVB	100151	81501	3.84%	0.422%
37	12.680	1814	1818	1826	rBV	1253342	1136830	53.49%	5.893%
38	12.933	1858	1861	1864	rVB	141647	122069	5.74%	0.633%
39	13.274	1916	1919	1922	rBV	139436	116025	5.46%	0.601%
40	13.598	1971	1974	1981	rVB2	170596	214458	10.09%	1.112%
41	13.727	1992	1996	1998	rBV	493302	507429	23.88%	2.630%
42	13.916	2026	2028	2031	rVB	137362	110486	5.20%	0.573%
43	14.221	2077	2080	2083	rBV	176094	184524	8.68%	0.956%
44	14.516	2127	2130	2136	rBV2	196662	248067	11.67%	1.286%
45	15.098	2226	2229	2233	rBV	284433	321503	15.13%	1.667%

Sum of corrected areas: 19291792

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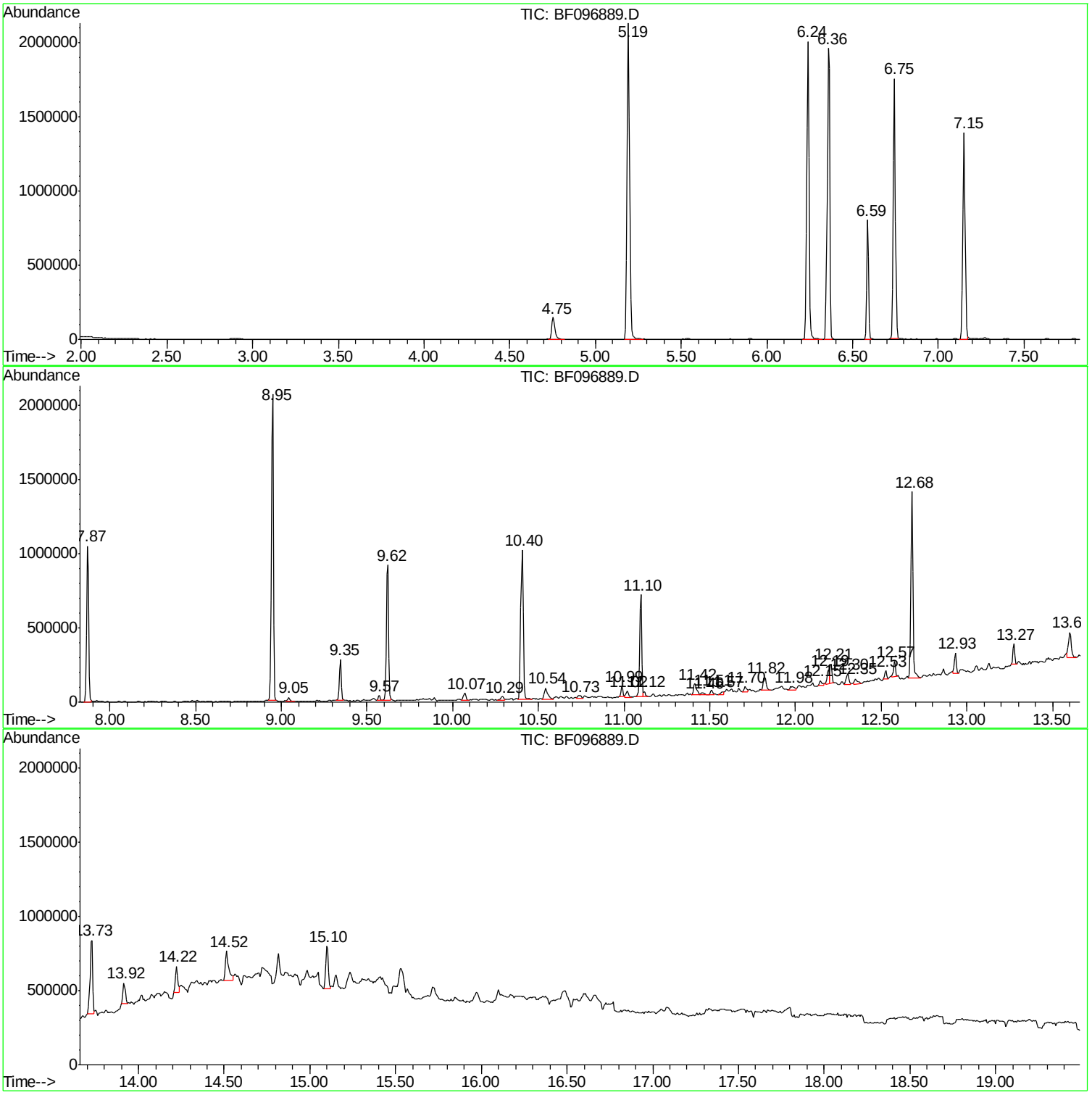
OK-02-071817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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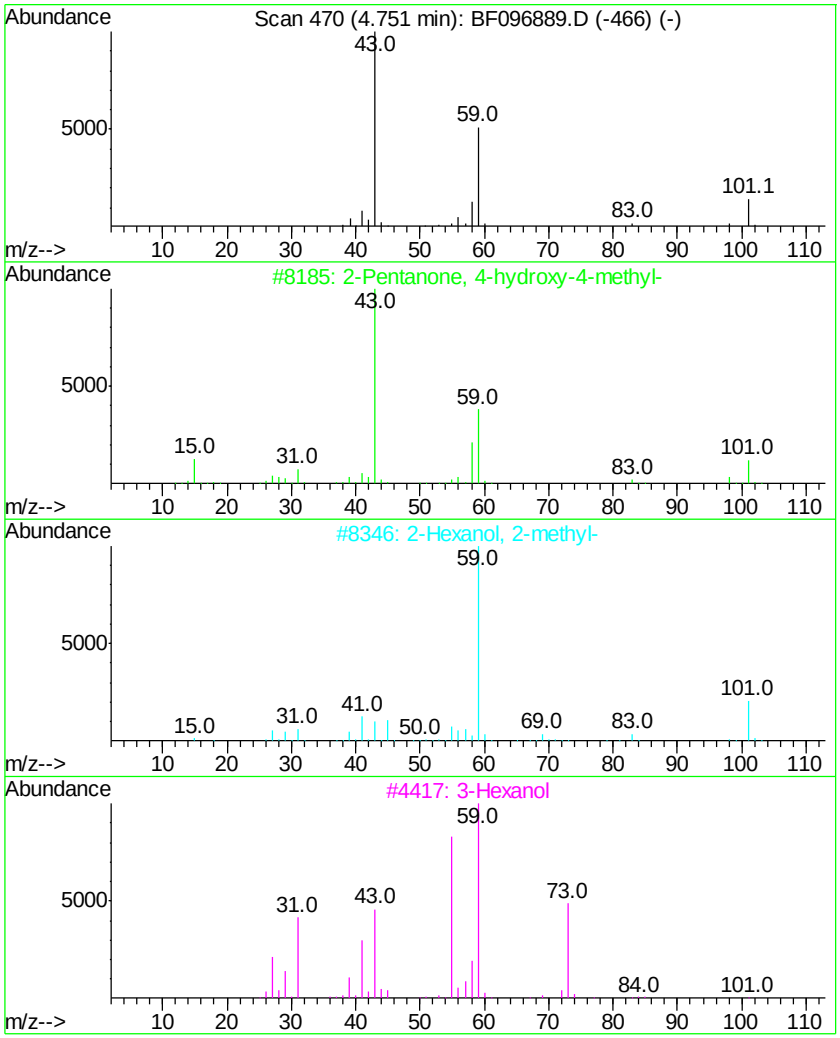
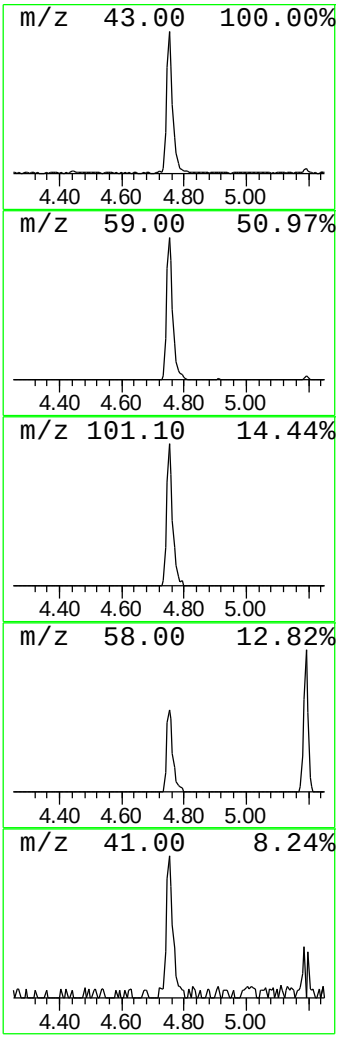
