LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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	2.146	5	10	19	rVB	321890	420786	21.28%	1.689%
2	5.498	575	580	599	rBV	1552448	1604570	81.16%	6.441%
3	6.504	747	751	766	rBV	1845945	1683522	85.15%	6.758%
4	6.645	771	775	779	rBV	2029005	1779035	89.98%	7.141%
5	6.881	811	815	818	rBV	1212045	1059210	53.57%	4.252%
6	7.034	837	841	845	rBV	1633076	1396596	70.64%	5.606%
7	7.434	905	909	921	rBV	1211819	1091827	55.22%	4.383%
8	8.163	1029	1033	1036	rBV	1406995	1298703	65.69%	5.213%
9	9.233	1211	1215	1226	rBV	2337330	1977080	100.00%	7.936%
10	9.622	1278	1281	1287	rBV	198850	184737	9.34%	0.742%
11	9.916	1327	1331	1345	rVB	1831254	1527407	77.26%	6.131%
12	10.698	1461	1464	1476	rBV	1010735	1060317	53.63%	4.256%
13	10.822	1482	1485	1494	rVB3	28433	47503	2.40%	0.191%
14	11.298	1564	1566	1572	rVB3	24443	23818	1.20%	0.096%
15	11.398	1580	1583	1586	rBV	1383299	1325968	67.07%	5.323%
16	11.422	1586	1587	1591	rVB	101762	72905	3.69%	0.293%
17	11.692	1630	1633	1636	rBV	34355	28207	1.43%	0.113%
18	11.792	1647	1650	1652	rBV	30040	24823	1.26%	0.100%
19	11.927	1666	1673	1685	rBV2	420196	595505	30.12%	2.390%
20	12.016	1685	1688	1690	rVV2	27749	29055	1.47%	0.117%
21	12.098	1700	1702	1707	rVB2	35038	29958	1.52%	0.120%
22	12.380	1748	1750	1755	rBV5	17163	23959	1.21%	0.096%
23	12.451	1759	1762	1764	rBV	28840	30777	1.56%	0.124%
24	12.474	1764	1766	1768	rVV	135713	131106	6.63%	0.526%
25	12.498	1768	1770	1775	rVB2	152892	135667	6.86%	0.545%
26	12.580	1781	1784	1787	rBV3	23189	25119	1.27%	0.101%
27	12.616	1787	1790	1794	rBV	169156	166203	8.41%	0.667%
28	12.716	1802	1807	1815	rBV	760653	974259	49.28%	3.911%
29	12.839	1825	1828	1831	rBV	137139	138438	7.00%	0.556%
30	12.980	1849	1852	1856	rBV	1731709	1470292	74.37%	5.902%
31	13.168	1882	1884	1888	rVB2	38865	34198	1.73%	0.137%
32	13.216	1889	1892	1894	rBV2	44133	43401	2.20%	0.174%
33	13.886	2004	2006	2010	rVB	63019	54597	2.76%	0.219%
34	14.039	2028	2032	2035	rBV	1223569	1181244	59.75%	4.742%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.204	2057	2060	2065	rVB	81526	75843	3.84%	0.304%
36	14.510	2109	2112	2116	rVB	151613	147235	7.45%	0.591%
37	14.815	2161	2164	2168	rBV	286458	260947	13.20%	1.047%
38	15.157	2218	2222	2227	rBV	419333	491498	24.86%	1.973%
39	15.521	2279	2284	2286	rBV	942595	1309592	66.24%	5.257%
40	15.980	2358	2362	2370	rBV	352780	539379	27.28%	2.165%
41	16.492	2445	2449	2457	rVB	232774	416589	21.07%	1.672%

Sum of corrected areas: 24911875

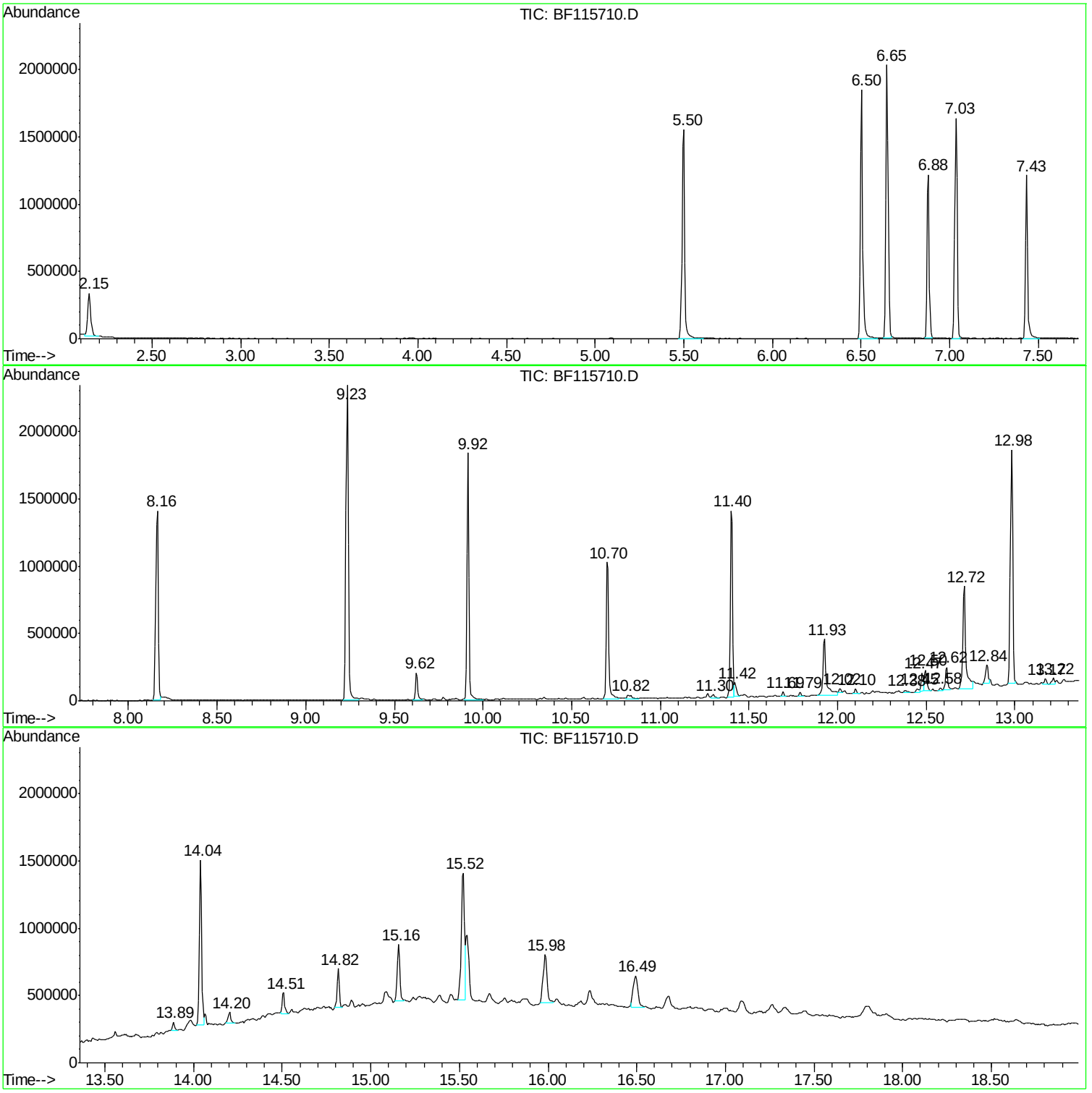
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

