LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

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-BF031816.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	5.053	240	242	249	rBV	40482	72712	1.79%	0.222%
2	5.453	274	277	280	rBV	2589575	2887733	70.92%	8.801%
3	6.481	364	367	370	rBV	2209104	3295802	80.94%	10.045%
4	6.619	376	379	382	rBV	2966413	3046046	74.81%	9.284%
5	6.847	397	399	402	rBV	681120	743906	18.27%	2.267%
6	7.007	410	413	416	rBV	2672021	2501559	61.44%	7.624%
7	7.419	446	449	451	rBV	2116993	2235344	54.90%	6.813%
8	7.510	454	457	464	rVB	66337	89893	2.21%	0.274%
9	8.139	509	512	514	rBV	1093148	1055618	25.93%	3.217%
10	9.213	603	606	609	rBV	3444795	3693625	90.71%	11.258%
11	9.602	638	640	642	rBV	319043	419977	10.31%	1.280%
12	9.887	663	665	668	rVB	1149889	1092453	26.83%	3.330%
13	10.322	699	703	705	rBV3	93211	125104	3.07%	0.381%
14	10.539	720	722	726	rBV	31698	55801	1.37%	0.170%
15	10.676	731	734	737	rBV2	1922598	2371273	58.24%	7.227%
16	10.790	743	744	749	rBV	81966	141976	3.49%	0.433%
17	11.248	782	784	785	rBV	69568	83366	2.05%	0.254%
18	11.373	793	795	797	rBV	1350014	1218242	29.92%	3.713%
19	11.442	798	801	803	rVB2	29765	58473	1.44%	0.178%
20	11.613	812	816	819	rBV	42275	98181	2.41%	0.299%
21	11.671	819	821	823	rVB	61998	57204	1.40%	0.174%
22	11.899	840	841	847	rBV2	198432	321158	7.89%	0.979%
23	12.585	898	901	902	rBV	63947	76761	1.89%	0.234%
24	12.688	907	910	916	rVV2	126875	165480	4.06%	0.504%
25	12.779	916	918	919	rVV	80444	73290	1.80%	0.223%
26	12.813	919	921	924	rVB2	42946	72715	1.79%	0.222%
27	12.962	931	934	936	rBV	3935883	4071722	100.00%	12.410%
28	13.191	952	954	958	rBV	33919	44862	1.10%	0.137%
29	13.431	973	975	981	rBV2	124072	355886	8.74%	1.085%
30	13.534	981	984	986	rVB2	24660	45869	1.13%	0.140%
31	13.865	1010	1013	1021	rBV	74234	182053	4.47%	0.555%
32	14.002	1022	1025	1028	rBV	1118913	1109479	27.25%	3.382%
33	14.848	1097	1099	1101	rBV	93951	91410	2.24%	0.279%
34	15.431	1147	1150	1153	rBV	722960	854657	20.99%	2.605%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-GRID-7A

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-BF031816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