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	6.28 ng	203880	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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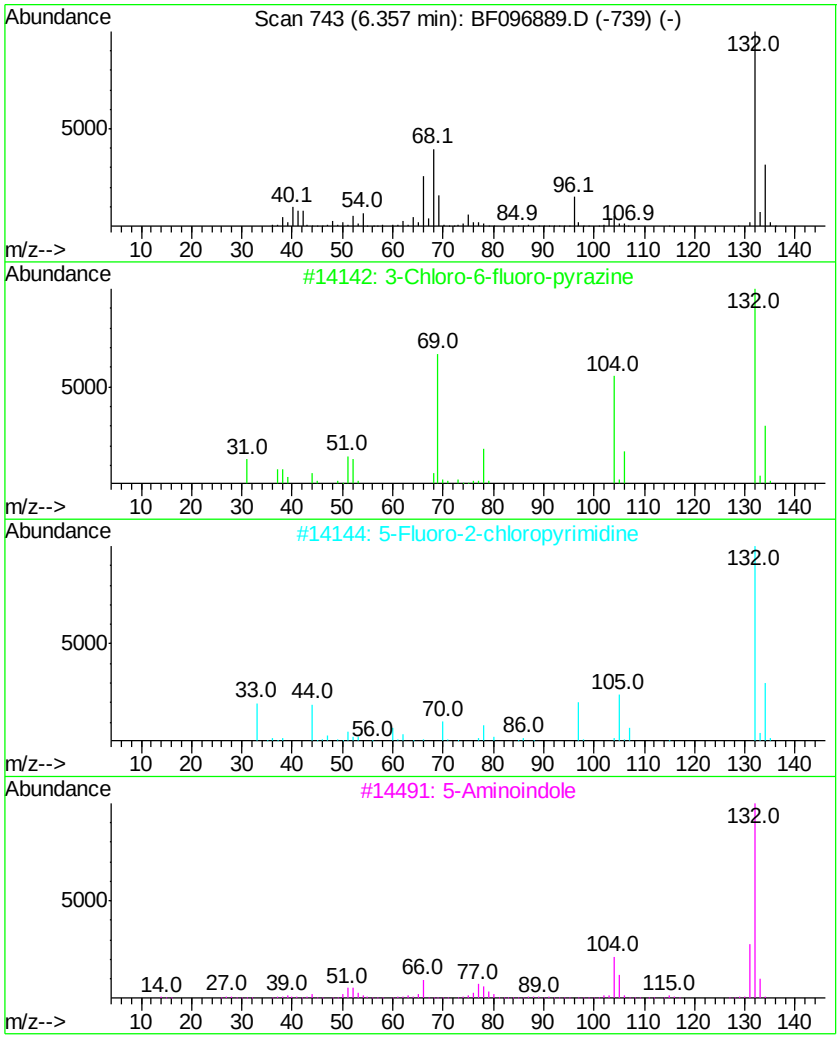
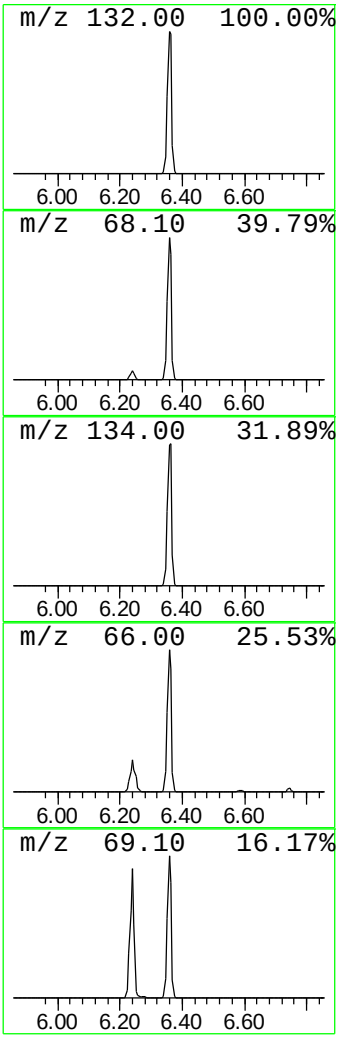
Peak Number 2 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	59.72 ng	1938370	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Operator : SJ/JU
Sample : I4258-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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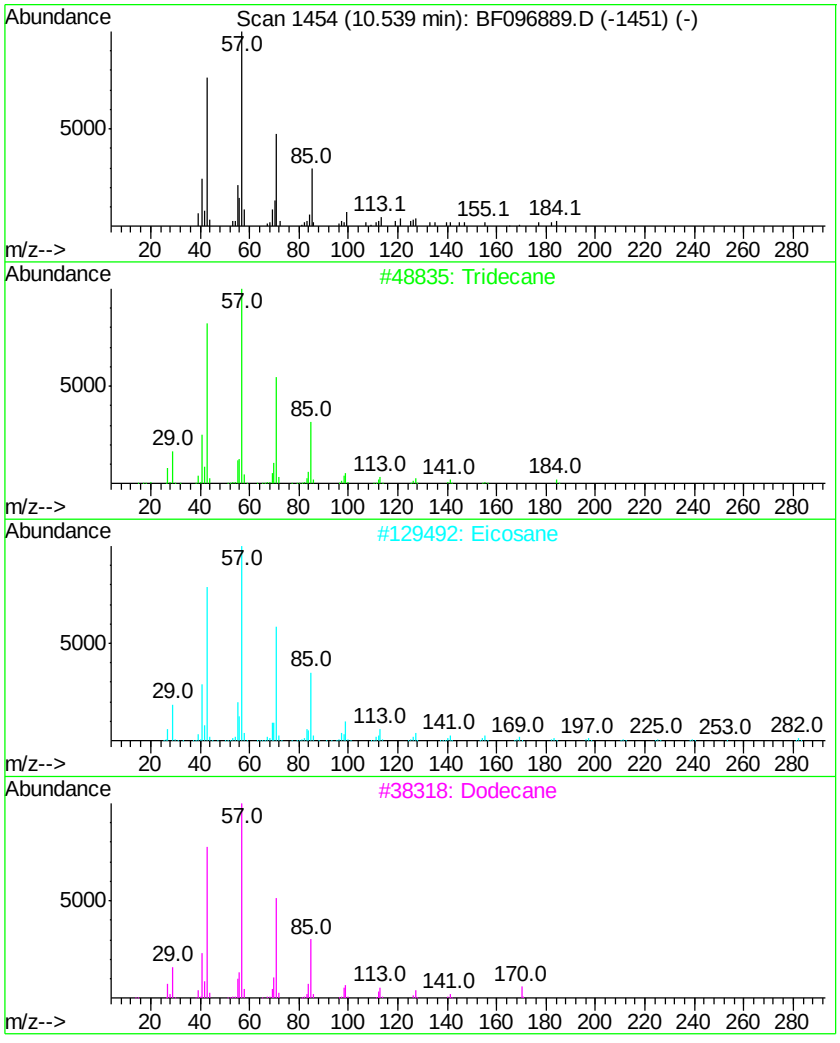
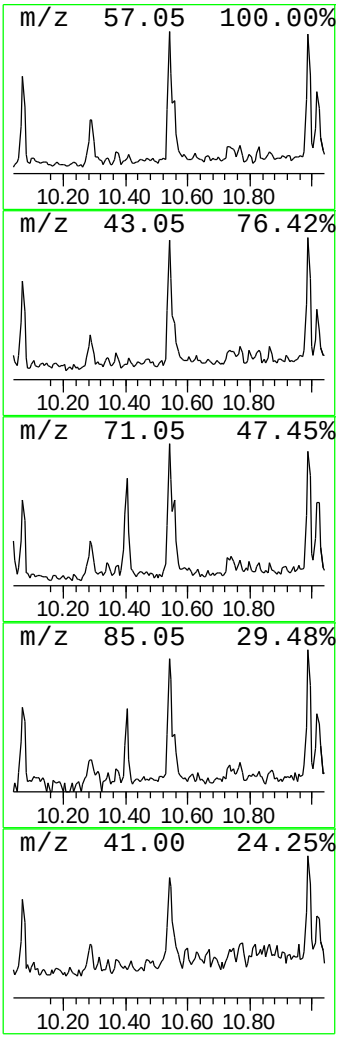
Peak Number 4 Tridecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	3.02 ng	94123	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Eicosane	282	C20H42	000112-95-8	86
3	Dodecane	170	C12H26	000112-40-3	86
4	Heptadecane	240	C17H36	000629-78-7	80
5	Heneicosane	296	C21H44	000629-94-7	80