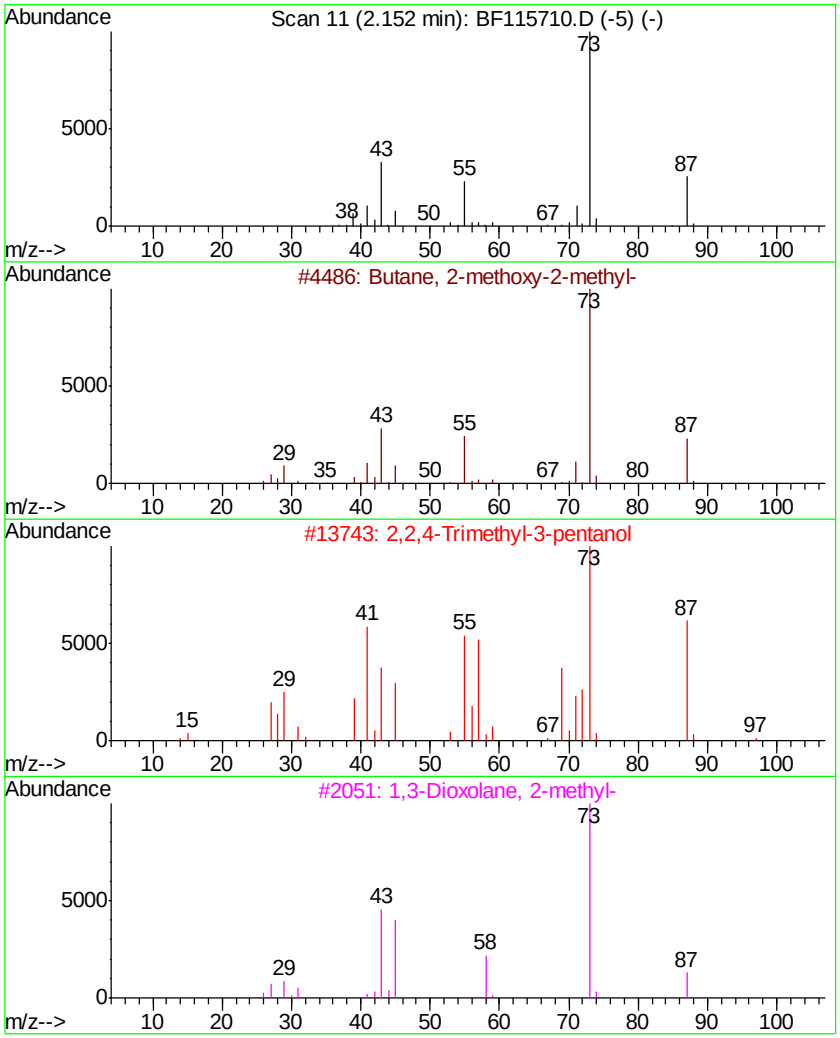
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

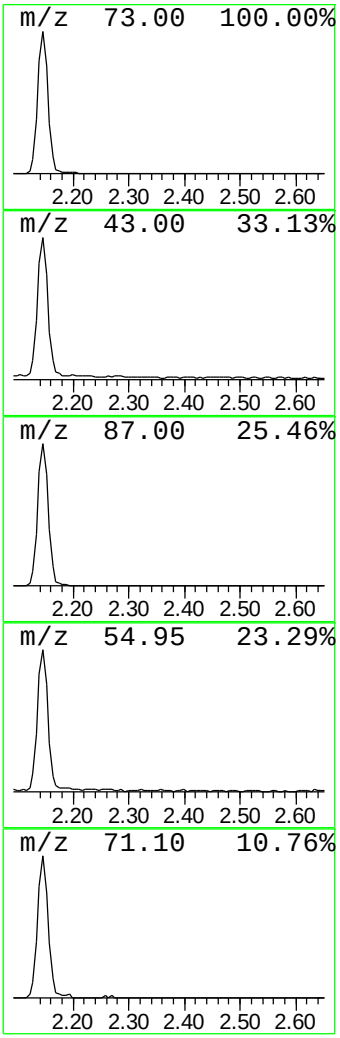
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	7.95 ng	420786	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

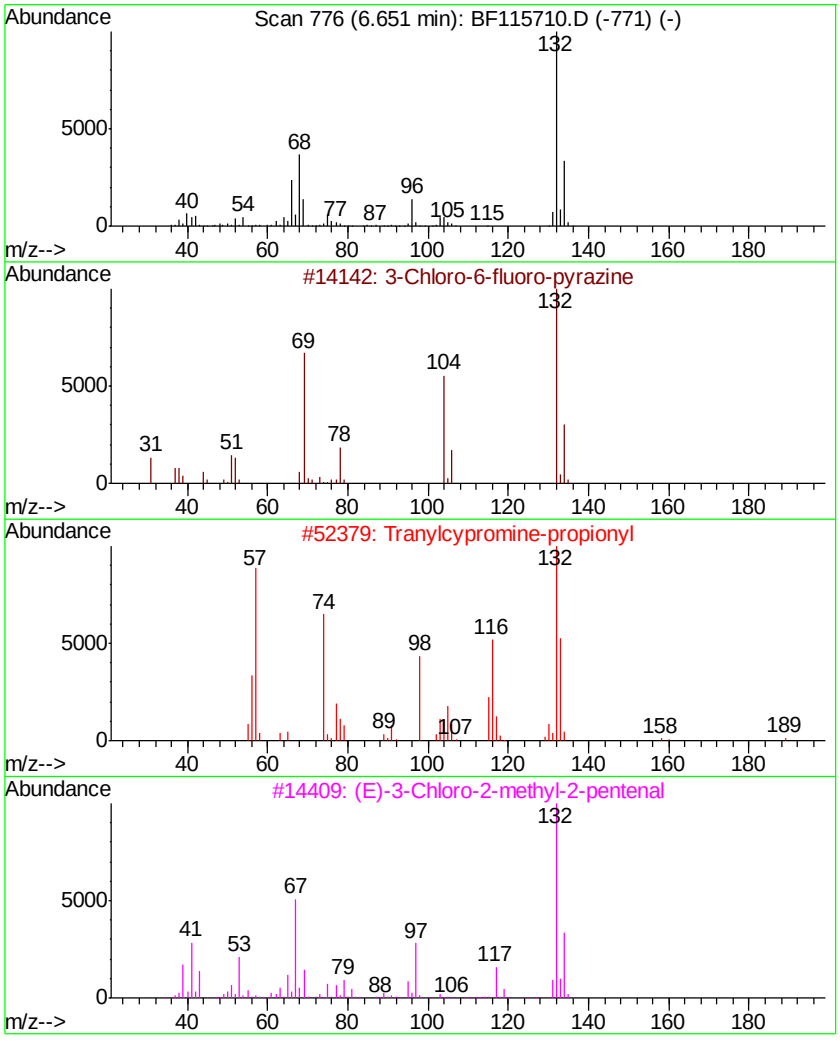
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

