LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	496	500	516	rBV	535458	787360	23.59%	2.792%
2	5.434	565	569	588	rBV	2792203	3083244	92.38%	10.933%
3	6.451	738	742	760	rBV	2820185	3337578	100.00%	11.835%
4	6.581	760	764	771	rVB	3118673	2952136	88.45%	10.469%
5	6.810	799	803	810	rBV	1013734	929258	27.84%	3.295%
6	6.963	825	829	844	rBV	2388674	2283366	68.41%	8.097%
7	7.375	895	899	917	rBV	1674003	1905052	57.08%	6.755%
8	8.092	1017	1021	1039	rVB	1197387	1190638	35.67%	4.222%
9	9.163	1199	1203	1213	rBV	2917996	2787842	83.53%	9.886%
10	9.563	1265	1271	1277	rBV	140083	143500	4.30%	0.509%
11	9.763	1302	1305	1309	rBV	69339	65692	1.97%	0.233%
12	9.845	1316	1319	1328	rVB	1122761	1119499	33.54%	3.970%
13	10.263	1387	1390	1393	rVB	98073	76308	2.29%	0.271%
14	10.639	1451	1454	1463	rBV	1307700	1430296	42.85%	5.072%
15	10.739	1468	1471	1480	rVB	75252	85758	2.57%	0.304%
16	11.339	1569	1573	1582	rBV	1051384	1029130	30.83%	3.649%
17	11.851	1655	1660	1662	rBV2	37160	50180	1.50%	0.178%
18	11.957	1674	1678	1680	rBV2	36053	37347	1.12%	0.132%
19	12.557	1776	1780	1784	rBV	258658	227397	6.81%	0.806%
20	12.786	1813	1819	1825	rVB	226547	273095	8.18%	0.968%
21	12.921	1838	1842	1846	rBV	2163349	1925628	57.70%	6.828%
22	13.004	1852	1856	1859	rBV3	24260	41825	1.25%	0.148%
23	13.133	1877	1878	1881	rVB	57416	41263	1.24%	0.146%
24	13.480	1933	1937	1940	rBV	108489	113456	3.40%	0.402%
25	13.810	1989	1993	1997	rBV2	188323	218121	6.54%	0.773%