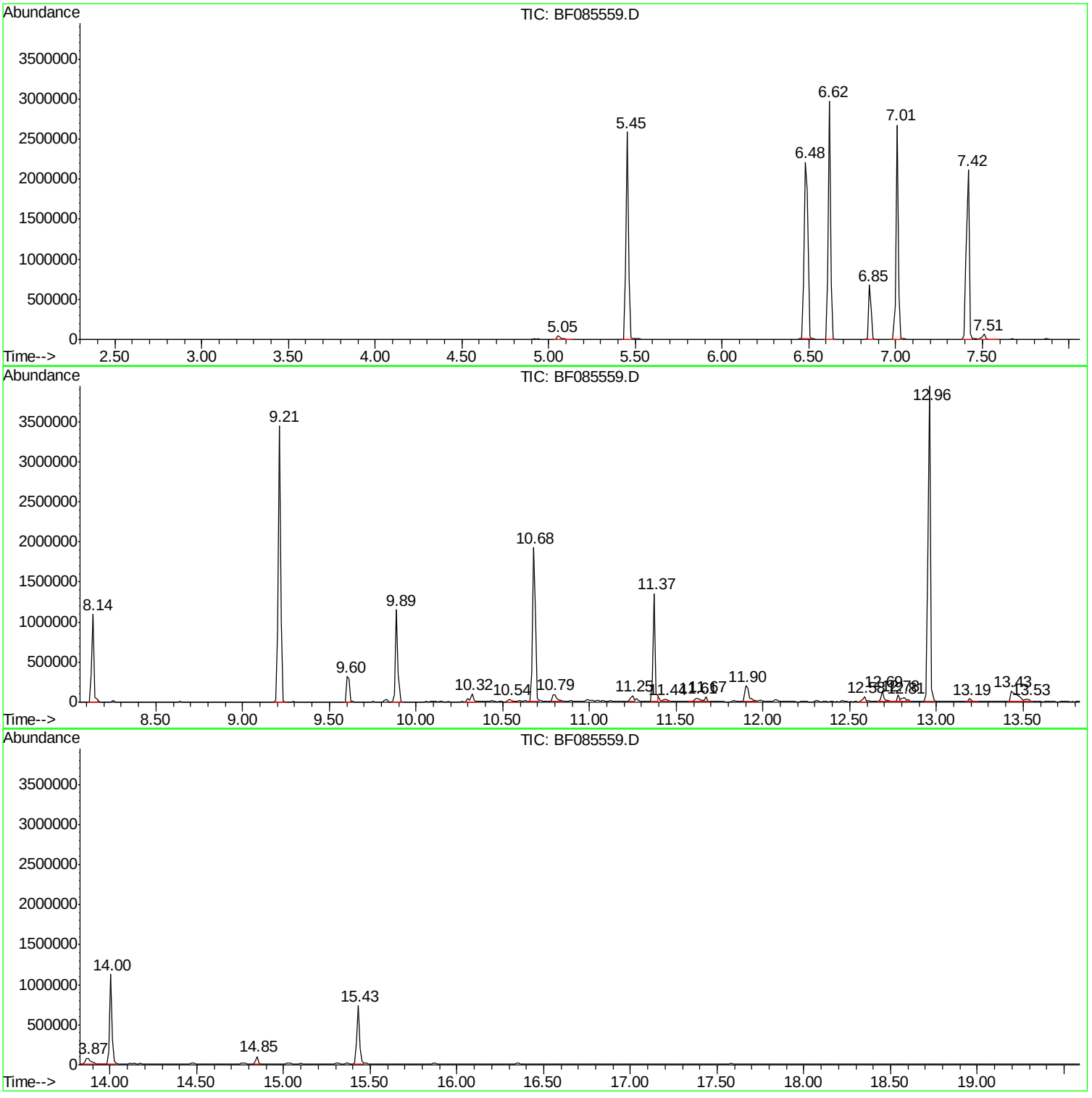
Sum of corrected areas: 32809630

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

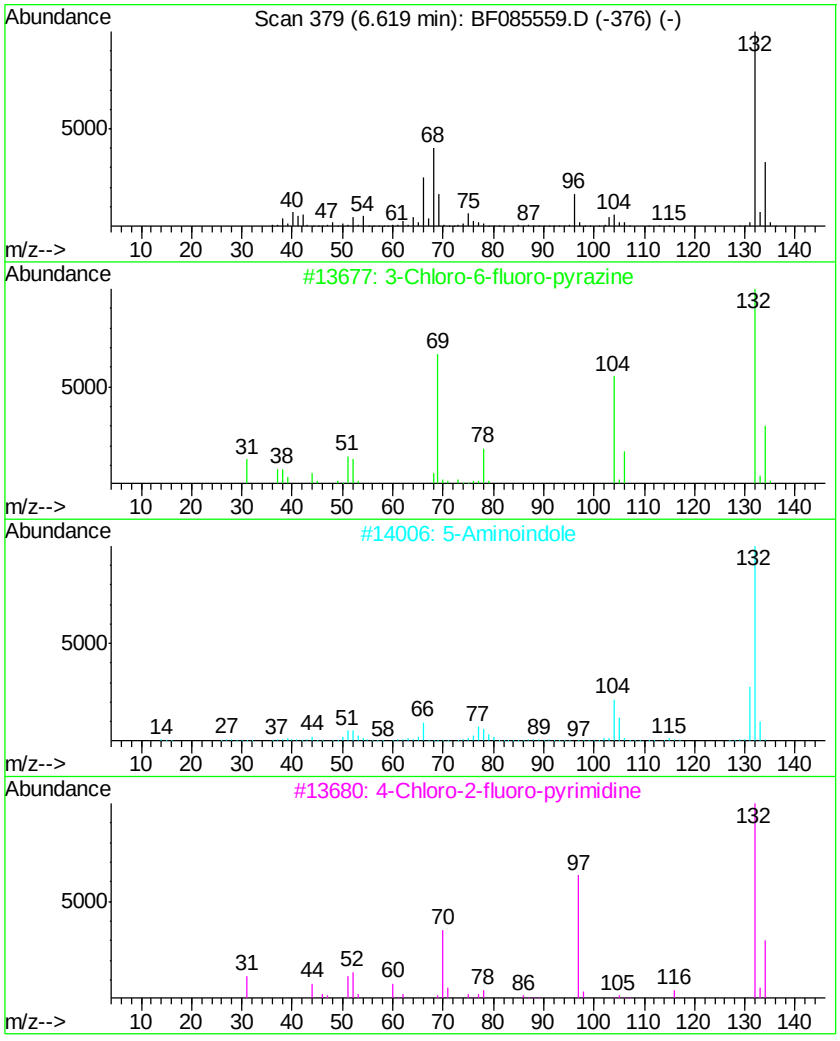
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

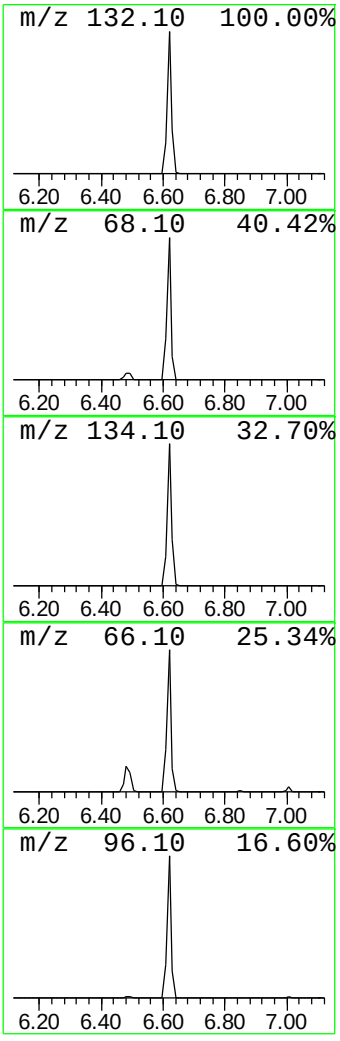
****

Peak Number 1 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	81.89 ng	3046050	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