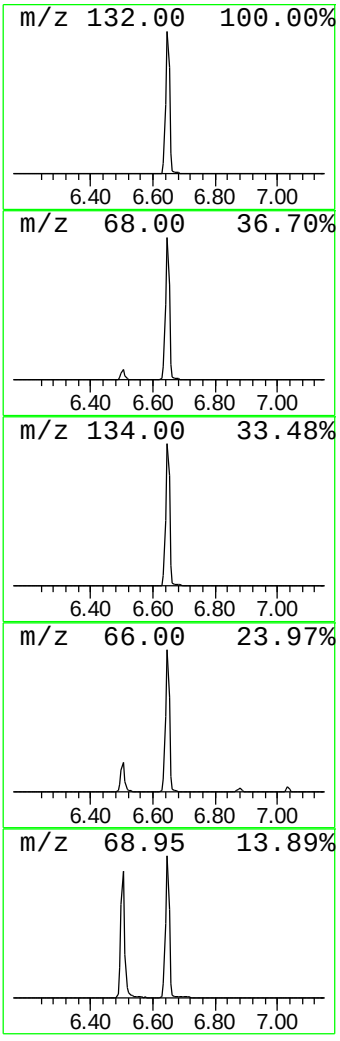
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	33.59 ng	1779040	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

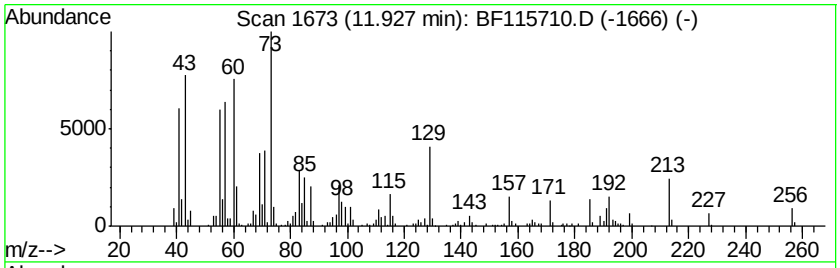
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

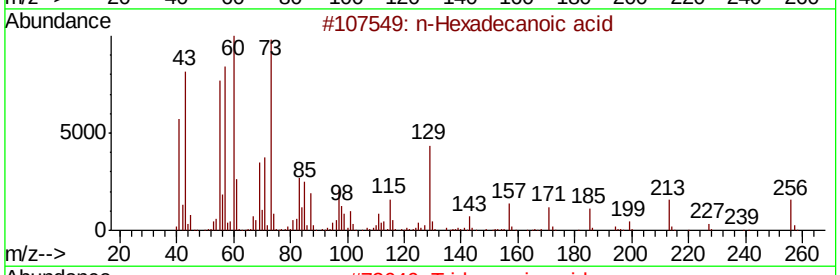
****

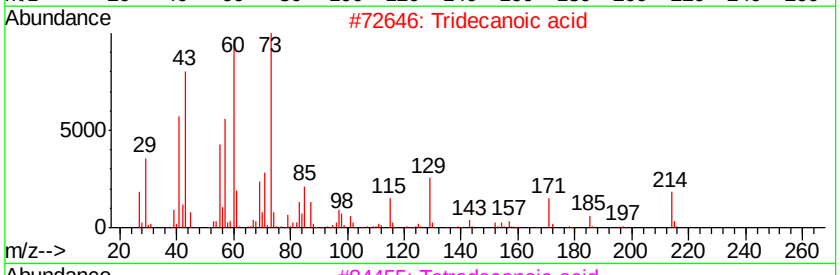
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

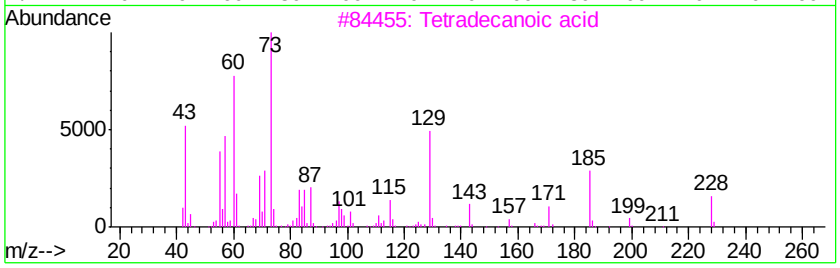
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	8.98 ng	595505	Phenanthrene-d10	11.40

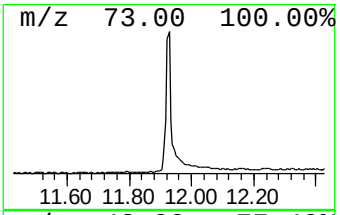
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68