26	13.992	2019	2024	2027	rBV	846689	955070	28.62%	3.387%
27	14.015	2027	2028	2032	rVB	105195	66211	1.98%	0.235%
28	14.121	2043	2046	2049	rBV	145242	124332	3.73%	0.441%
29	14.427	2095	2098	2100	rBV	124873	103681	3.11%	0.368%
30	14.727	2147	2149	2153	rVB	110023	102822	3.08%	0.365%
31	15.057	2203	2205	2210	rVB	124555	135441	4.06%	0.480%
32	15.462	2270	2274	2279	rVB	467301	577563	17.30%	2.048%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

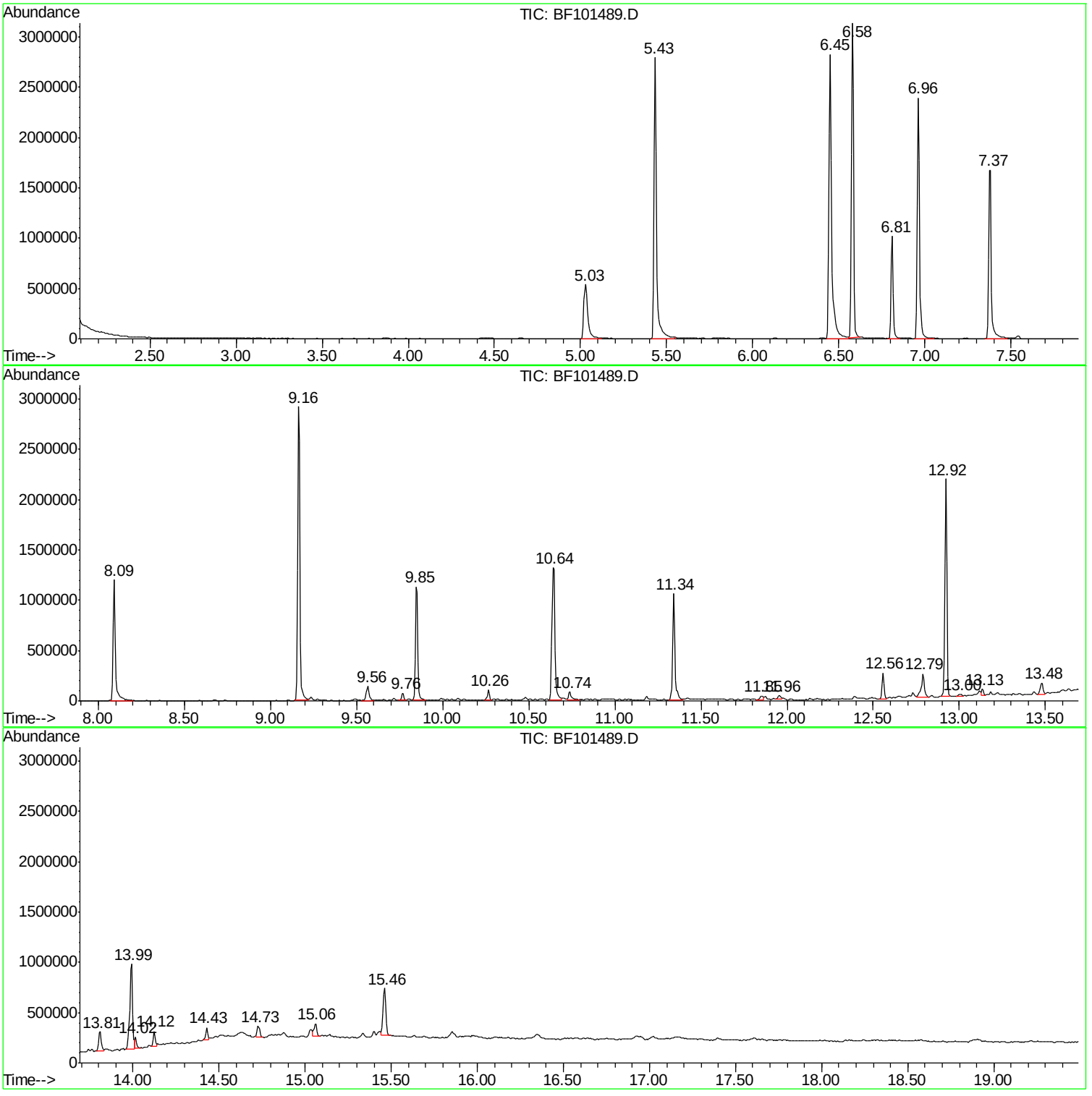
Sum of corrected areas: 28200089

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

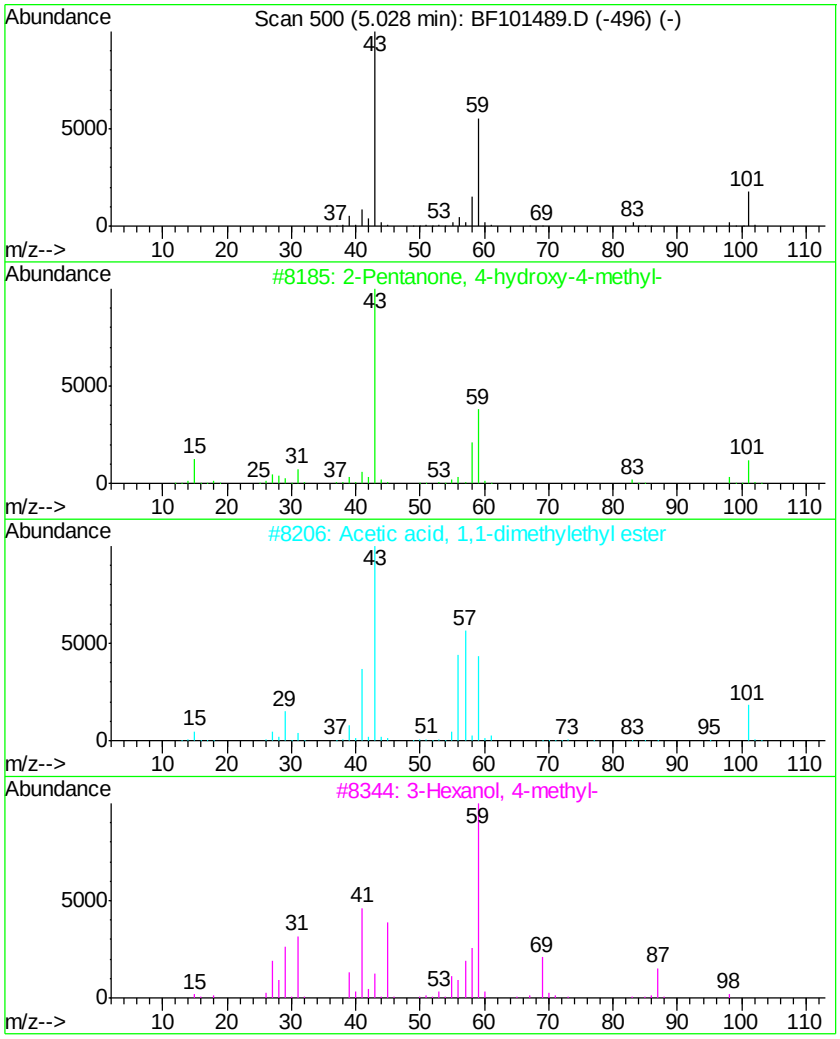
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