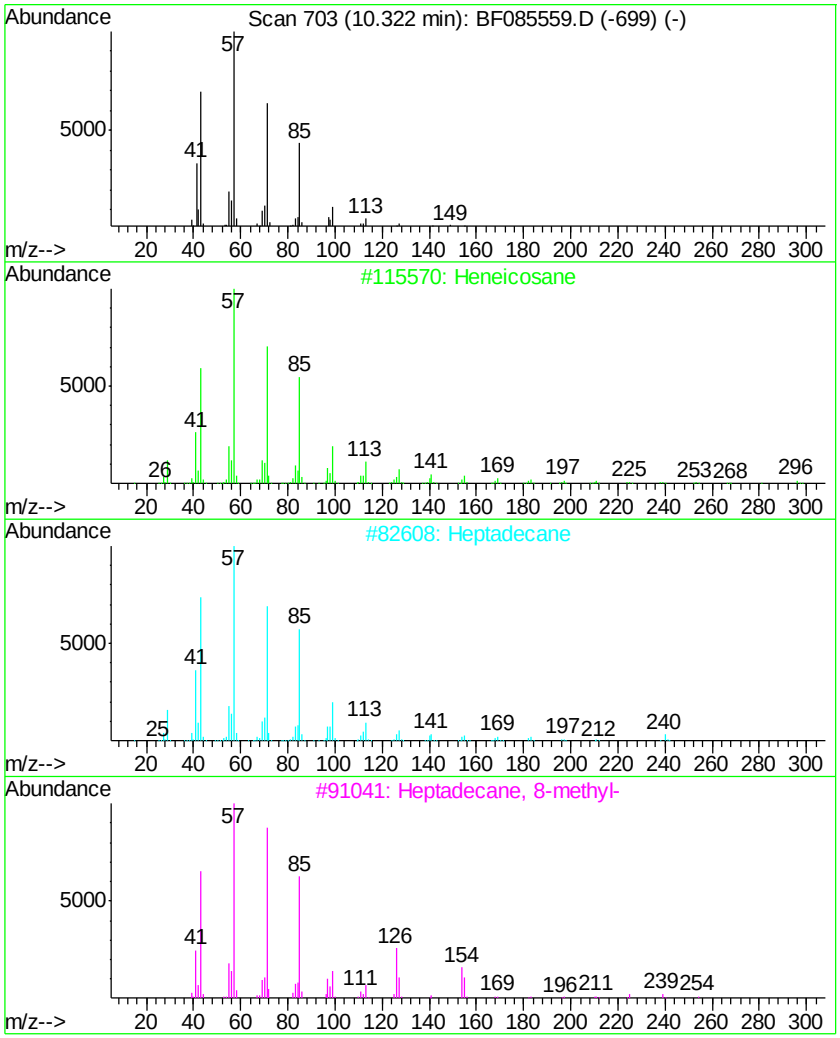
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