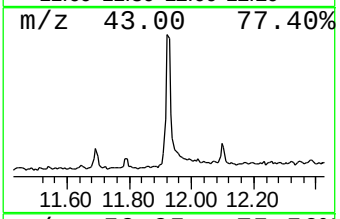


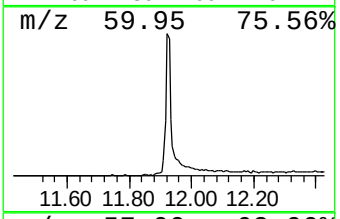


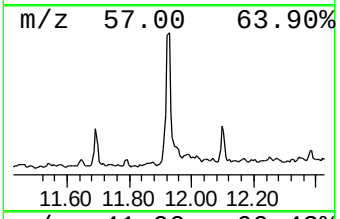


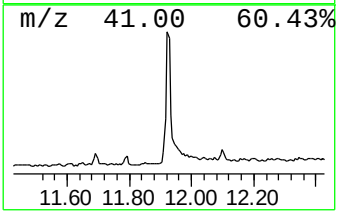












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

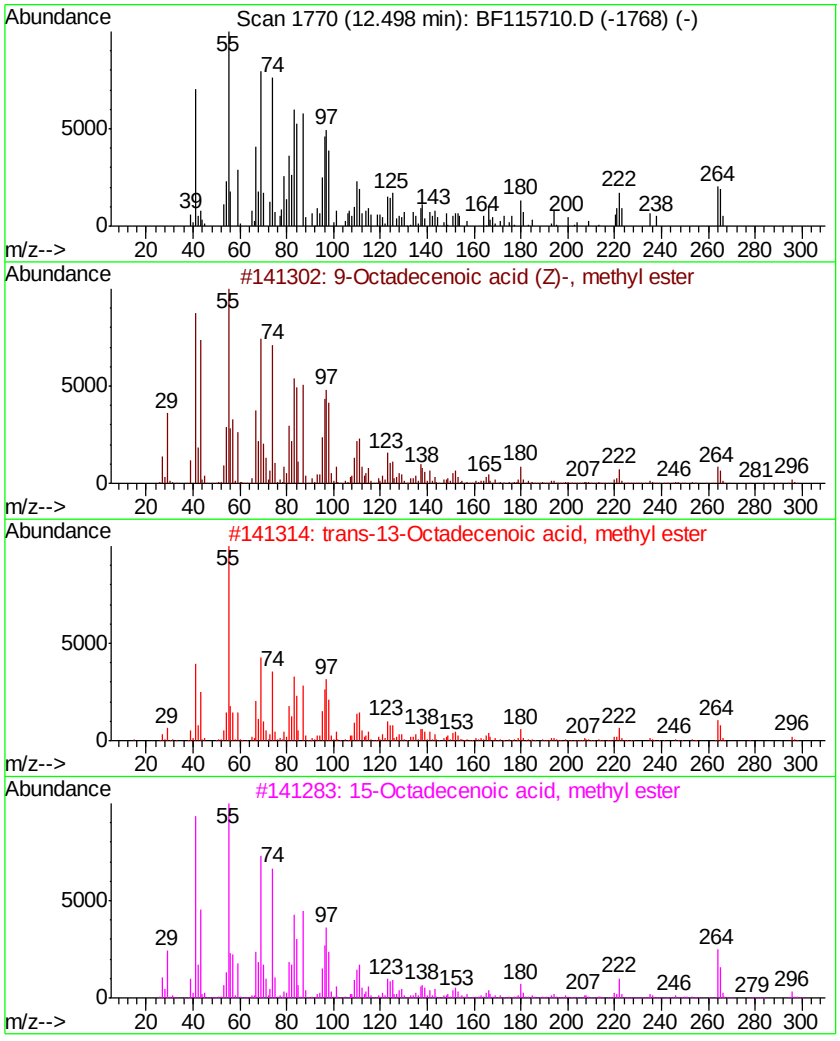
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

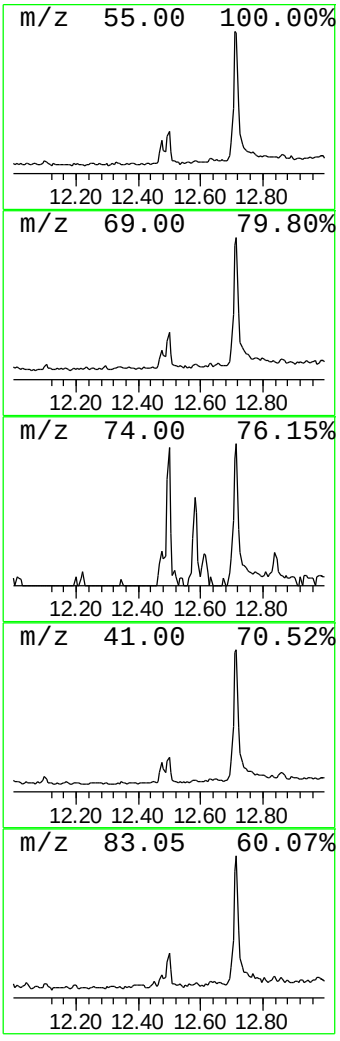
****

Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	2.05 ng	135667	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	74
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	72
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	72
5	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	72





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

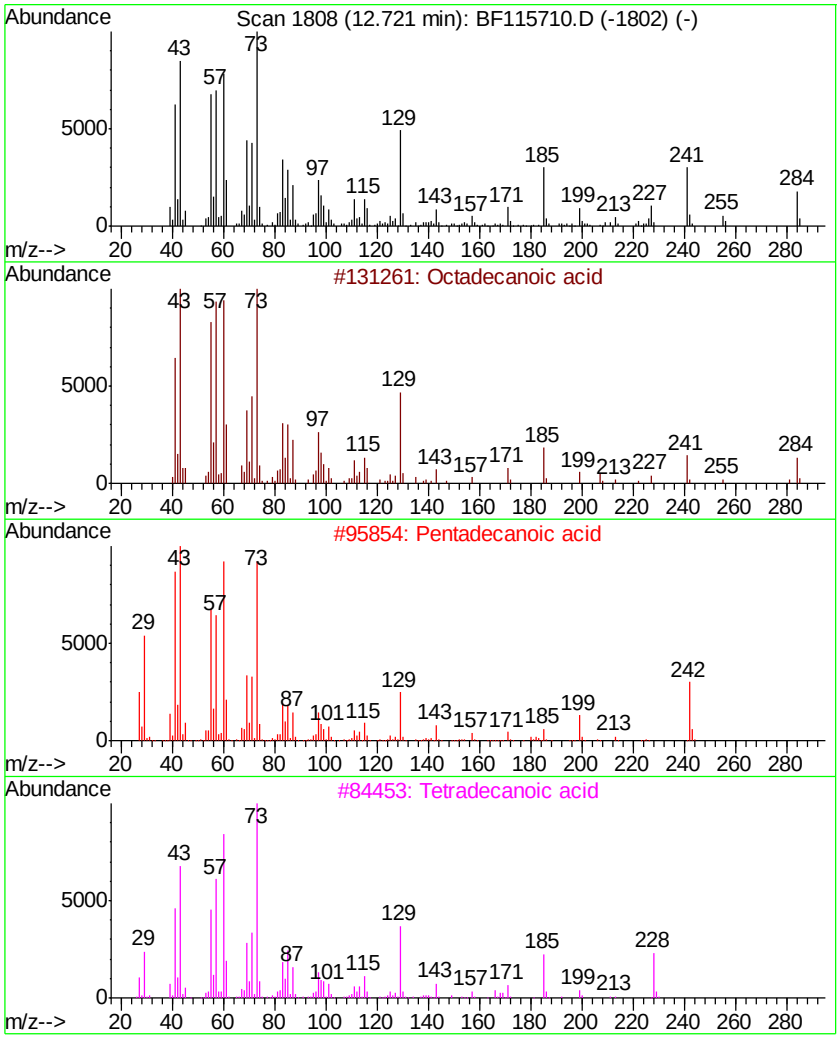
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