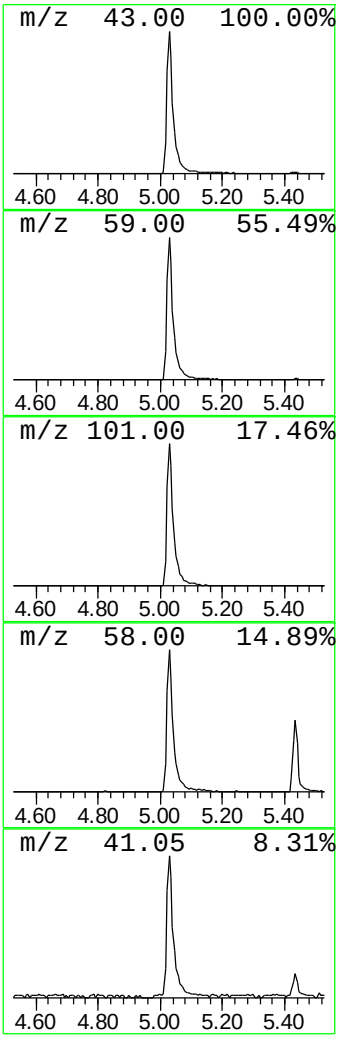
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	16.95 ng	787360	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

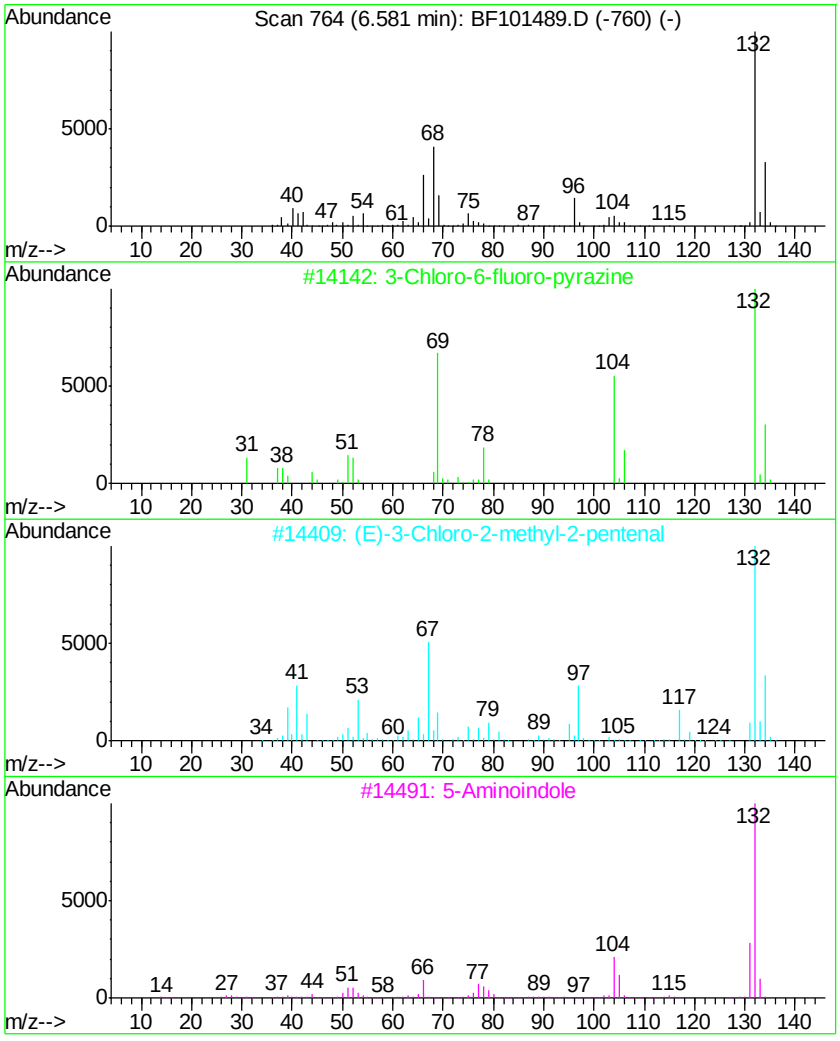
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

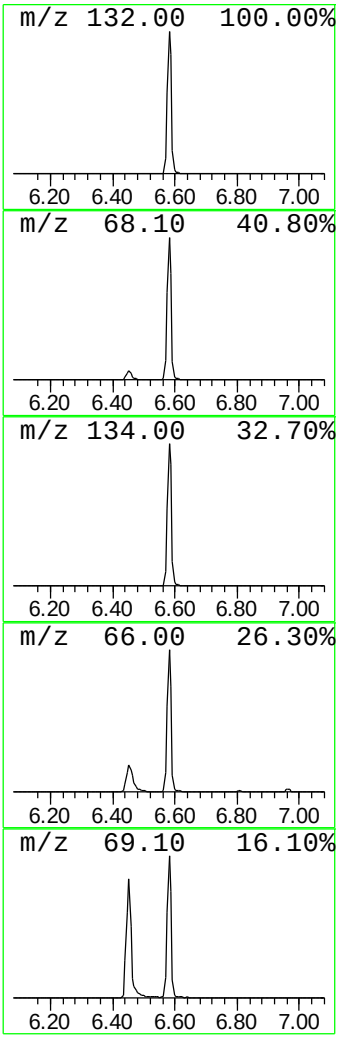
****

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	63.54 ng	2952140	1,4-Dichlorobenzene-d4	6.81

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	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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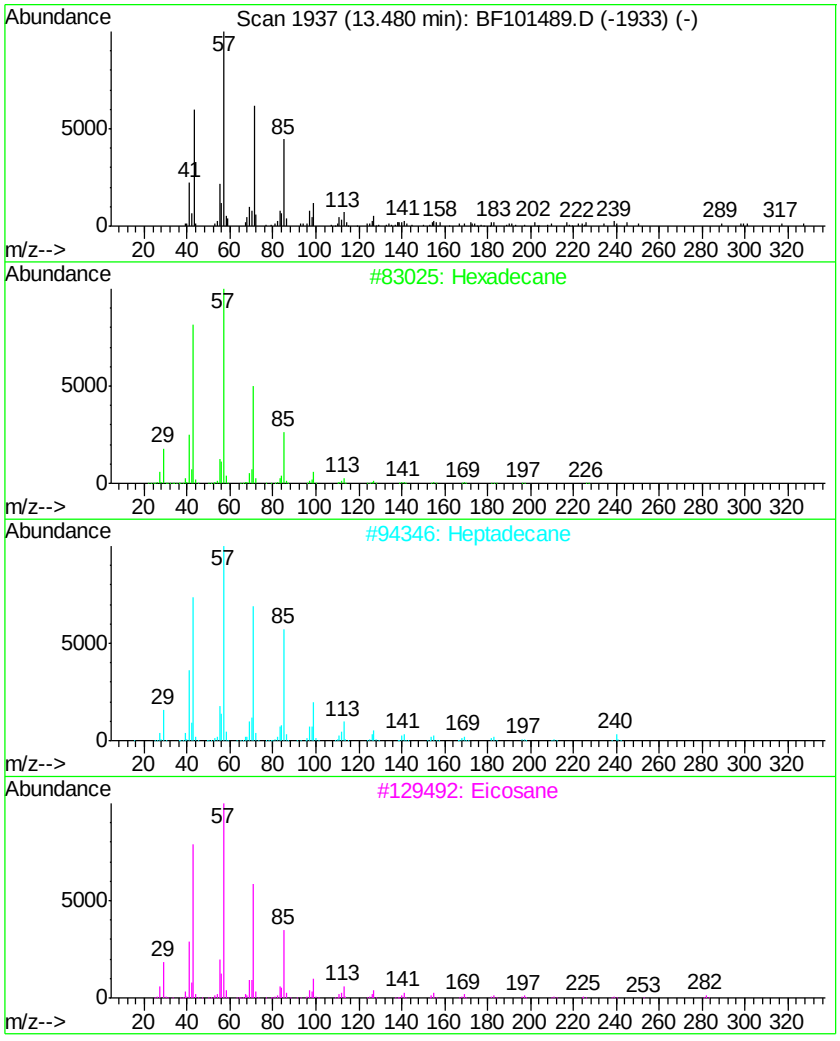
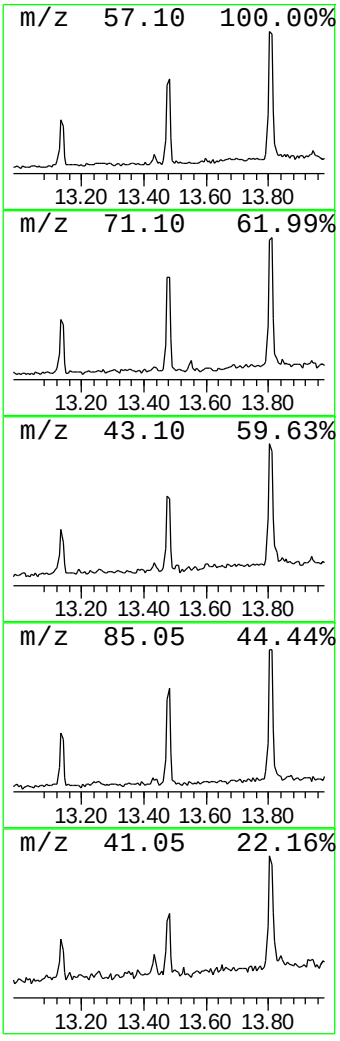
Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	2.38 ng	113456	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Heptadecane	240	C17H36	000629-78-7	95
3	Eicosane	282	C20H42	000112-95-8	83
4	Tetracosane	338	C24H50	000646-31-1	83
5	Pentadecane	212	C15H32	000629-62-9	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

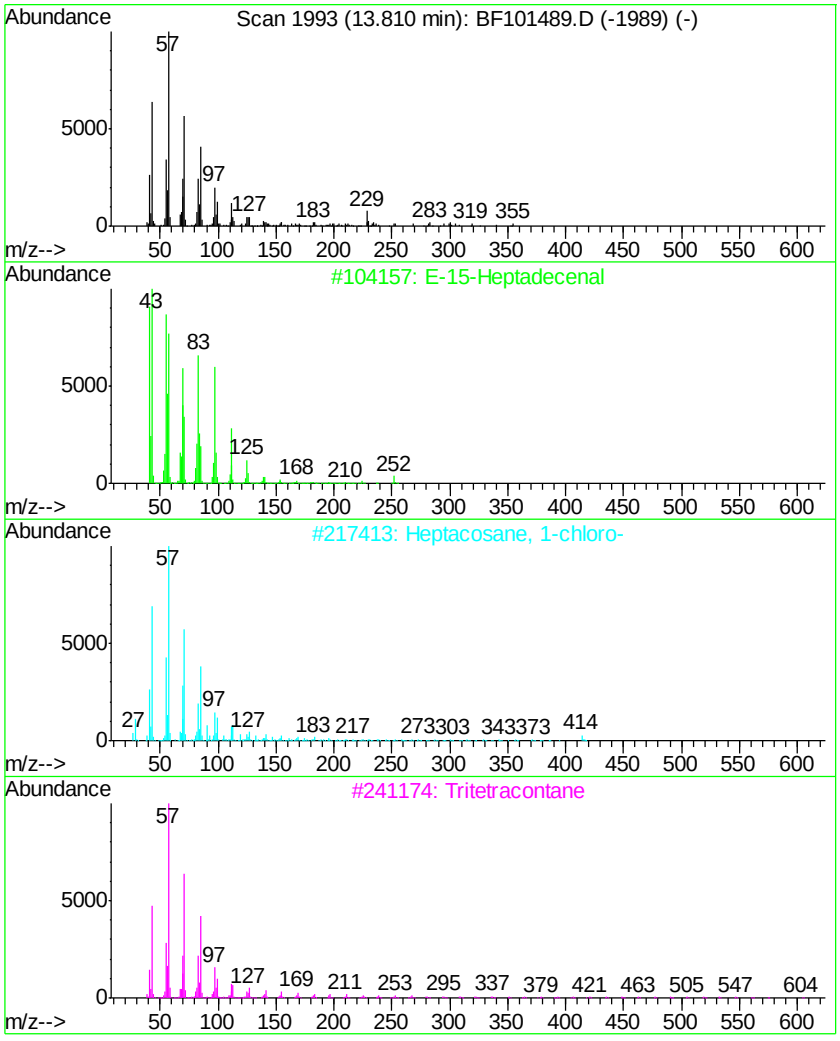
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

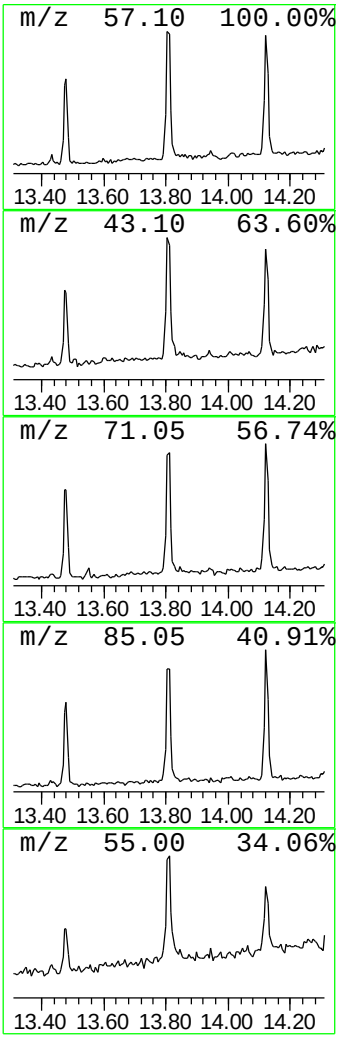
****

Peak Number 5 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	4.57 ng	218121	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	94
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
3	Tritetracontane	605	C43H88	007098-21-7	90
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	86