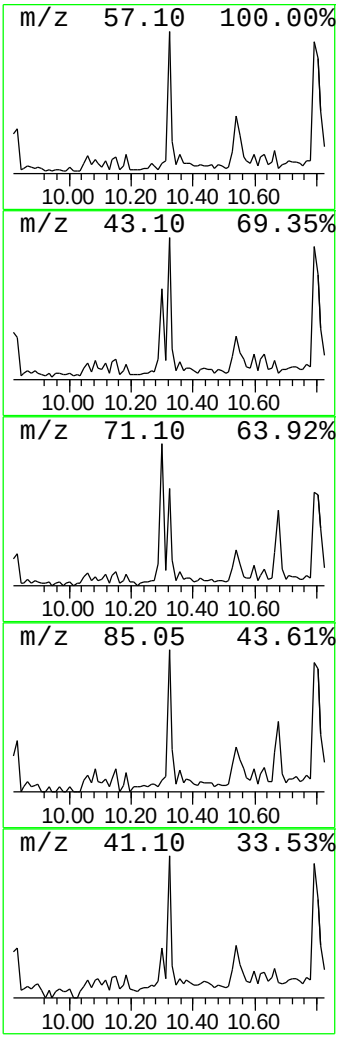
****

Peak Number 3 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	2.29 ng	125104	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5	Eicosane	282	C20H42	000112-95-8	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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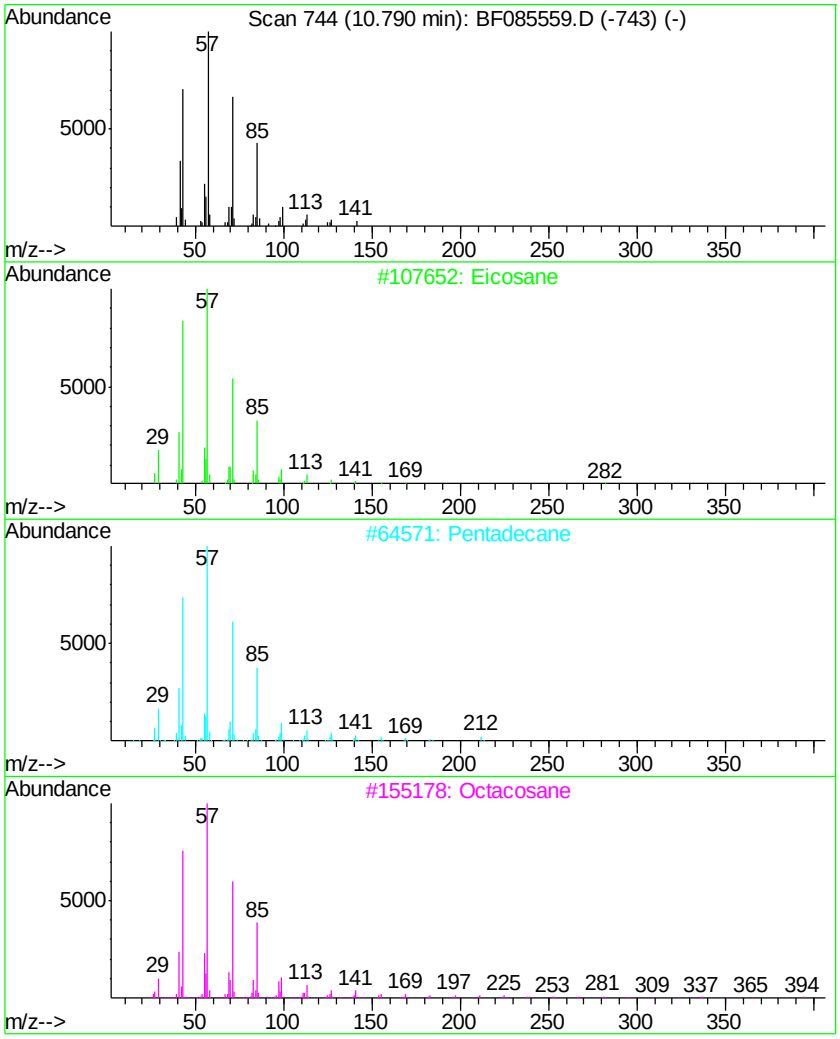
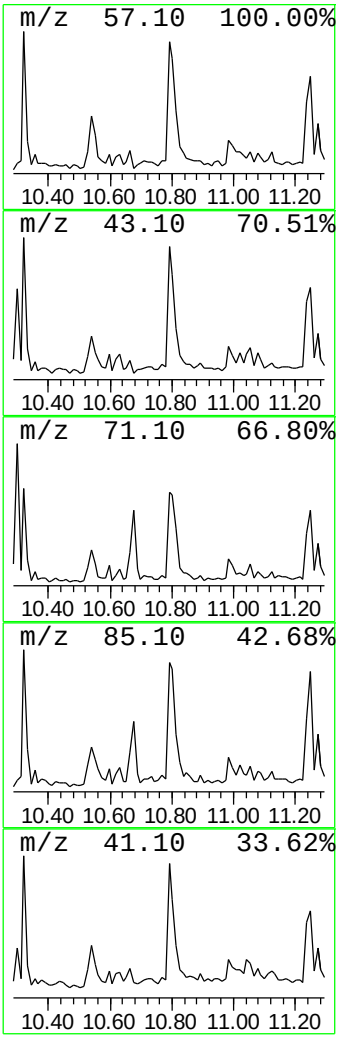
Peak Number 4 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	2.33 ng	141976	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Hexadecane	226	C16H34	000544-76-3	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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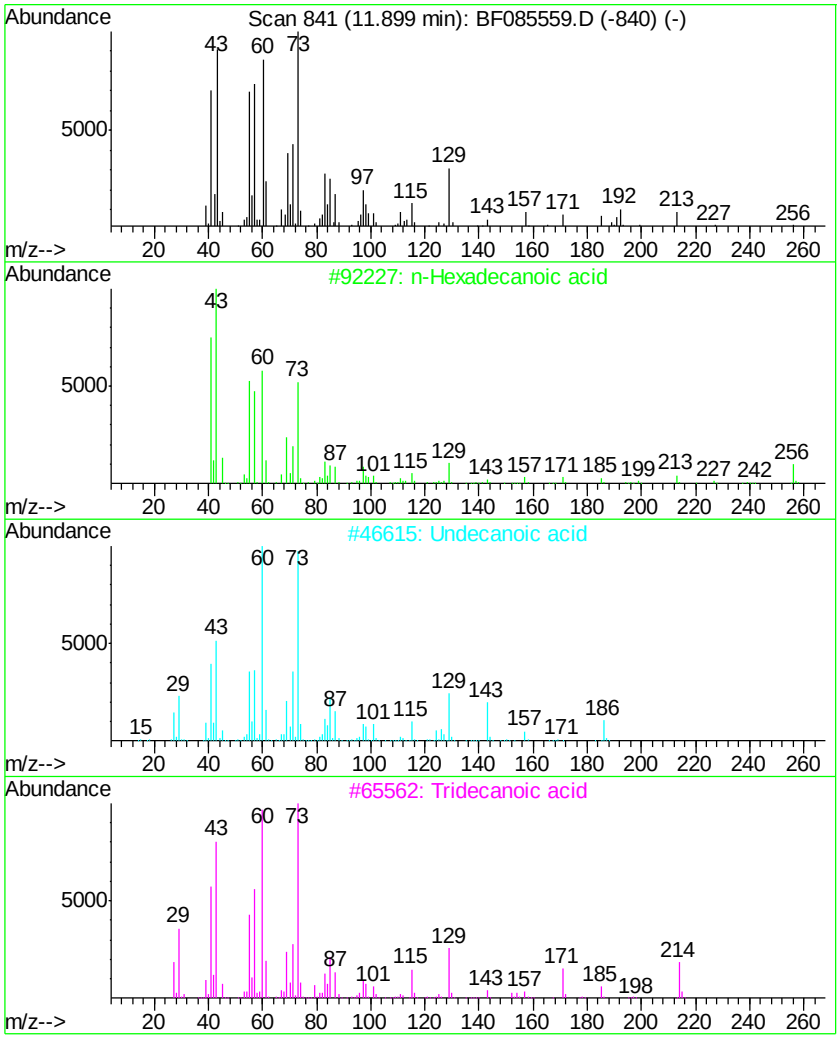
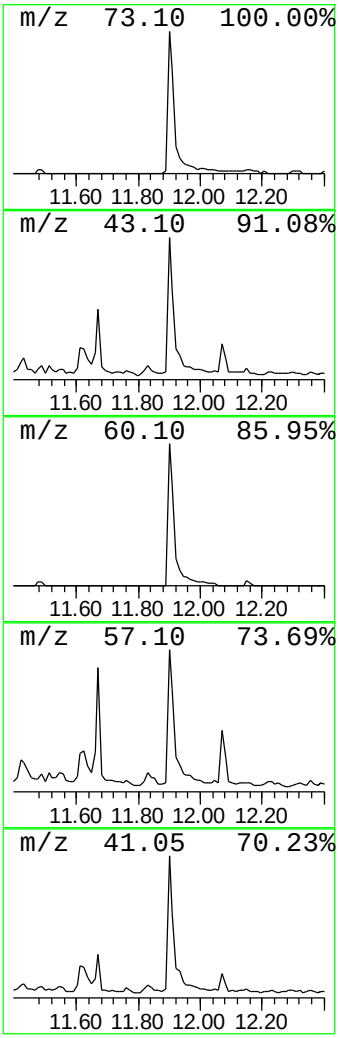
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	5.27 ng	321158	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Undecanoic acid	186	C11H22O2	000112-37-8	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Hexadecane	226	C16H34	000544-76-3	11