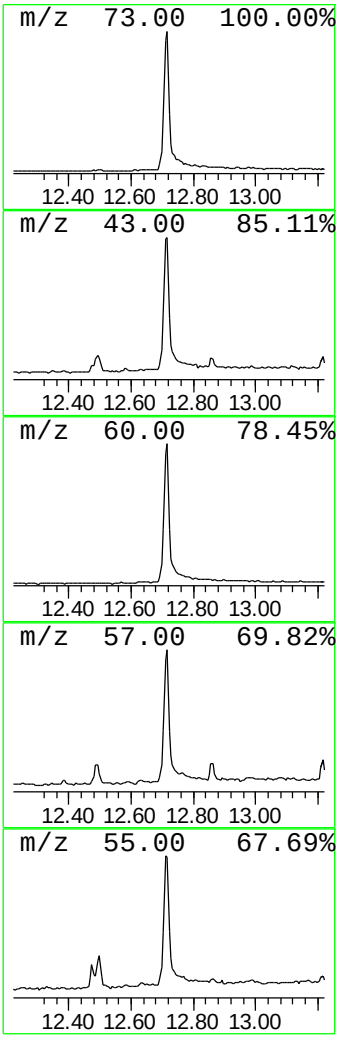
****

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	14.70 ng	974259	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Undecanoic acid	186	C11H22O2	000112-37-8	74
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74





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Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

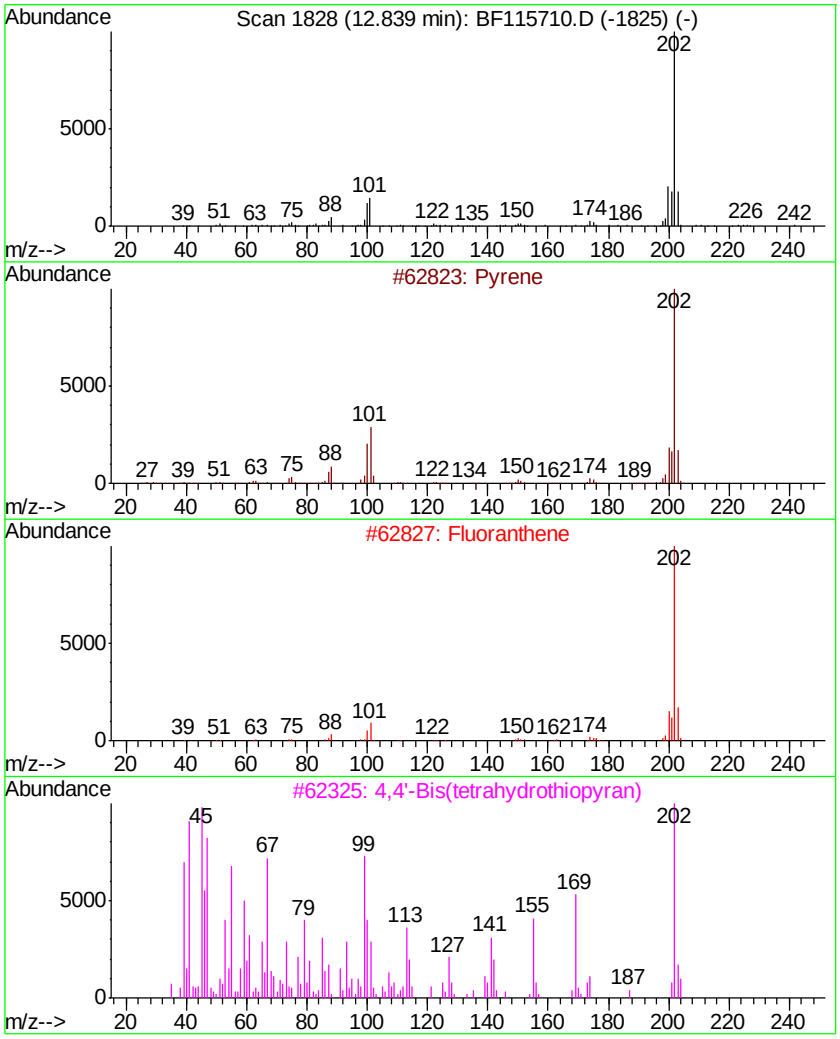
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

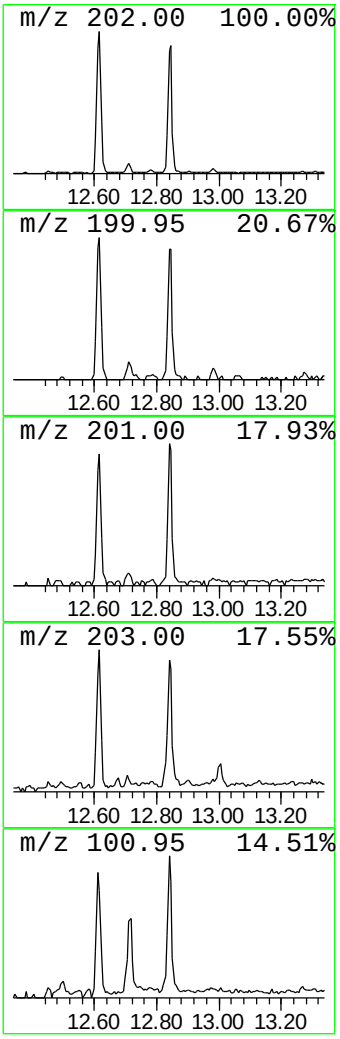
****

Peak Number 7 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.34 ng	138438	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	95
2	Fluoranthene	202	C16H10	000206-44-0	81
3	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	64
4	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	59
5	l-Leucyl-l-leucine, N,N'-dimethy...	528	C29H56N2O6	1000328-59-7	40





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

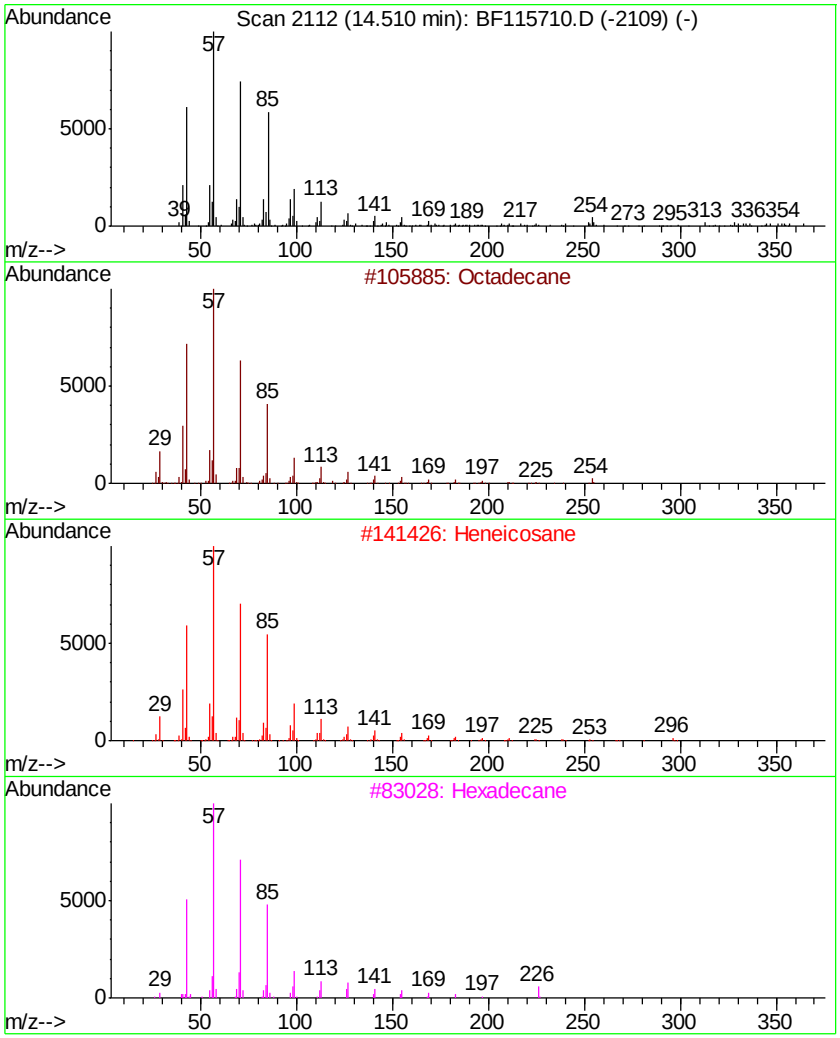
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

