LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

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-BF013017.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	5.024	254	257	265	rBV	1156583	1527294	37.70%	3.910%
2	5.447	292	294	297	rBV	2670574	3378313	83.39%	8.649%
3	6.487	382	385	388	rBV	2552257	3787150	93.48%	9.695%
4	6.624	394	397	399	rBV	3317544	3614444	89.22%	9.253%
5	6.853	414	417	419	rBV	1080991	958829	23.67%	2.455%
6	7.013	428	431	433	rBV	2236445	2744232	67.74%	7.025%
7	7.413	464	466	469	rBV	1587701	2293878	56.62%	5.872%
8	8.133	527	529	532	rBV	1173299	1223565	30.20%	3.132%
9	9.219	621	624	626	rBV	3053187	4051251	100.00%	10.371%
10	9.608	656	658	660	rBV	862510	708009	17.48%	1.813%
11	9.813	673	676	679	rBV2	49570	90228	2.23%	0.231%
12	9.893	680	683	685	rVV	1227948	1388812	34.28%	3.555%
13	10.293	716	718	719	rBV	46596	41294	1.02%	0.106%
14	10.316	719	720	722	rVB	80461	71994	1.78%	0.184%
15	10.533	737	739	743	rBV	26610	49400	1.22%	0.126%
16	10.682	749	752	754	rBV	1963481	2240070	55.29%	5.735%
17	10.796	760	762	768	rVB	99837	147750	3.65%	0.378%
18	11.242	798	801	802	rBV	113434	110692	2.73%	0.283%
19	11.265	802	803	806	rVB	38289	41302	1.02%	0.106%
20	11.368	810	812	816	rBV	1194358	1589566	39.24%	4.069%
21	11.448	816	819	821	rVB	52016	65333	1.61%	0.167%
22	11.665	836	838	840	rBV	133172	105303	2.60%	0.270%
23	11.985	864	866	870	rVB2	50982	71585	1.77%	0.183%
24	12.076	872	874	876	rVB	43717	52310	1.29%	0.134%
25	12.579	916	918	921	rBV	294830	284750	7.03%	0.729%
26	12.808	933	938	941	rBV	252810	310726	7.67%	0.795%
27	12.957	948	951	954	rVV	3162599	3504194	86.50%	8.971%
28	13.139	963	967	968	rBV	45802	58106	1.43%	0.149%
29	13.848	1027	1029	1035	rVB2	272189	354512	8.75%	0.908%
30	14.008	1040	1043	1045	rBV	1556905	1610893	39.76%	4.124%
31	14.168	1055	1057	1061	rBV3	29600	63374	1.56%	0.162%
32	14.477	1081	1084	1087	rBV	84203	169212	4.18%	0.433%
33	14.751	1106	1108	1112	rBV2	159172	209108	5.16%	0.535%
34	14.911	1120	1122	1124	rBV	74454	70398	1.74%	0.180%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

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-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.025	1129	1132	1136	rBV	101799	189349	4.67%	0.485%
36	15.094	1136	1138	1139	rBV	86176	90260	2.23%	0.231%
37	15.128	1139	1141	1143	rVB2	45515	70247	1.73%	0.180%
38	15.311	1155	1157	1161	rVB	45701	68629	1.69%	0.176%
39	15.380	1161	1163	1165	rBV	62871	84094	2.08%	0.215%
40	15.437	1165	1168	1174	rBV	824280	1080225	26.66%	2.765%
41	15.654	1184	1187	1189	rVB	52192	75225	1.86%	0.193%
42	15.871	1203	1206	1208	rBV	89279	125444	3.10%	0.321%
43	15.917	1208	1210	1213	rVV4	20683	41208	1.02%	0.105%
44	16.625	1269	1272	1276	rBV4	28681	58685	1.45%	0.150%
45	16.843	1288	1291	1294	rBV	30536	62420	1.54%	0.160%
46	16.911	1294	1297	1300	rVB2	23556	47372	1.17%	0.121%
47	16.980	1300	1303	1307	rBV4	32173	80372	1.98%	0.206%