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Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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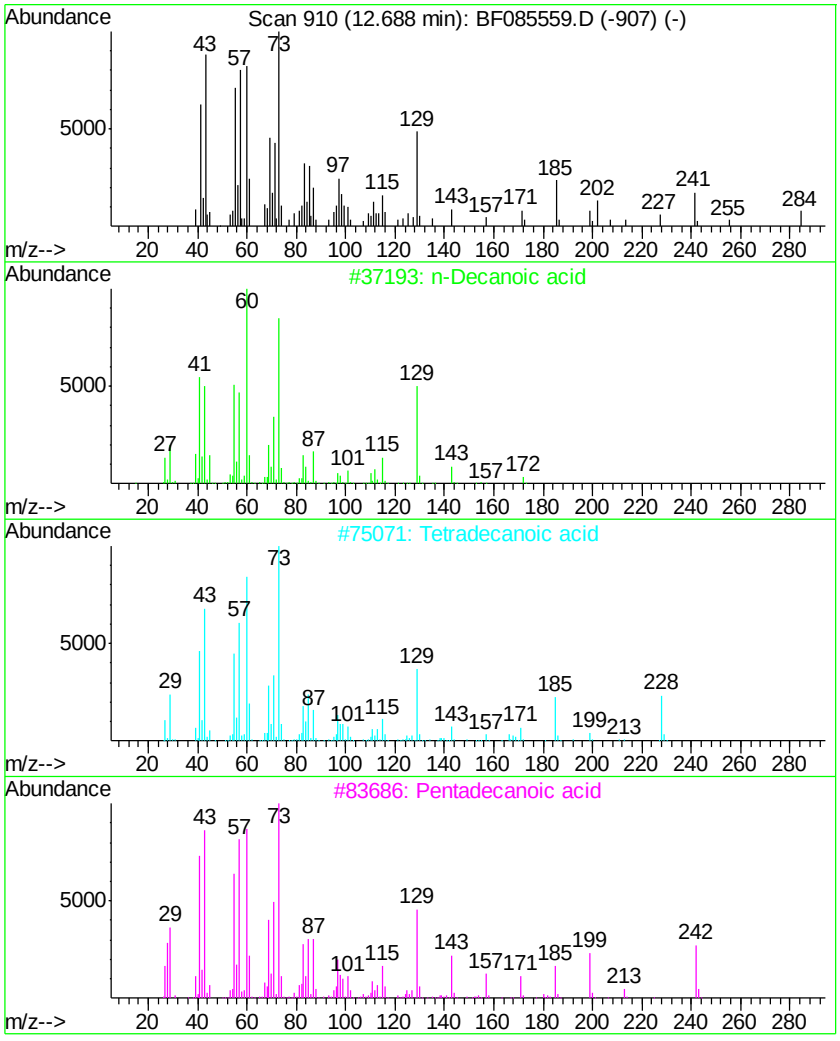
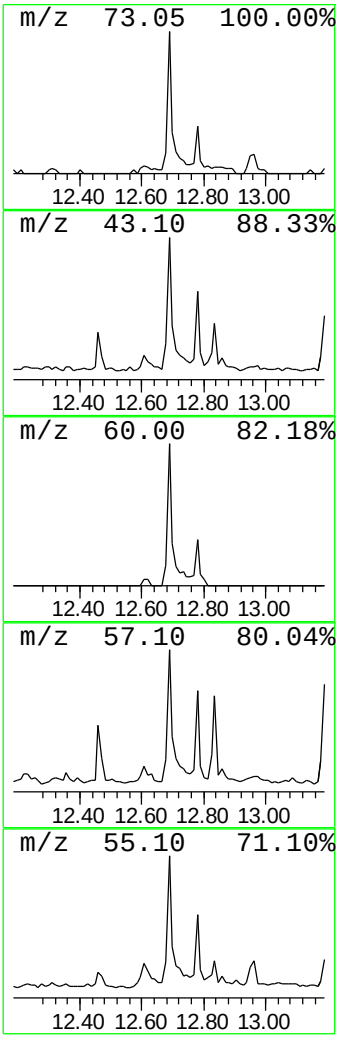
Peak Number 6 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	2.72 ng	165480	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	92
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
5	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	11