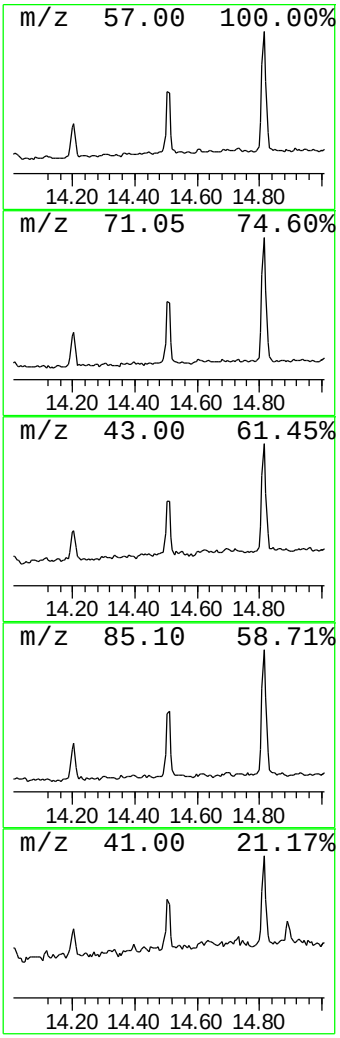
****

Peak Number 8 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.49 ng	147235	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	97
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexadecane	226	C16H34	000544-76-3	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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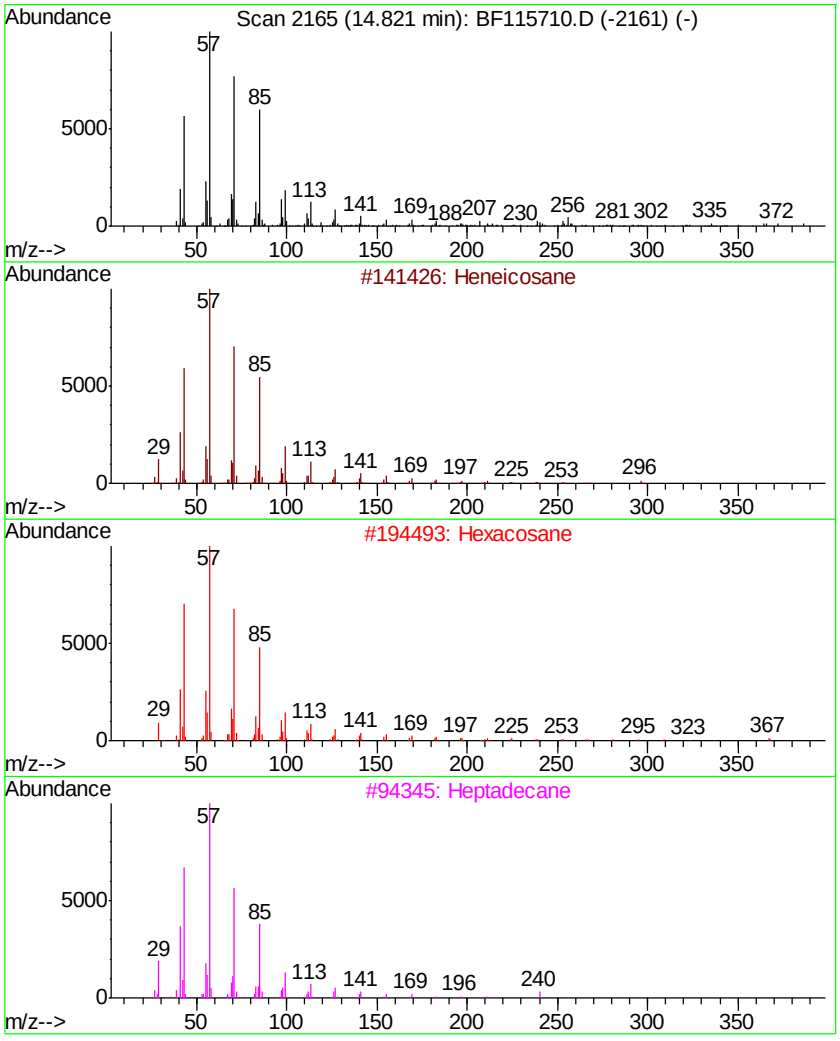
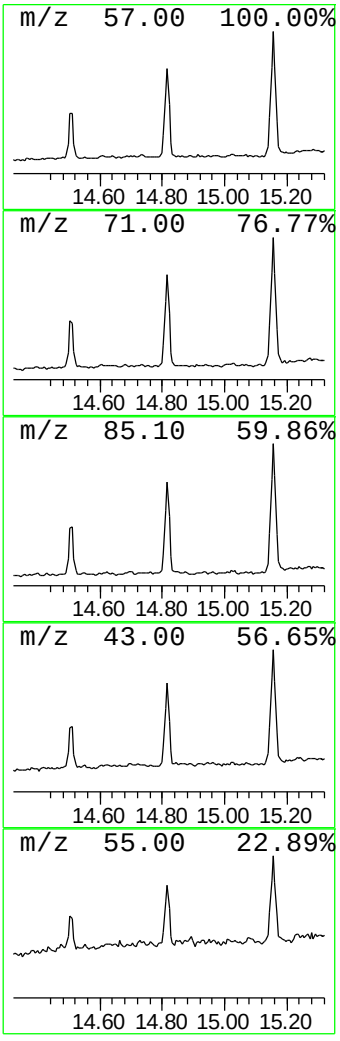
Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	3.99 ng	260947	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane	240	C17H36	000629-78-7	90
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Hexadecane	226	C16H34	000544-76-3	87