Library Search Compound Report

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Instrument : BNA_F
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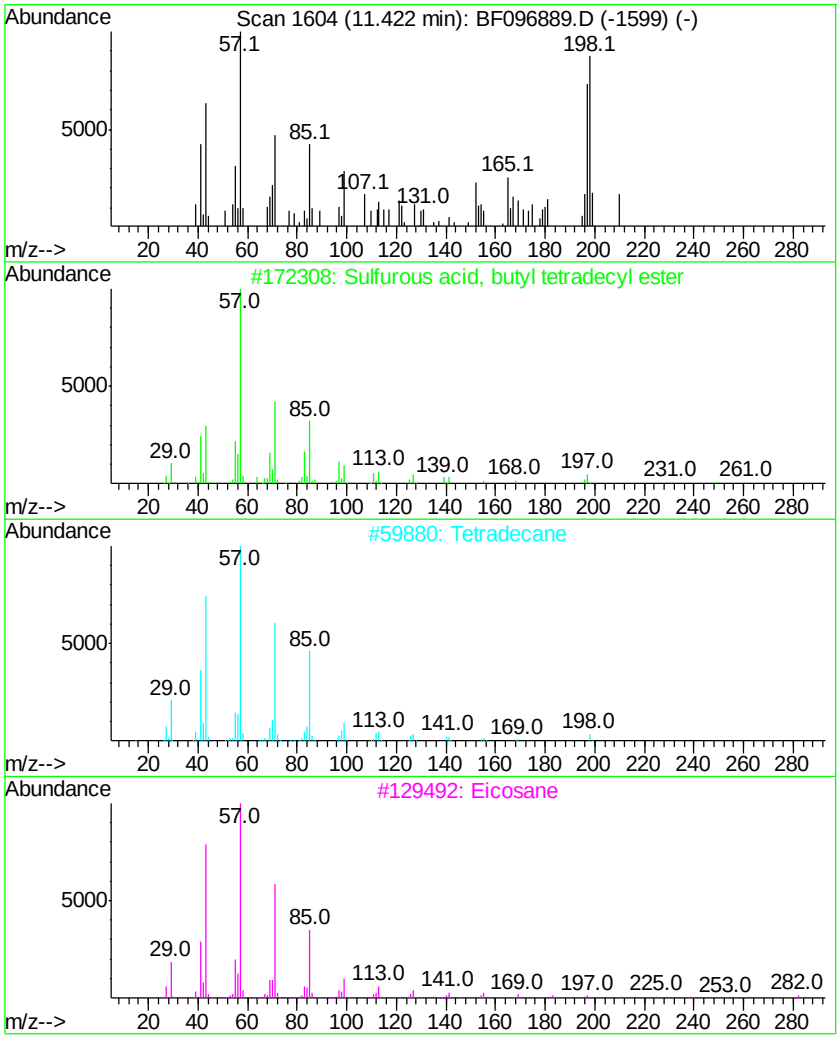
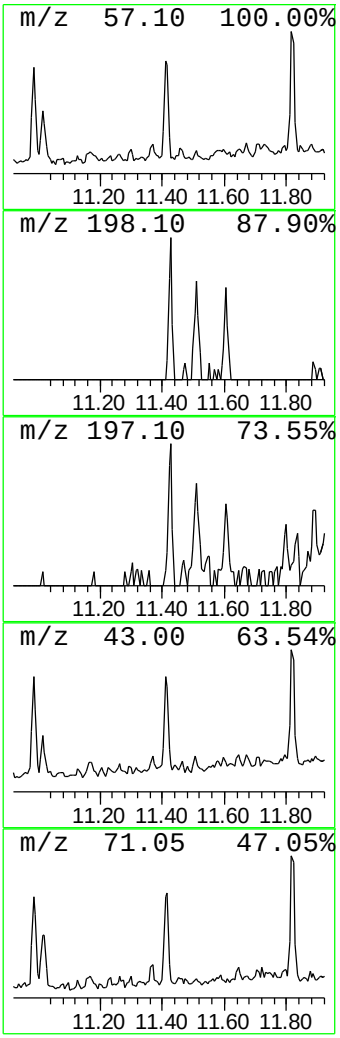
Peak Number 5 Sulfurous acid, butyl tetra... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	2.81 ng	87790	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
2	Tetradecane	198	C14H30	000629-59-4	70
3	Eicosane	282	C20H42	000112-95-8	68
4	Hexadecane	226	C16H34	000544-76-3	68
5	Pentadecane	212	C15H32	000629-62-9	64





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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-B

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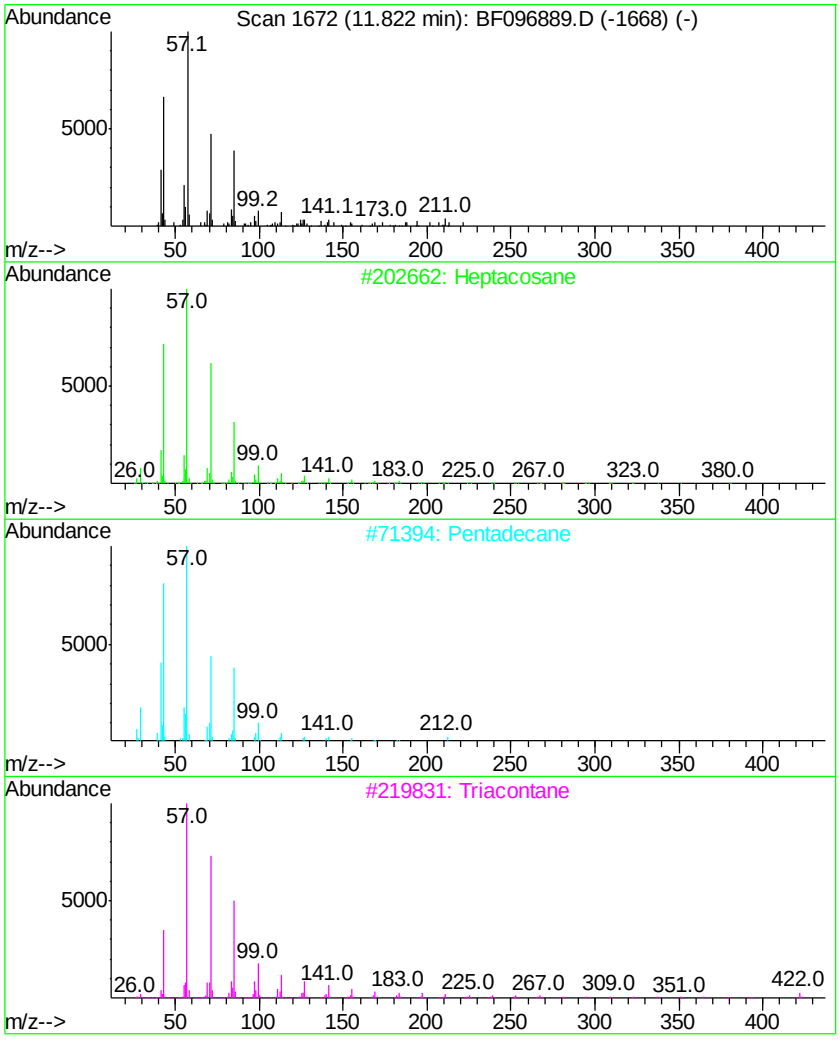
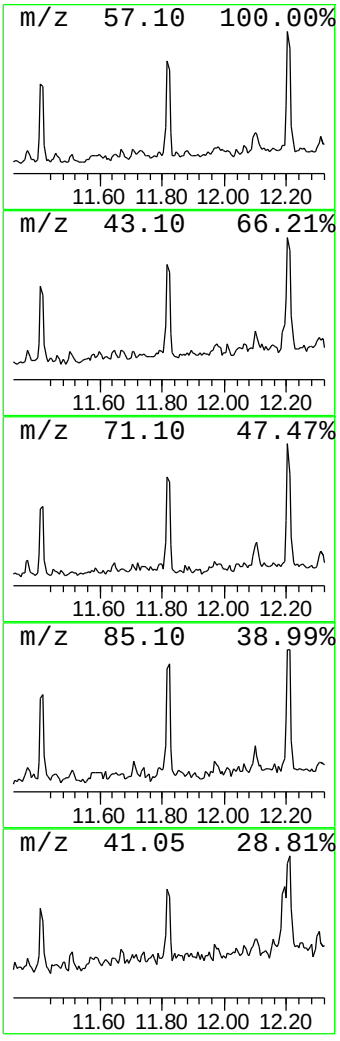
Peak Number 6 Heptacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	3.03 ng	94554	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Pentadecane	212	C15H32	000629-62-9	80
3	Triacontane	422	C30H62	000638-68-6	72
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	72