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

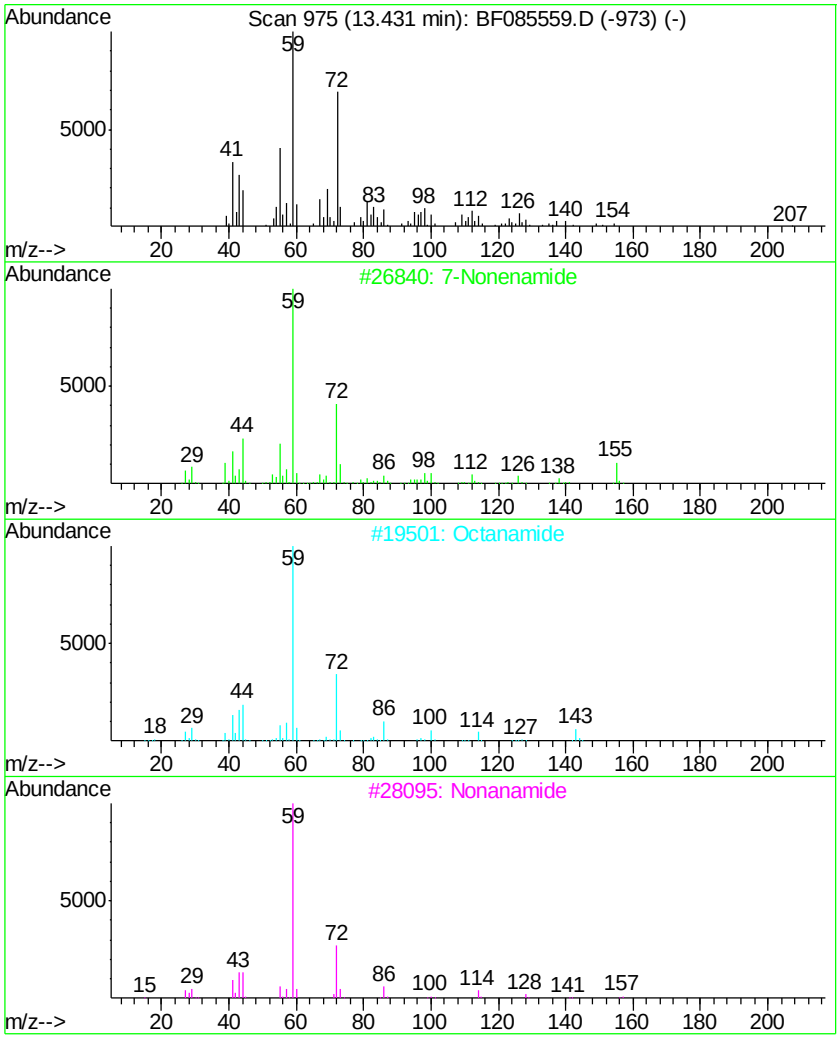
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