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Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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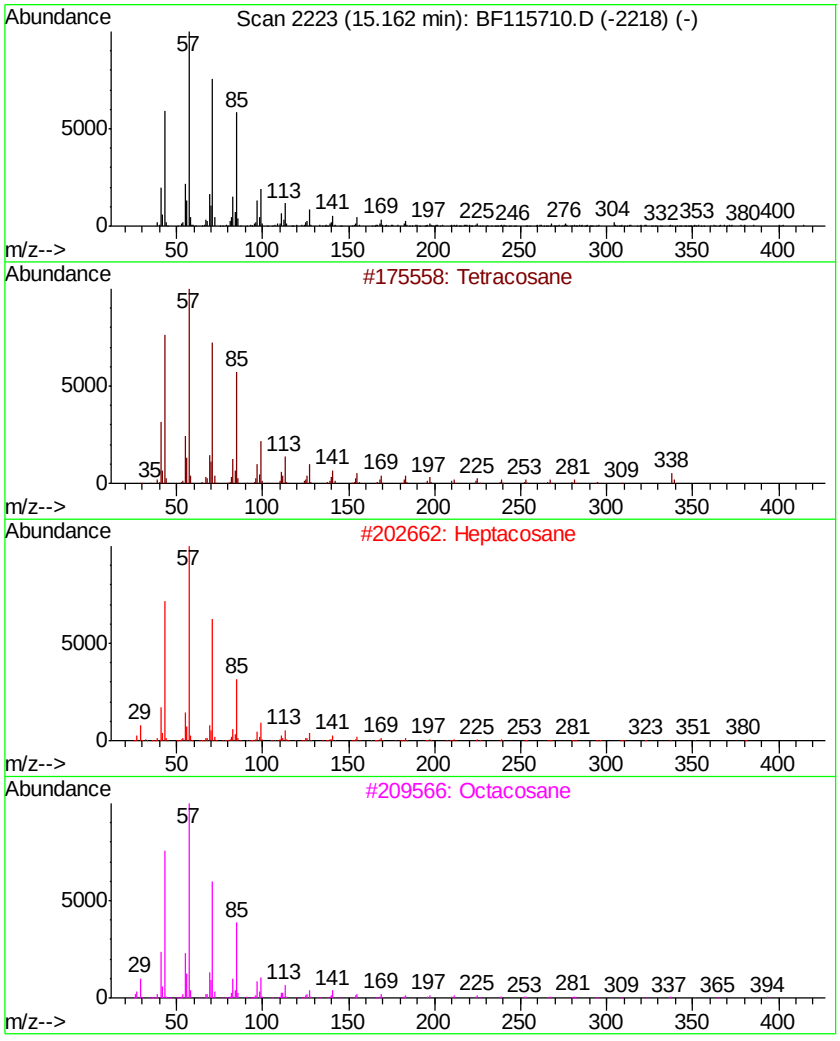
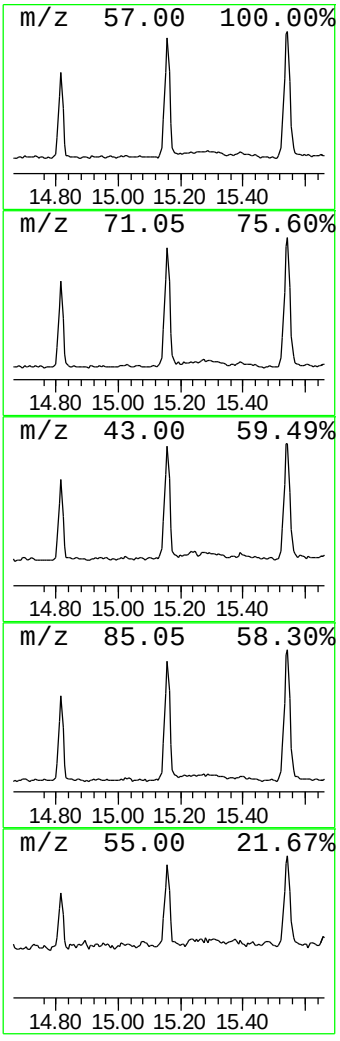
Peak Number 10 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	7.51 ng	491498	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	97
2	Heptacosane	380	C27H56	000593-49-7	94
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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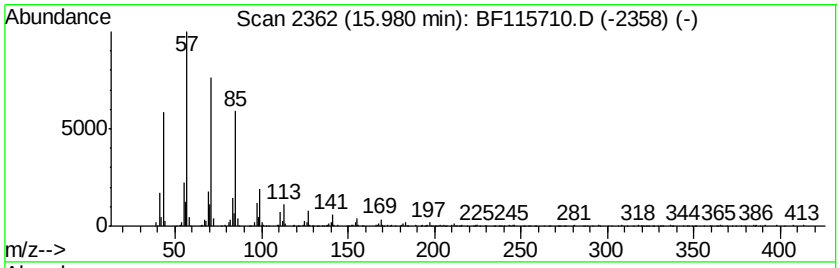
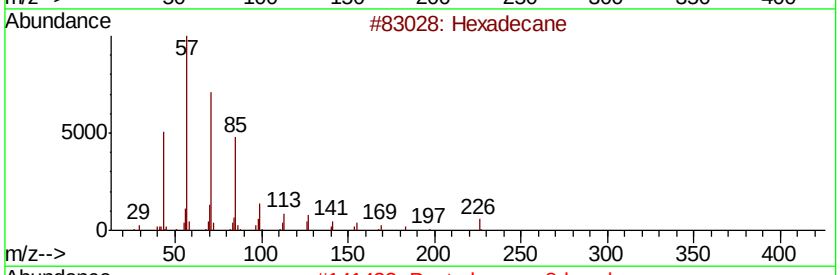
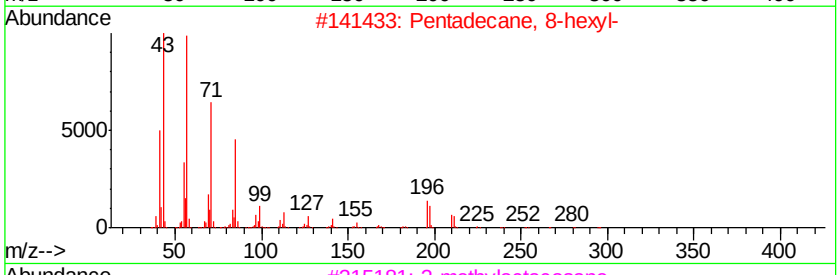
Peak Number 11 Hexadecane Concentration Rank 5

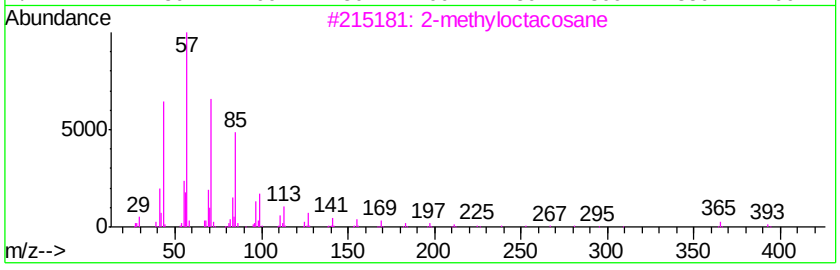
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	8.24 ng	539379	Perylene-d12	15.52