Sum of corrected areas: 39061407

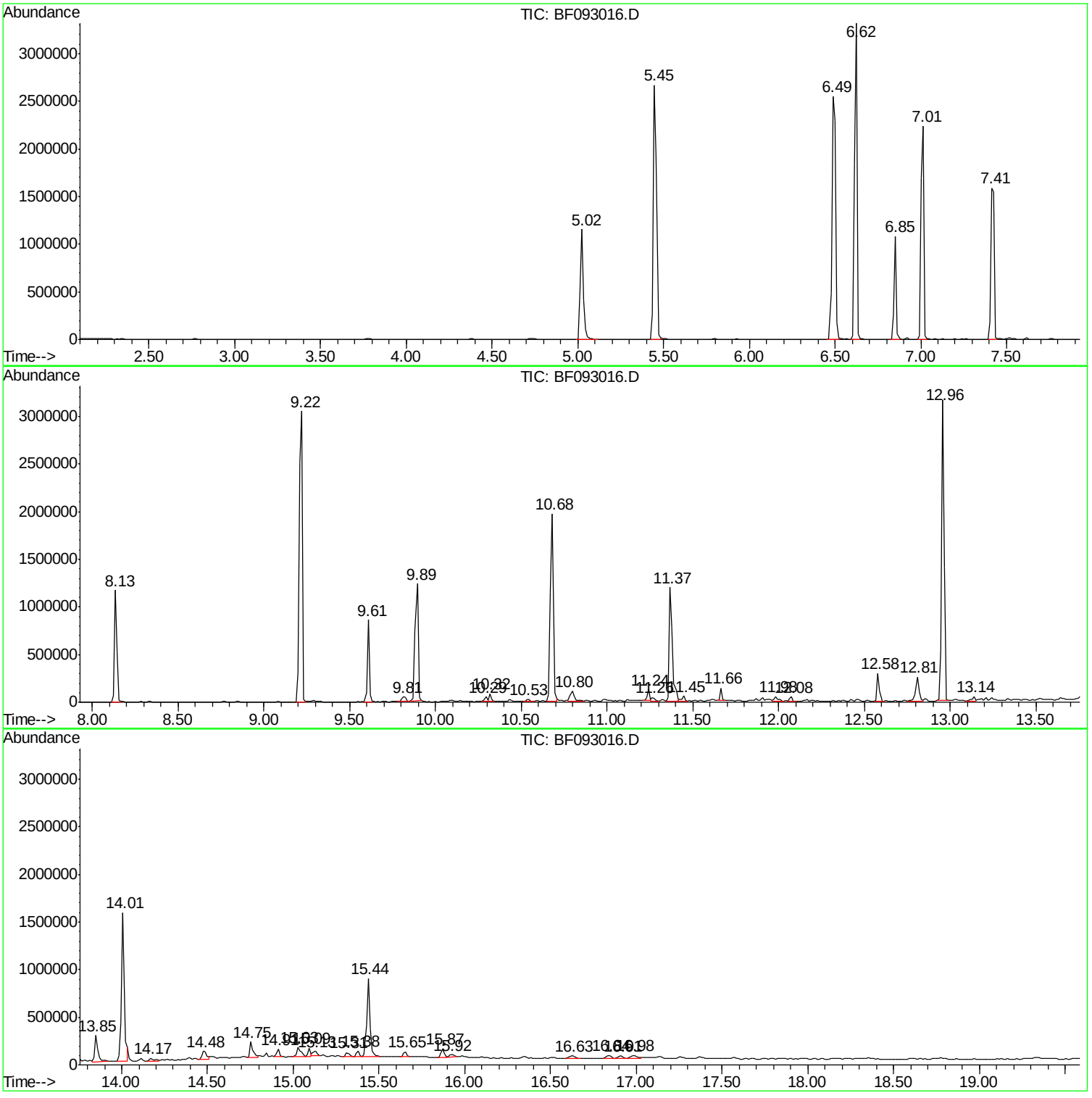
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