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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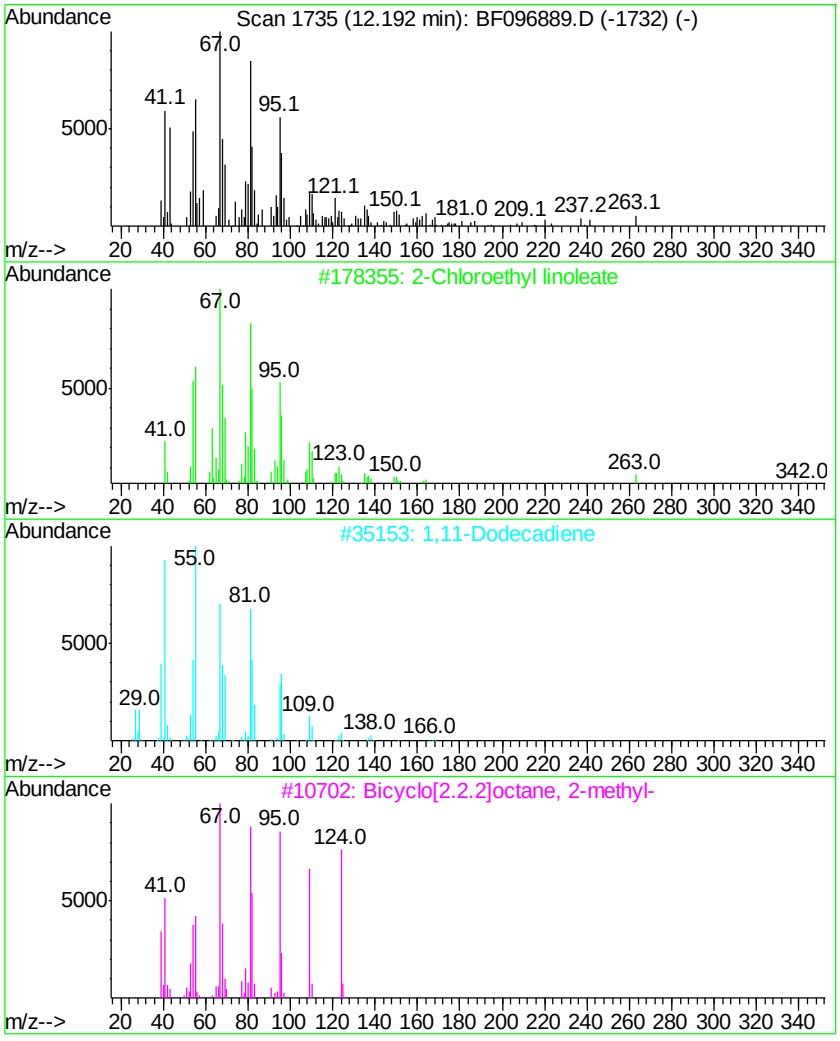
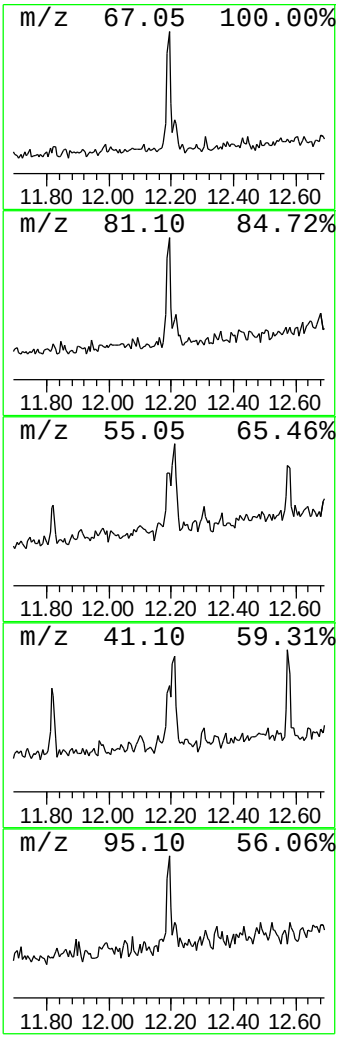
Peak Number 7 2-Chloroethyl linoleate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	3.21 ng	100113	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94
2	1,11-Dodecadiene	166	C12H22	005876-87-9	91
3	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	86
4	8-Hexadecyne	222	C16H30	019781-86-3	80
5	7-Hexadecyne	222	C16H30	074685-28-2	80





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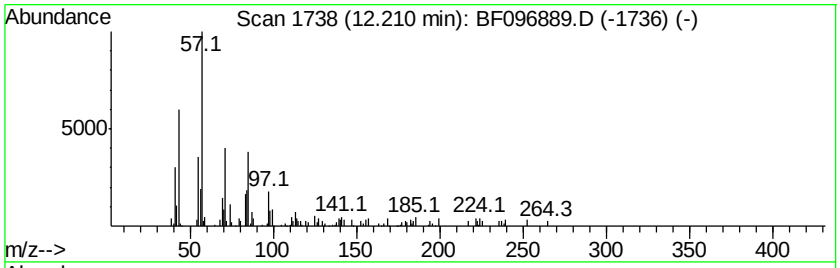
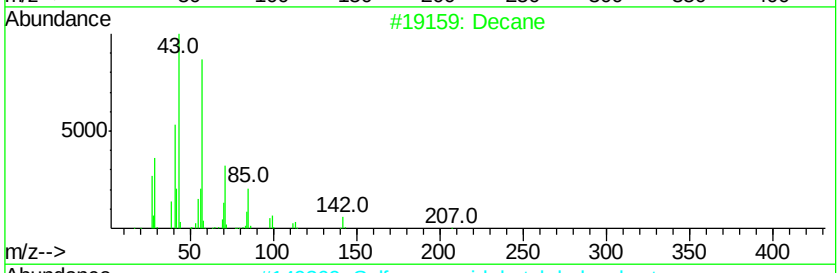
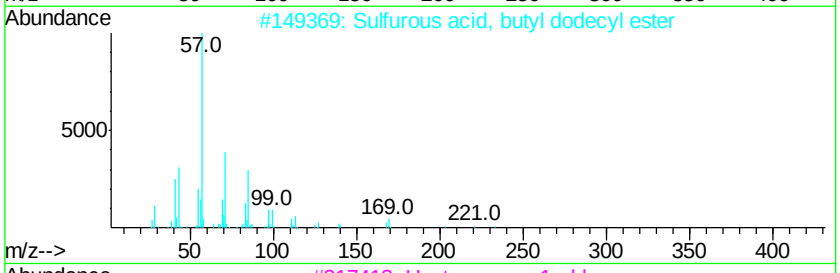
Peak Number 8 Decane Concentration Rank 10

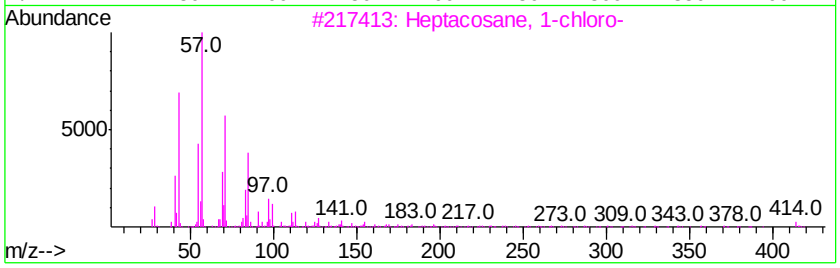
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.21	3.57 ng	111314	Phenanthrene-d10	11.10

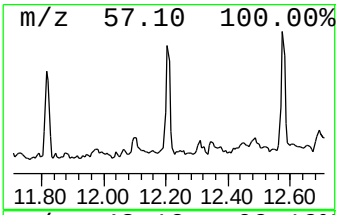
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	76
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	74
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	72
4	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72
5	Tritetracontane	605	C43H88	007098-21-7	64