5	1-Pentadecene	210	C15H30	013360-61-7	80





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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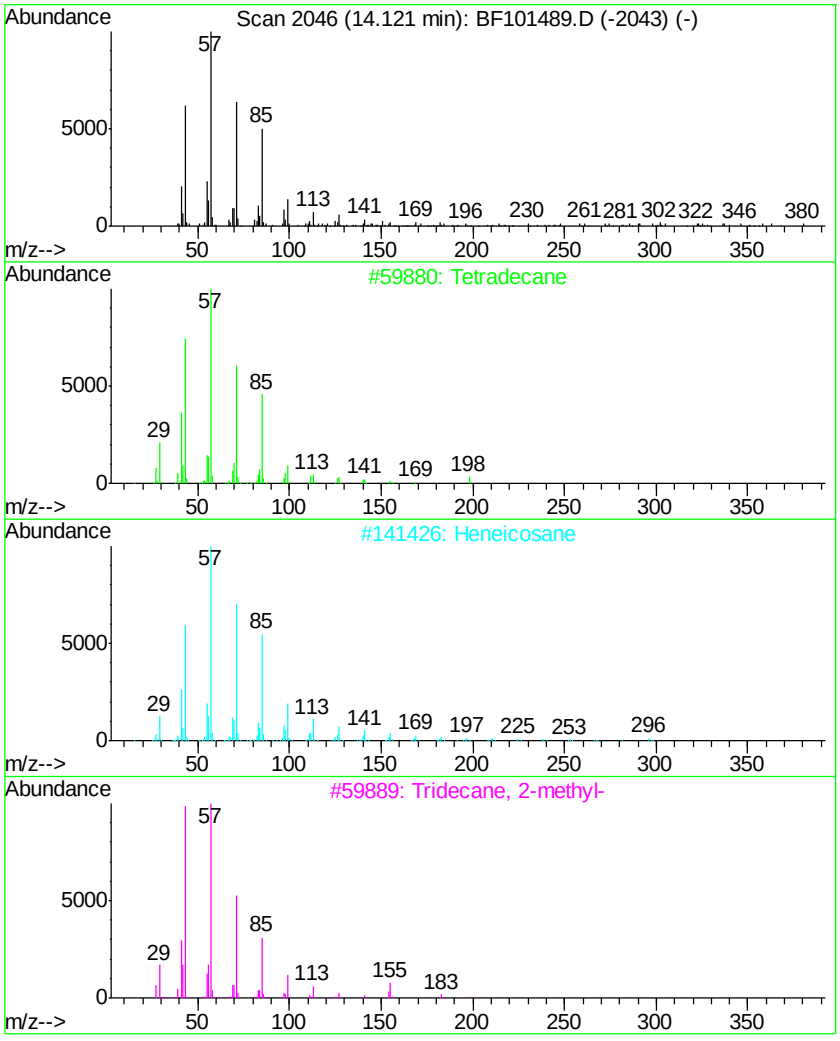
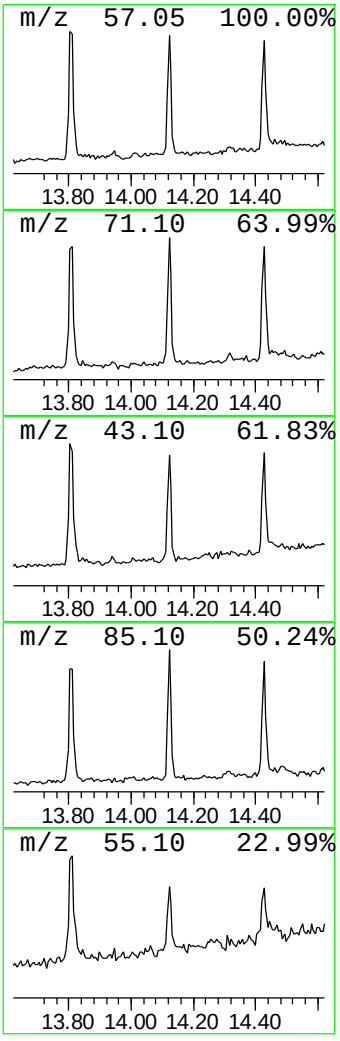
Peak Number 6 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.12	2.60 ng	124332	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	83
2	Heneicosane	296	C21H44	000629-94-7	83
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5	Nonadecane	268	C19H40	000629-92-5	80





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Acq On : 18 Dec 2017 19:09
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Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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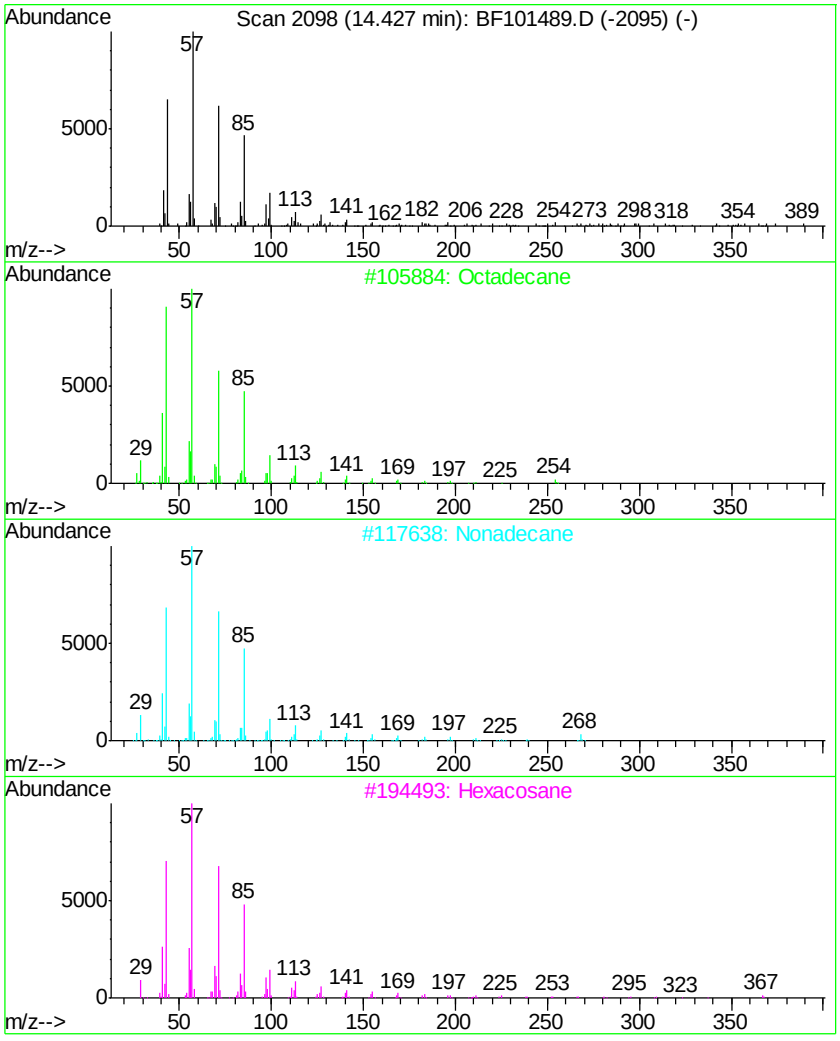