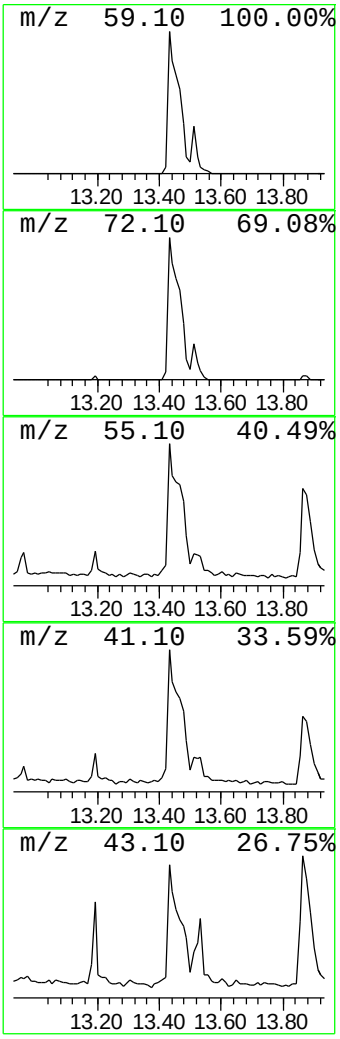
****

Peak Number 7 7-Nonenamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	6.42 ng	355886	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Nonenamide	155	C9H17NO	090949-53-4	72
2	Octanamide	143	C8H17NO	000629-01-6	64
3	Nonanamide	157	C9H19NO	001120-07-6	64
4	Hexadecanamide	255	C16H33NO	000629-54-9	64
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

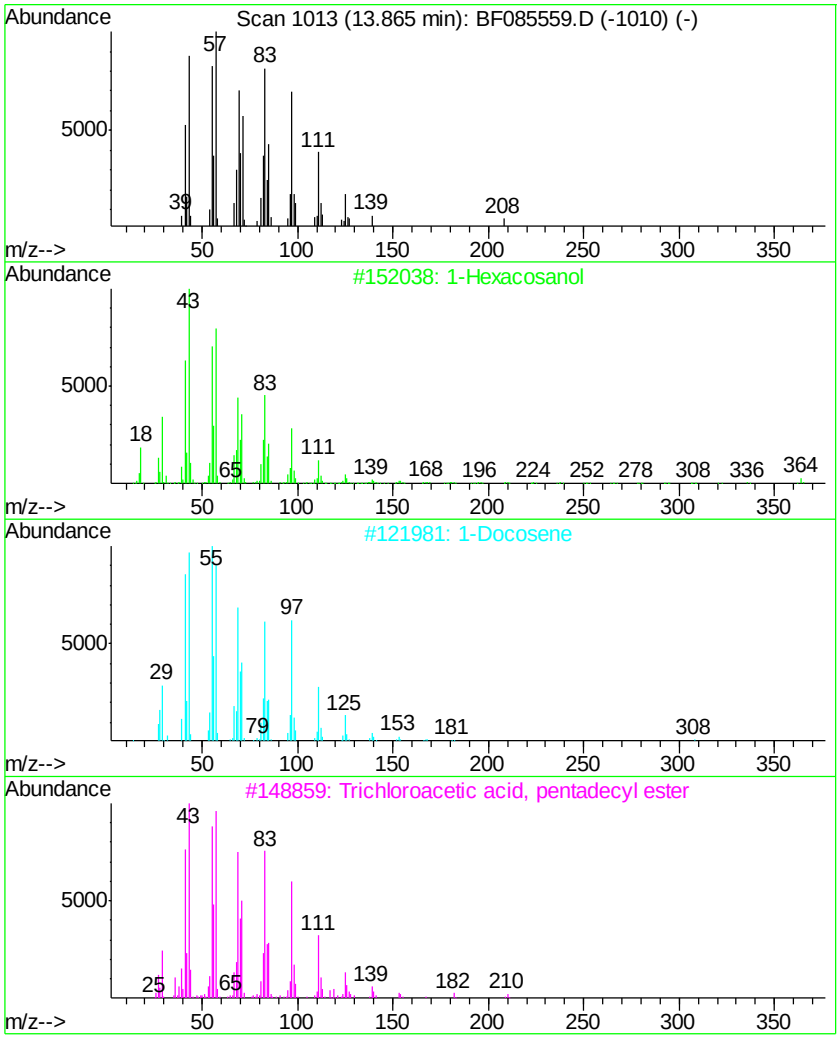
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

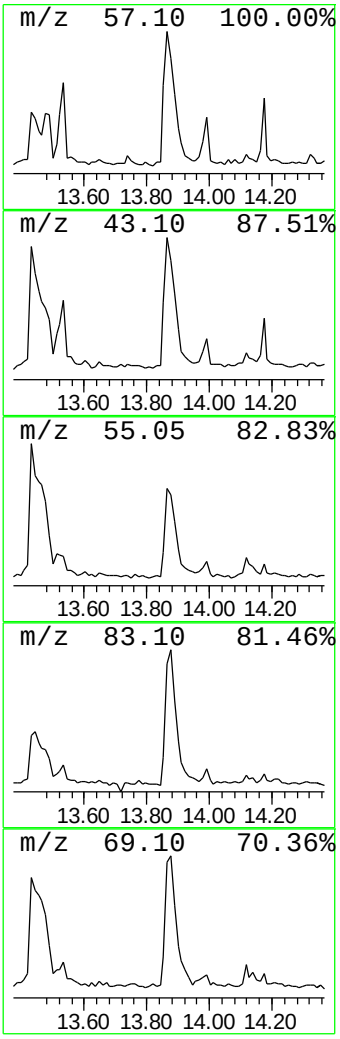
****

Peak Number 8 1-Hexacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.28 ng	182053	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	90
2	1-Docosene	308	C22H44	001599-67-3	90
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	1-Tetracosanol	354	C24H50O	000506-51-4	90