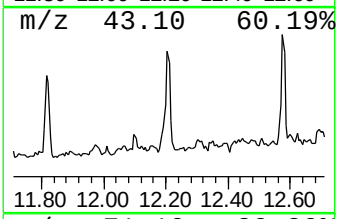


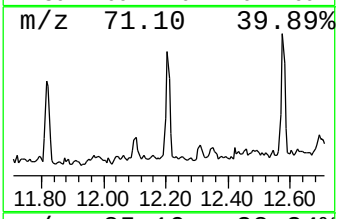


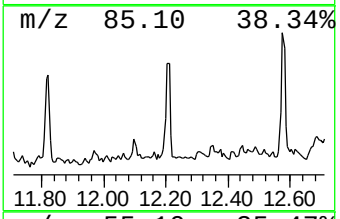


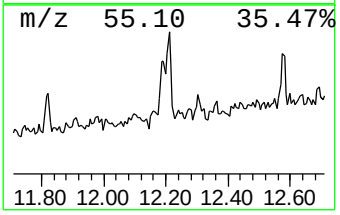












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Data Path : Z:\HPCHEM1\BNA F\DATA\BF071917\
Data File : BF096889.D
Acq On : 20 Jul 2017 00:12
Operator : SJ/JU
Sample : I4258-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

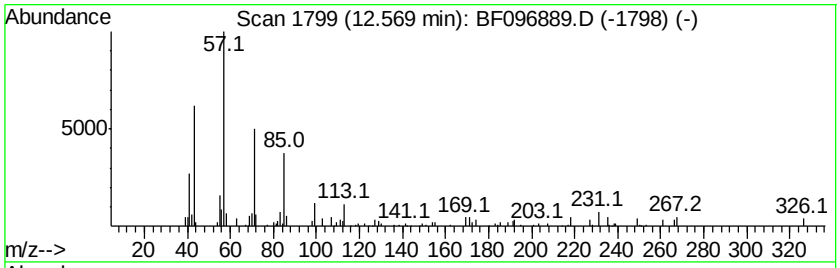
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

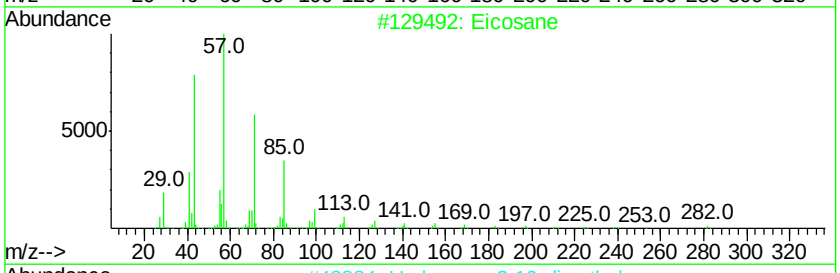
****

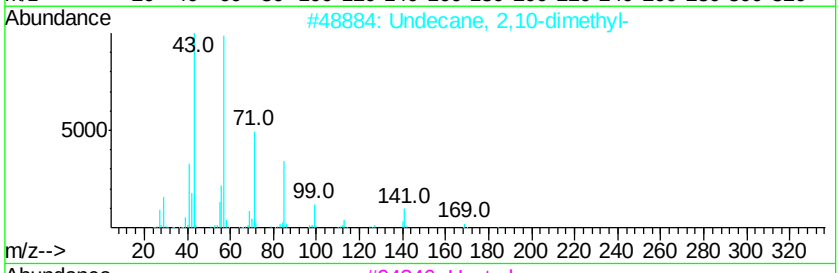
Peak Number 10 Eicosane Concentration Rank 11

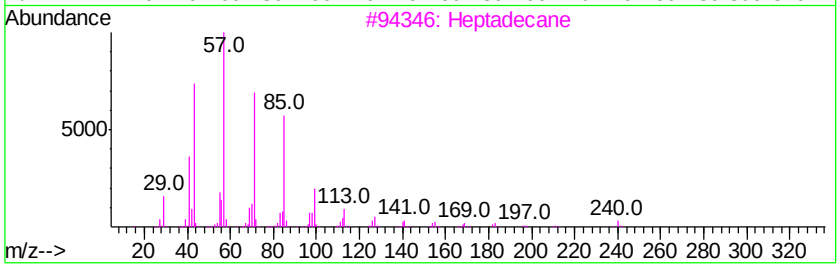
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.21 ng	81501	Chrysene-d12	13.73

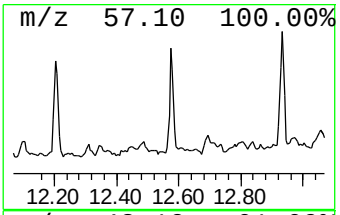
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	72
2	Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	72
3	Heptadecane	240	C17H36	000629-78-7	64
4	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64

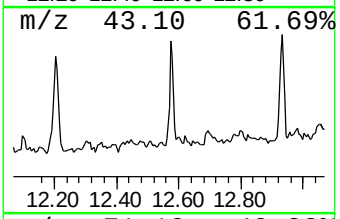


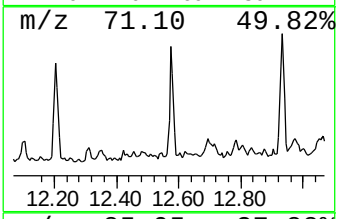


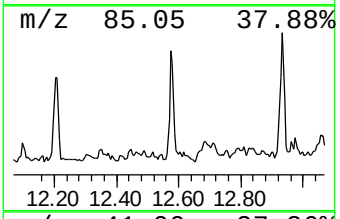


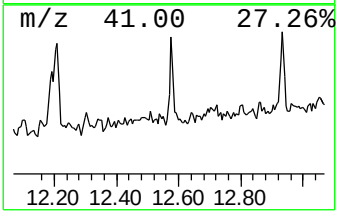












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Data File : BF096889.D
Acq On : 20 Jul 2017 00:12
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Sample : I4258-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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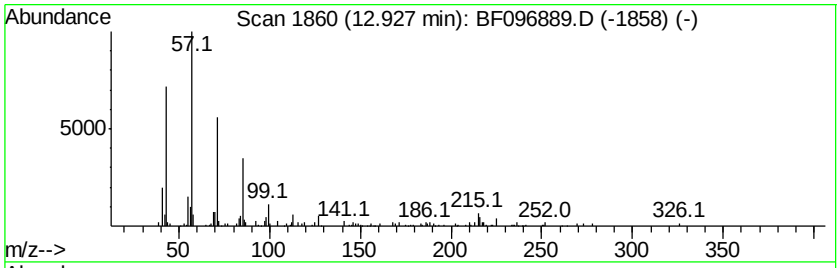
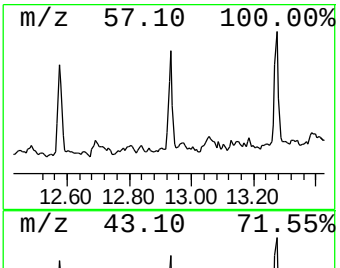
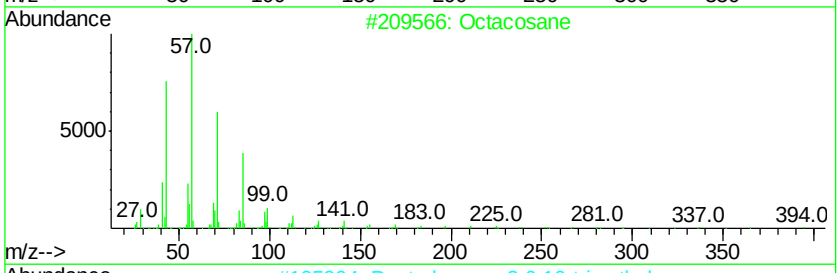
Peak Number 11 Octacosane Concentration Rank 7

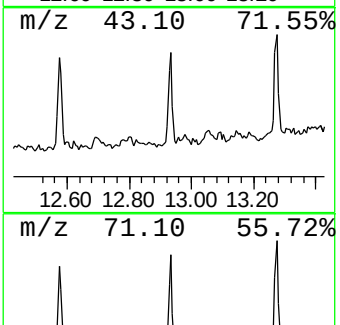
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.93	4.81 ng	122069	Chrysene-d12	13.73