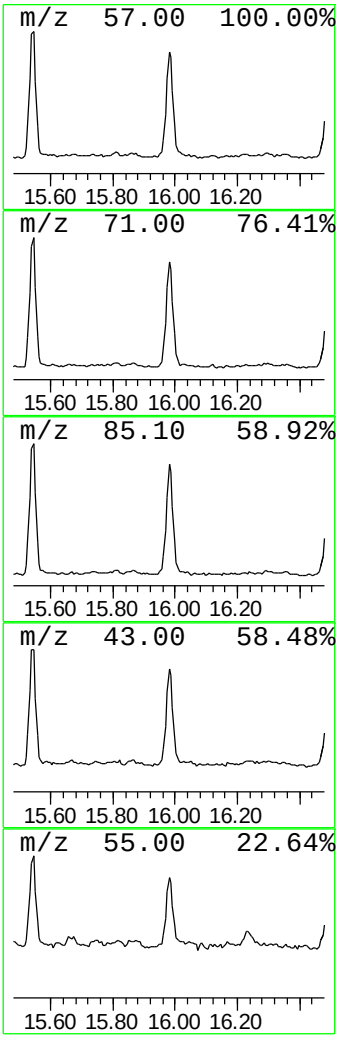
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91











Library Search Compound Report

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Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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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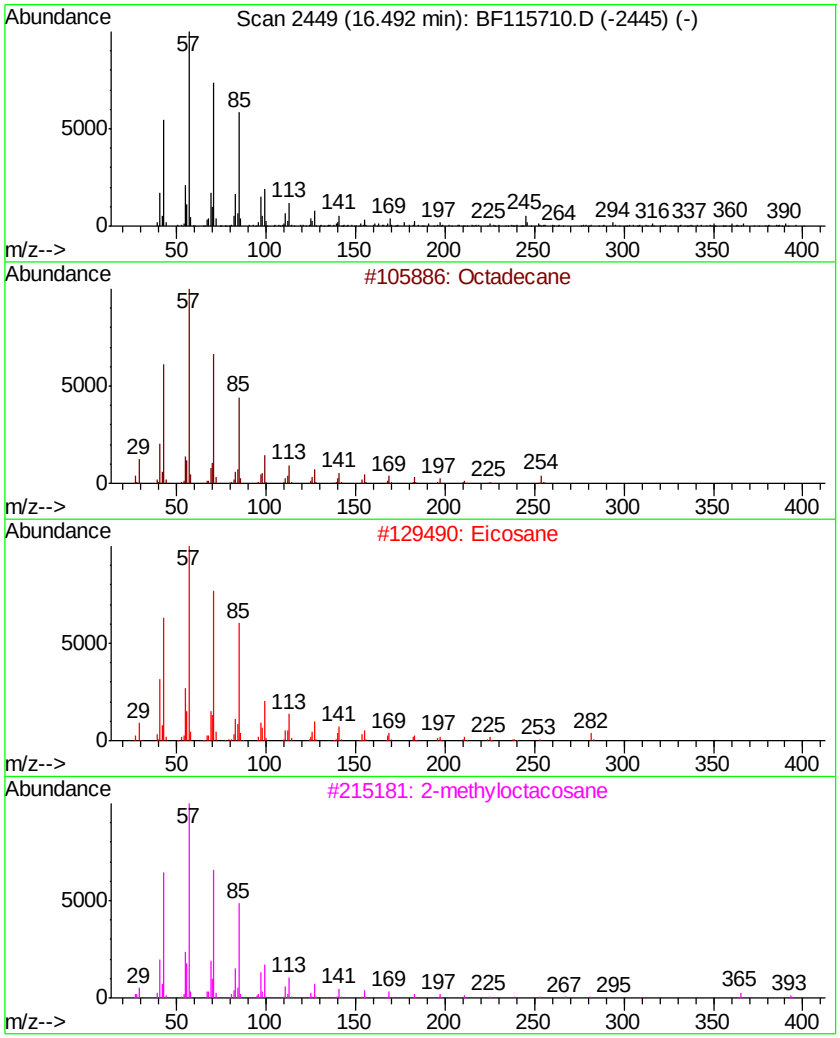
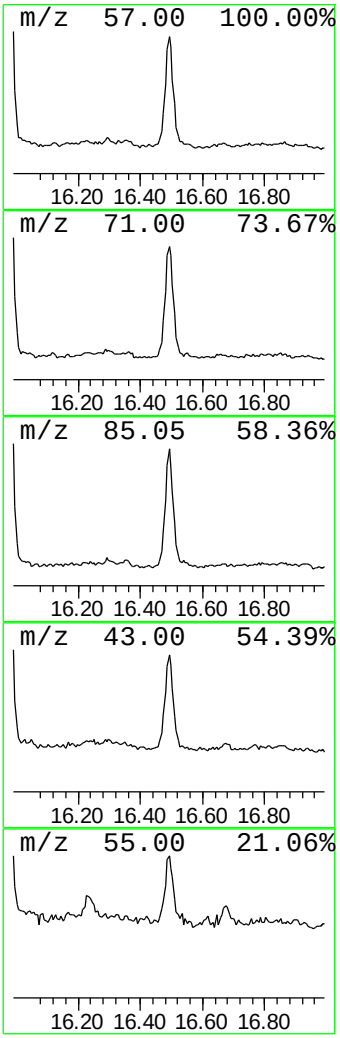
Peak Number 12 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	6.36 ng	416589	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Eicosane	282	C20H42	000112-95-8	90
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Heneicosane	296	C21H44	000629-94-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072219\
Data File : BF115710.D
Acq On : 22 Jul 2019 15:39
Operator : HP/JU
Sample : K3621-05 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OK-02-071919

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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
Butane, 2-methoxy...	2.15	8.0	ng	420786	1	6.88	1059210	20.0
unknown6.65	6.65	33.6	ng	1779040	1	6.88	1059210	20.0
n-Hexadecanoic acid	11.93	9.0	ng	595505	4	11.40	1325970	20.0
9-Octadecenoic ac...	12.50	2.0	ng	135667	4	11.40	1325970	20.0
Octadecanoic acid	12.72	14.7	ng	974259	4	11.40	1325970	20.0
4,4'-Bis(tetrahyd...	12.84	2.3	ng	138438	5	14.04	1181240	20.0
Octadecane	14.51	2.5	ng	147235	5	14.04	1181240	20.0
Heneicosane	14.82	4.0	ng	260947	6	15.52	1309590	20.0
Tetracosane	15.16	7.5	ng	491498	6	15.52	1309590	20.0
Hexadecane	15.98	8.2	ng	539379	6	15.52	1309590	20.0
Eicosane	16.49	6.4	ng	416589	6	15.52	1309590	20.0