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Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

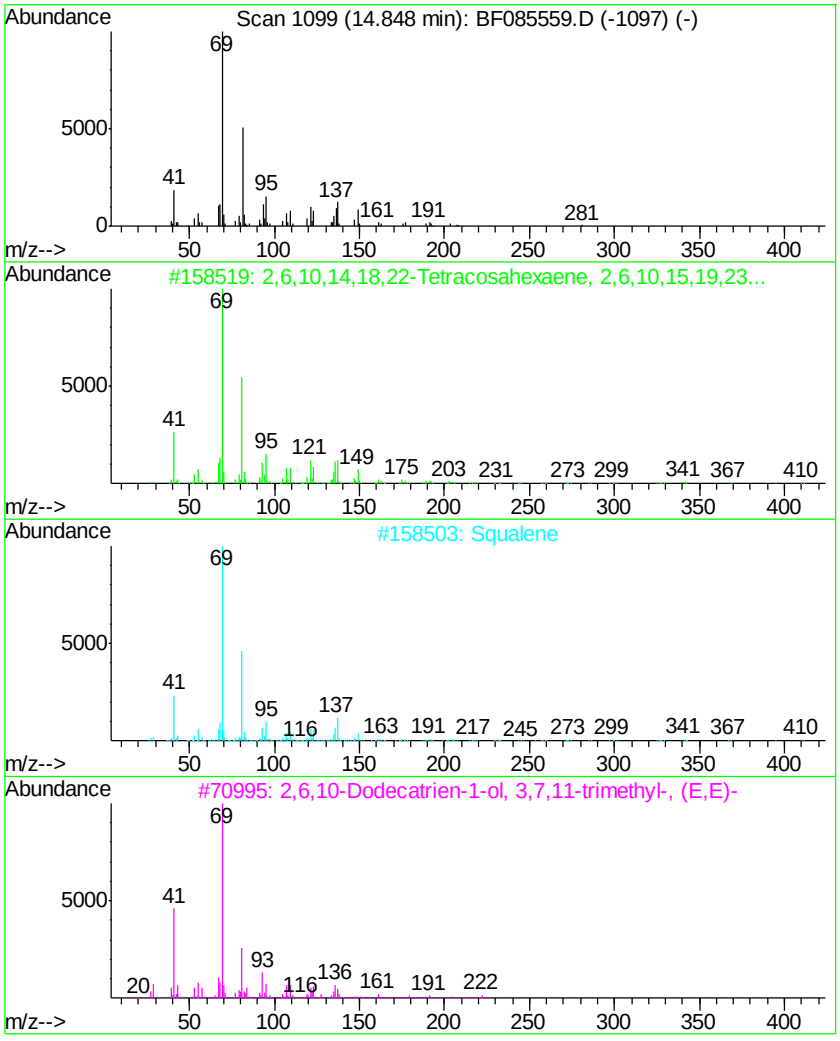
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

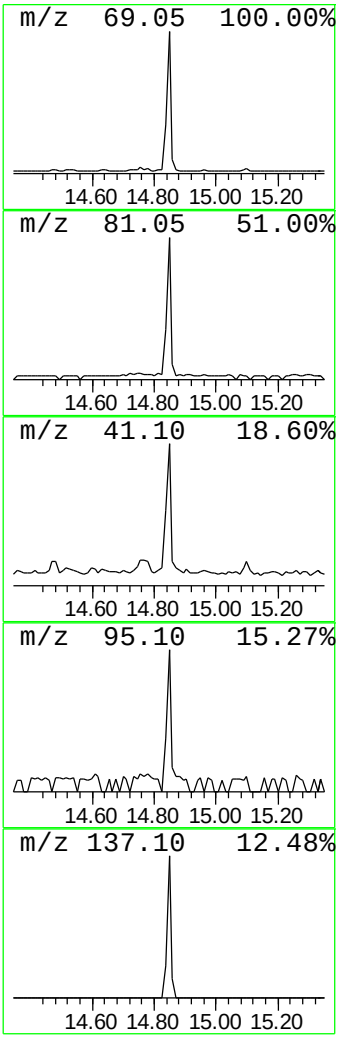
****

Peak Number 9 2,6,10,14,18,22-Tetracosahe... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	2.14 ng	91410	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
2	Squalene	410	C30H50	007683-64-9	91
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	59
4	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50
5	Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085559.D
Acq On : 19 Mar 2016 7:31
Operator : UM/SJ
Sample : H1804-01
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-7A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.62	6.62	81.9	ng	3046050	1	6.85	743906	20.0
Heneicosane	10.32	2.3	ng	125104	3	9.89	1092450	20.0
Eicosane	10.79	2.3	ng	141976	4	11.37	1218240	20.0
n-Hexadecanoic acid	11.90	5.3	ng	321158	4	11.37	1218240	20.0
n-Decanoic acid	12.69	2.7	ng	165480	4	11.37	1218240	20.0
7-Nonenamide	13.43	6.4	ng	355886	5	14.00	1109480	20.0
1-Hexacosanol	13.87	3.3	ng	182053	5	14.00	1109480	20.0
2,6,10,14,18,22-T...	14.85	2.1	ng	91410	6	15.43	854657	20.0