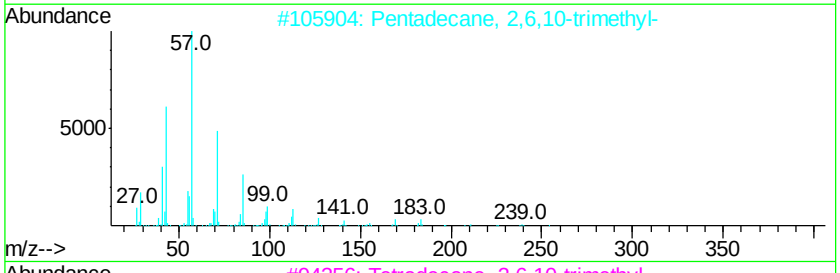
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heneicosane	296	C21H44	000629-94-7	86

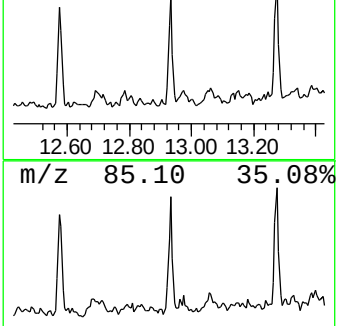


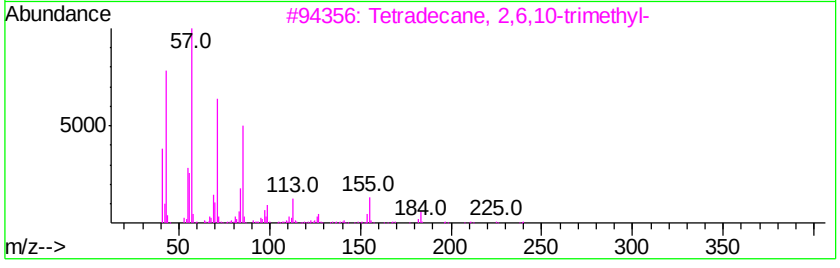


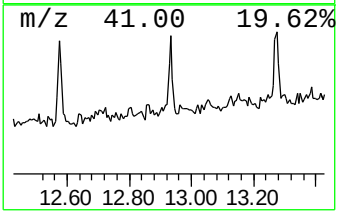












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Data File : BF096889.D
Acq On : 20 Jul 2017 00:12
Operator : SJ/JU
Sample : I4258-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

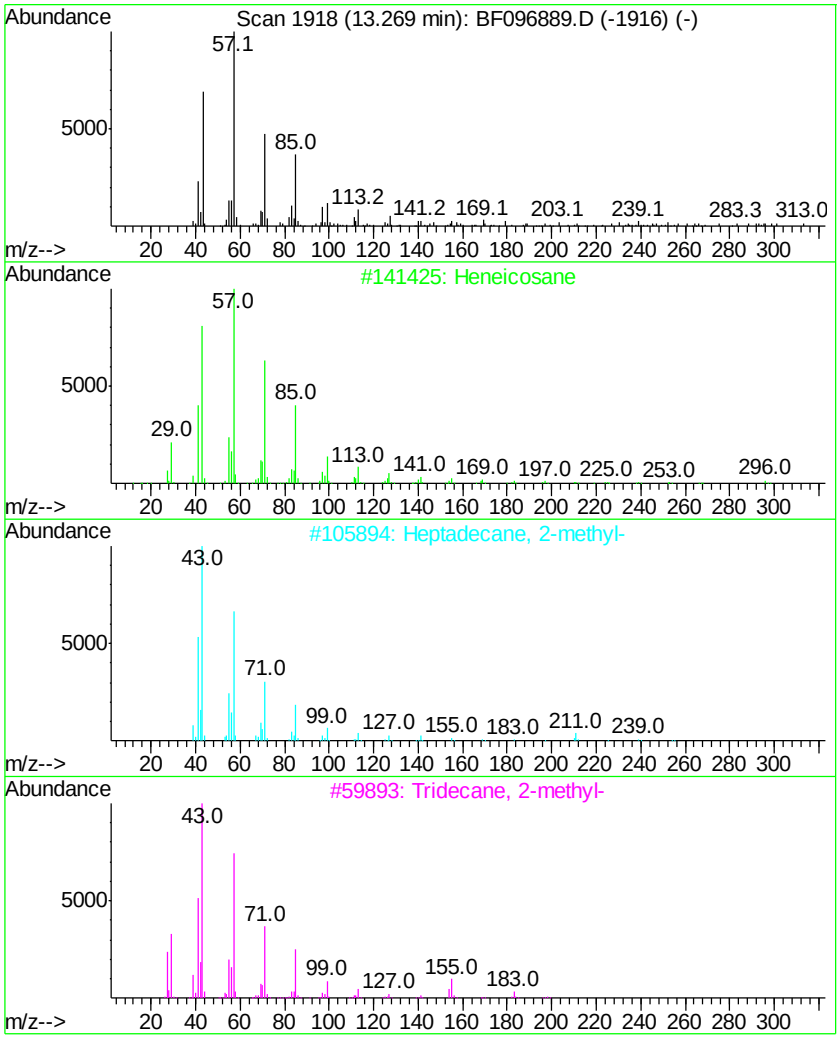
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