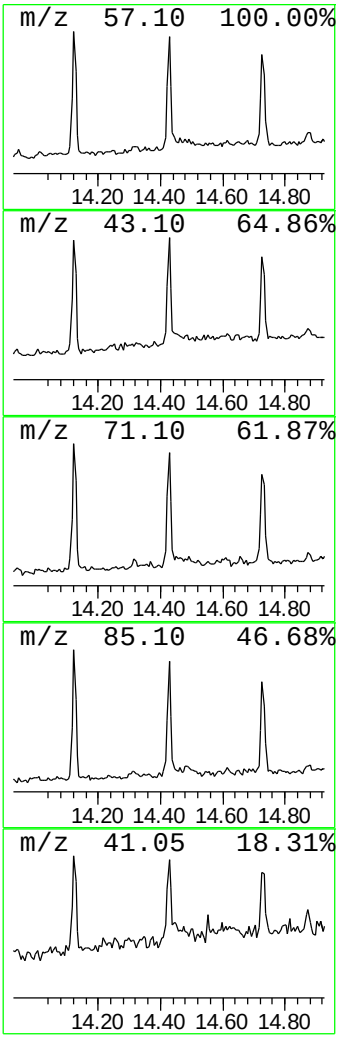
Peak Number 7 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.17 ng	103681	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Nonadecane	268	C19H40	000629-92-5	95
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane	296	C21H44	000629-94-7	86
5	Eicosane	282	C20H42	000112-95-8	80





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Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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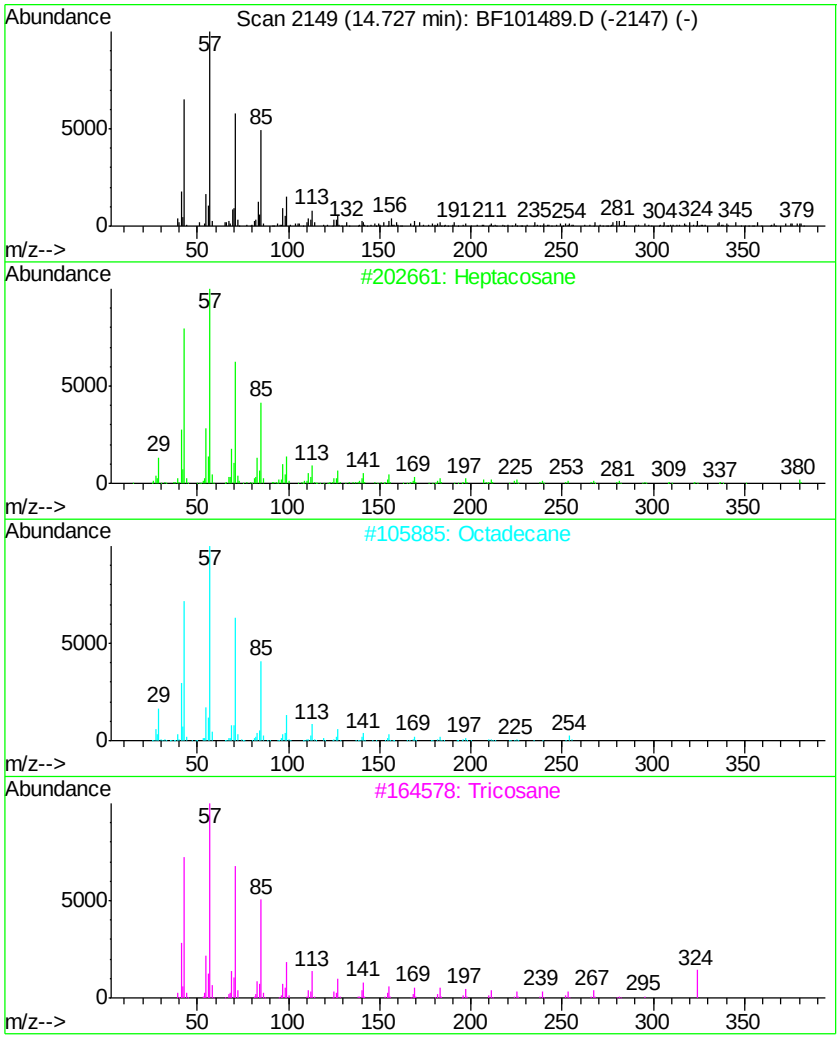
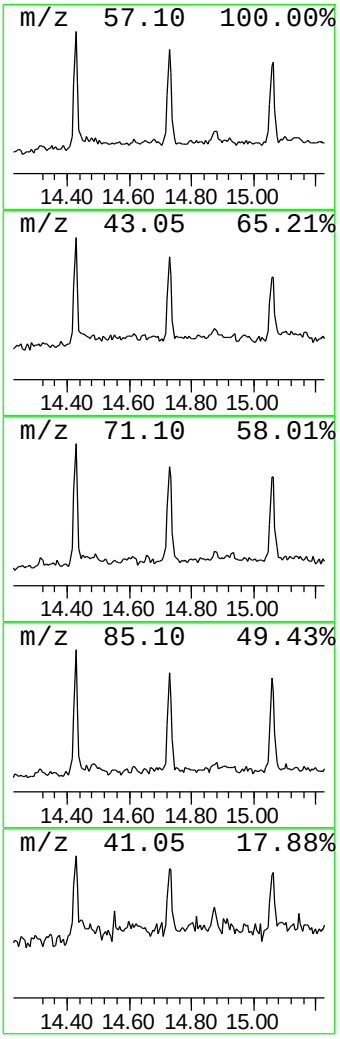
Peak Number 8 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.15 ng	102822	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	93
2	Octadecane	254	C18H38	000593-45-3	90
3	Tricosane	324	C23H48	000638-67-5	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101489.D
Acq On : 18 Dec 2017 19:09
Operator : SJ/JU
Sample : I6908-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	16.9	ng	787360	1	6.81	929258	20.0
unknown6.58	6.58	63.5	ng	2952140	1	6.81	929258	20.0
Hexadecane	13.48	2.4	ng	113456	5	13.99	955070	20.0
E-15-Heptadecenal	13.81	4.6	ng	218121	5	13.99	955070	20.0
Tetradecane	14.12	2.6	ng	124332	5	13.99	955070	20.0
Octadecane	14.43	2.2	ng	103681	5	13.99	955070	20.0
Heptacosane	14.73	2.1	ng	102822	5	13.99	955070	20.0