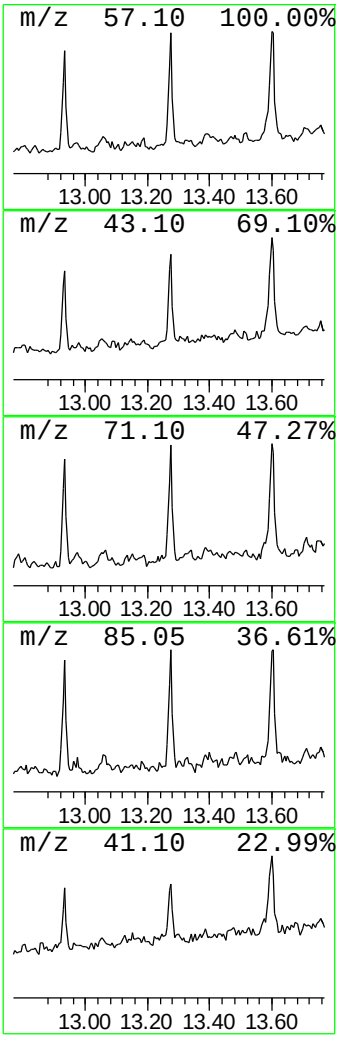
****

Peak Number 12 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	4.57 ng	116025	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
5	Tridecane, 6-methyl-	198	C14H30	013287-21-3	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071917\
Data File : BF096889.D
Acq On : 20 Jul 2017 00:12
Operator : SJ/JU
Sample : I4258-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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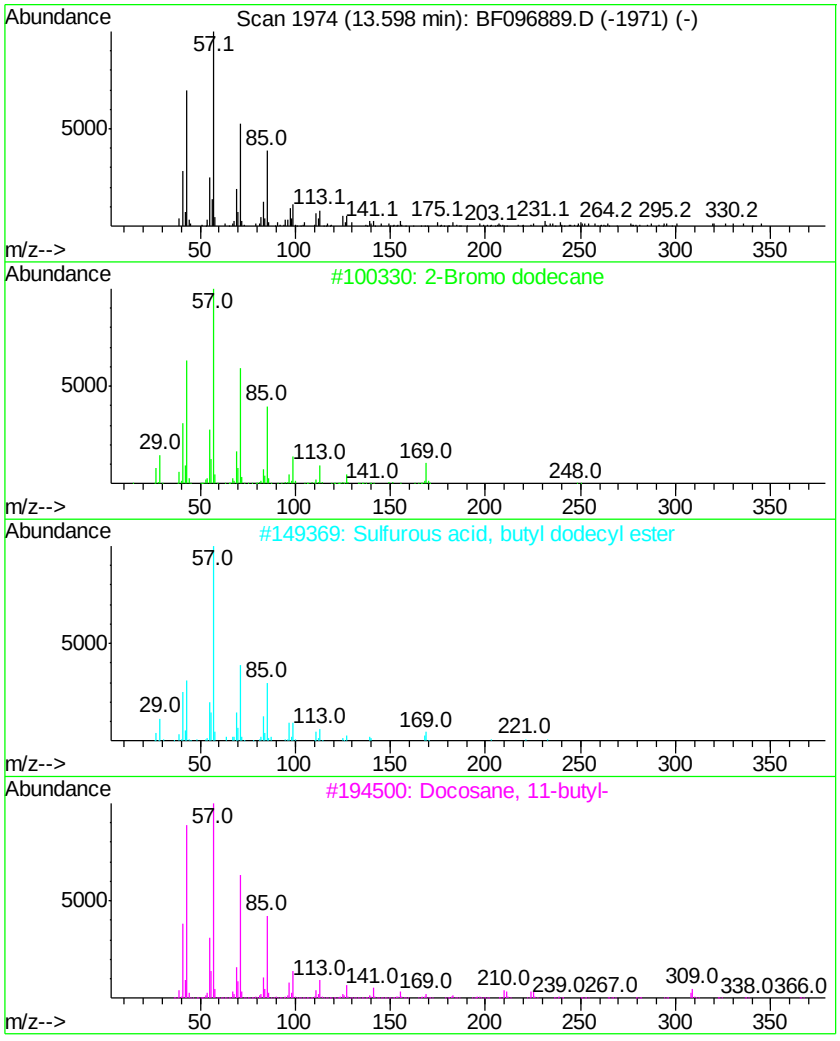
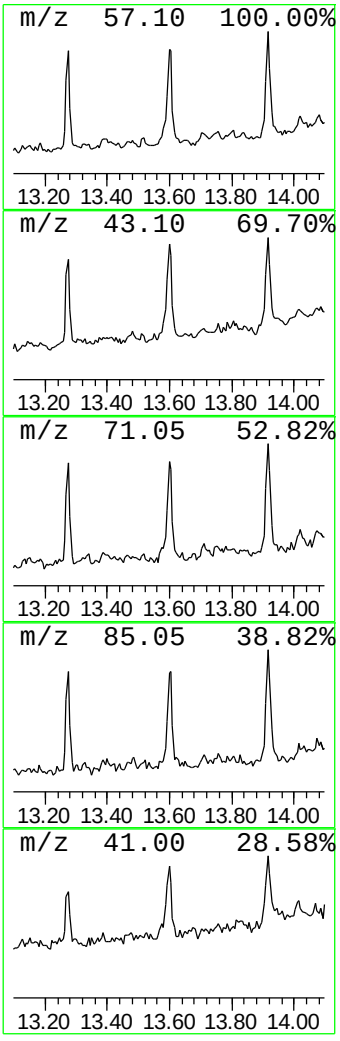
Peak Number 13 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	8.45 ng	214458	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	94
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	87
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
4	Hexacosane	366	C26H54	000630-01-3	81
5	Heptacosane	380	C27H56	000593-49-7	80





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Acq On : 20 Jul 2017 00:12
Operator : SJ/JU
Sample : I4258-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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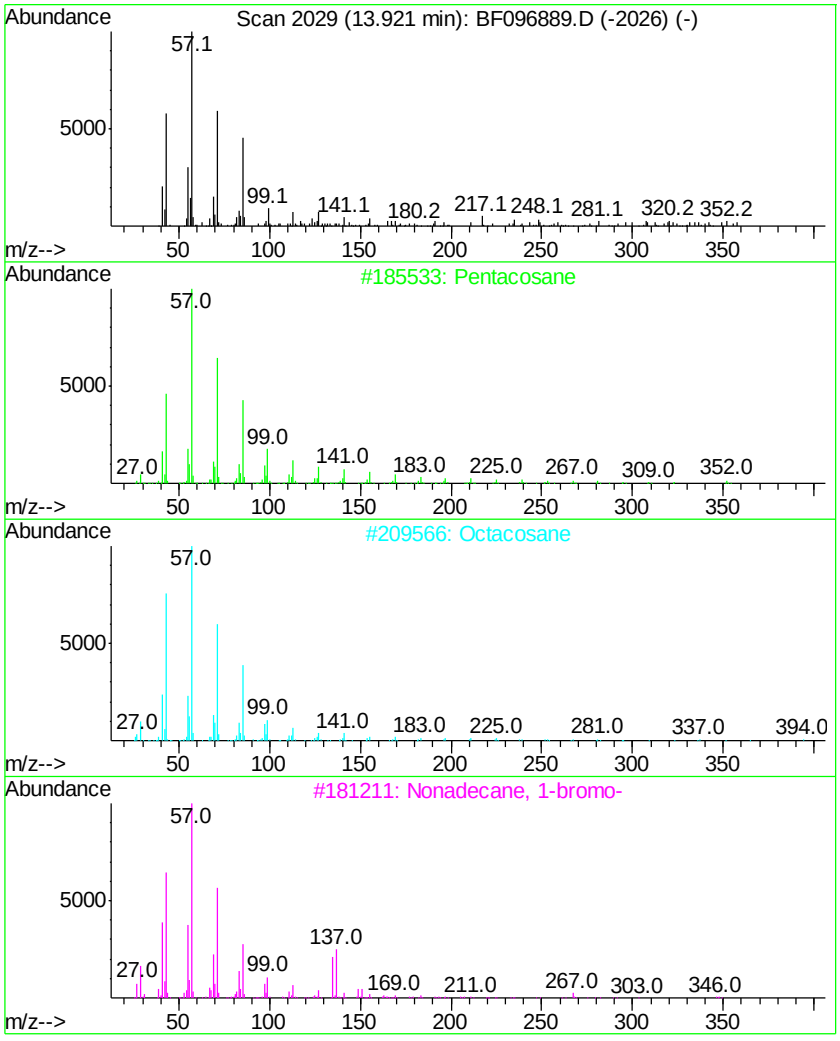
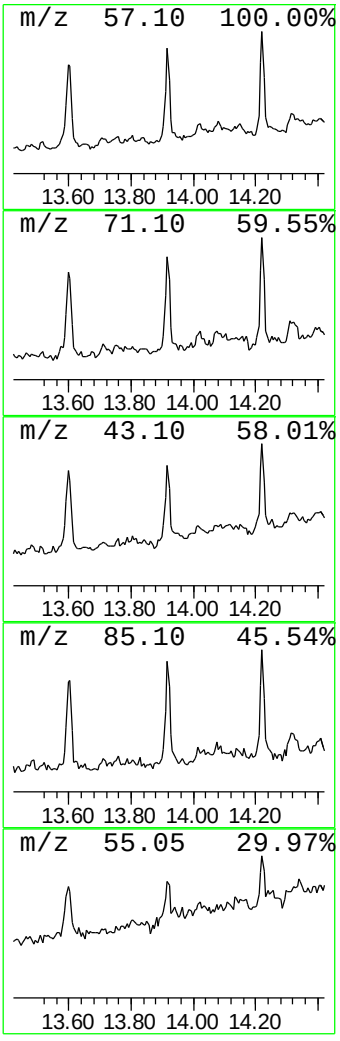
Peak Number 14 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	4.35 ng	110486	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	83
2	Octacosane	394	C28H58	000630-02-4	83
3	Nonadecane, 1-bromo-	346	C19H39Br	004434-66-6	83
4	Tridecane, 2-methyl-	198	C14H30	001560-96-9	80
5	Heptacosane	380	C27H56	000593-49-7	80





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071817-B

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TIC Library : C:\DATABASE\NIST11.L
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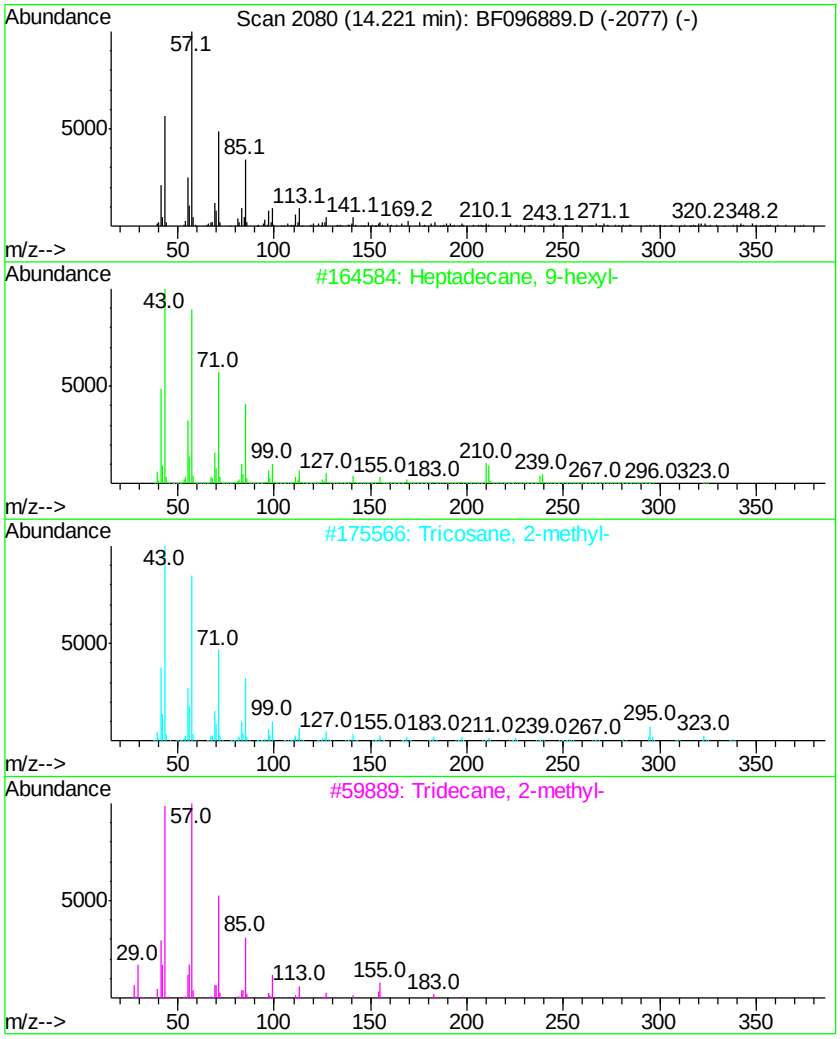
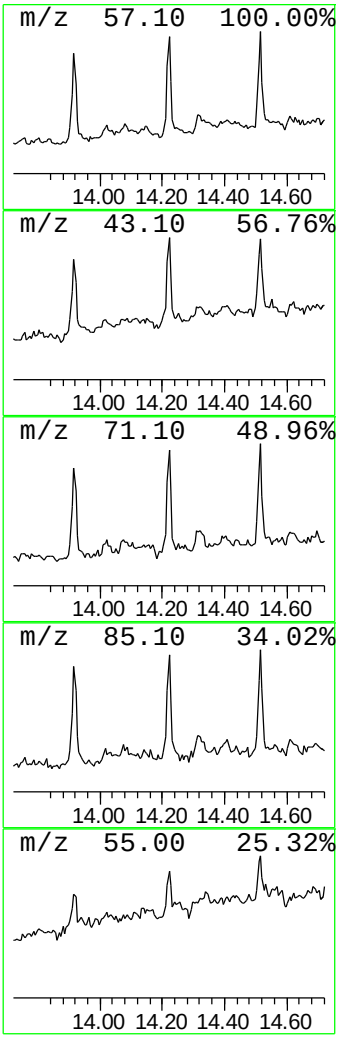
Peak Number 15 Heptadecane, 9-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	7.27 ng	184524	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91
2	Tricosane, 2-methyl-	338	C24H50	001928-30-9	91
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
4	Eicosane	282	C20H42	000112-95-8	83
5	Hexatriacontane	507	C36H74	000630-06-8	83





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Sample : I4258-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

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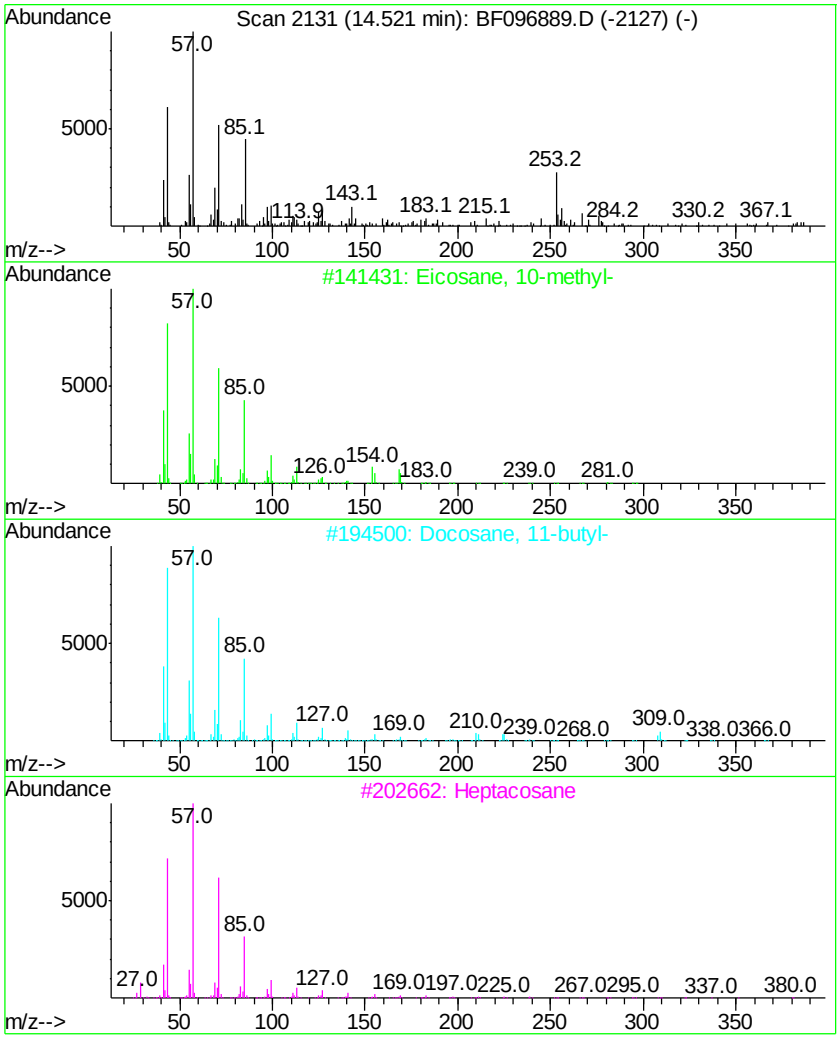
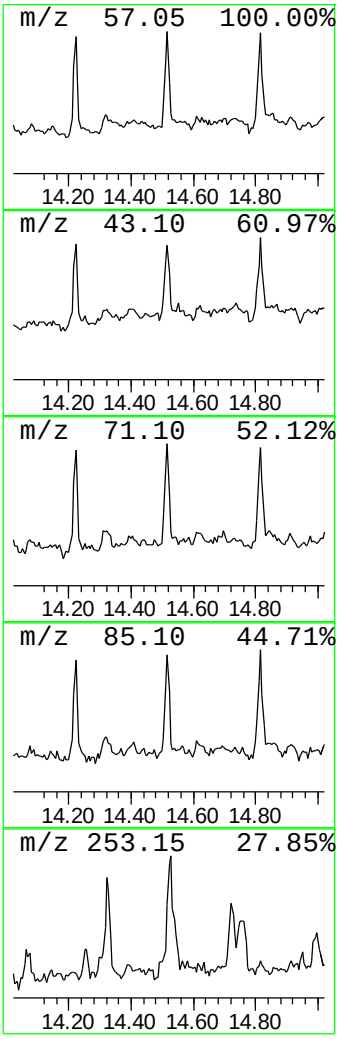
Peak Number 16 Eicosane, 10-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	15.43 ng	248067	Perylene-d12	15.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	89
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	87
3	Heptacosane	380	C27H56	000593-49-7	83
4	Hentriacontane	437	C31H64	000630-04-6	80
5	Hexadecane	226	C16H34	000544-76-3	80





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...	4.75	6.3	ng	203880	1	6.59	649126	20.0
unknown6.36	6.36	59.7	ng	1938370	1	6.59	649126	20.0
Tridecane	10.54	3.0	ng	94123	4	11.10	624287	20.0
Sulfurous acid, b...	11.42	2.8	ng	87790	4	11.10	624287	20.0
Heptacosane	11.82	3.0	ng	94554	4	11.10	624287	20.0
2-Chloroethyl lin...	12.19	3.2	ng	100113	4	11.10	624287	20.0
Decane	12.21	3.6	ng	111314	4	11.10	624287	20.0
Eicosane	12.57	3.2	ng	81501	5	13.73	507429	20.0
Octacosane	12.93	4.8	ng	122069	5	13.73	507429	20.0
Heneicosane	13.27	4.6	ng	116025	5	13.73	507429	20.0
2-Bromo dodecane	13.60	8.4	ng	214458	5	13.73	507429	20.0
Pentacosane	13.92	4.3	ng	110486	5	13.73	507429	20.0
Heptadecane, 9-he...	14.22	7.3	ng	184524	5	13.73	507429	20.0
Eicosane, 10-methyl-	14.52	15.4	ng	248067	6	15.10	321503	20.0