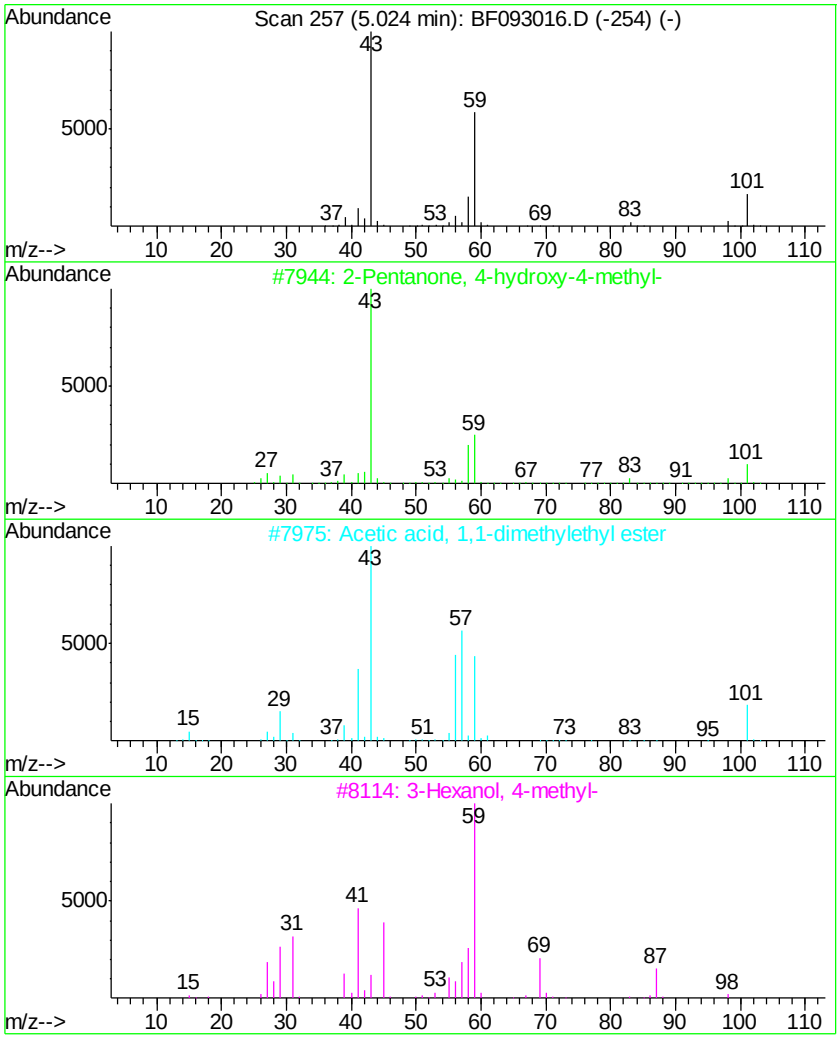
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

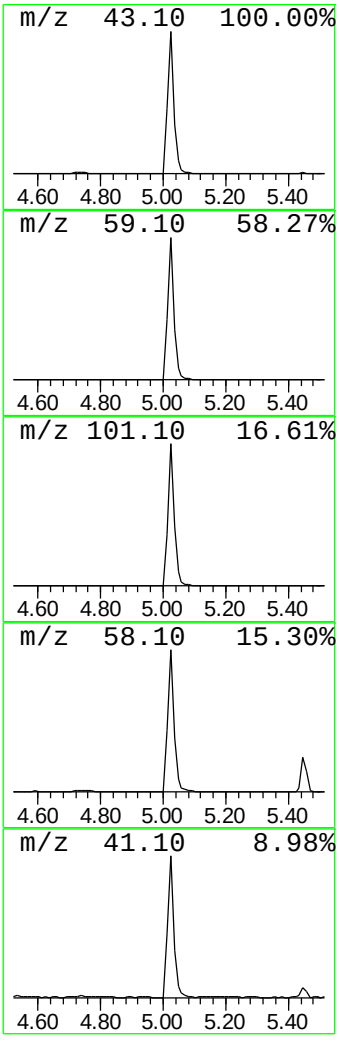
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	31.86 ng	1527290	1,4-Dichlorobenzene-d4	6.85

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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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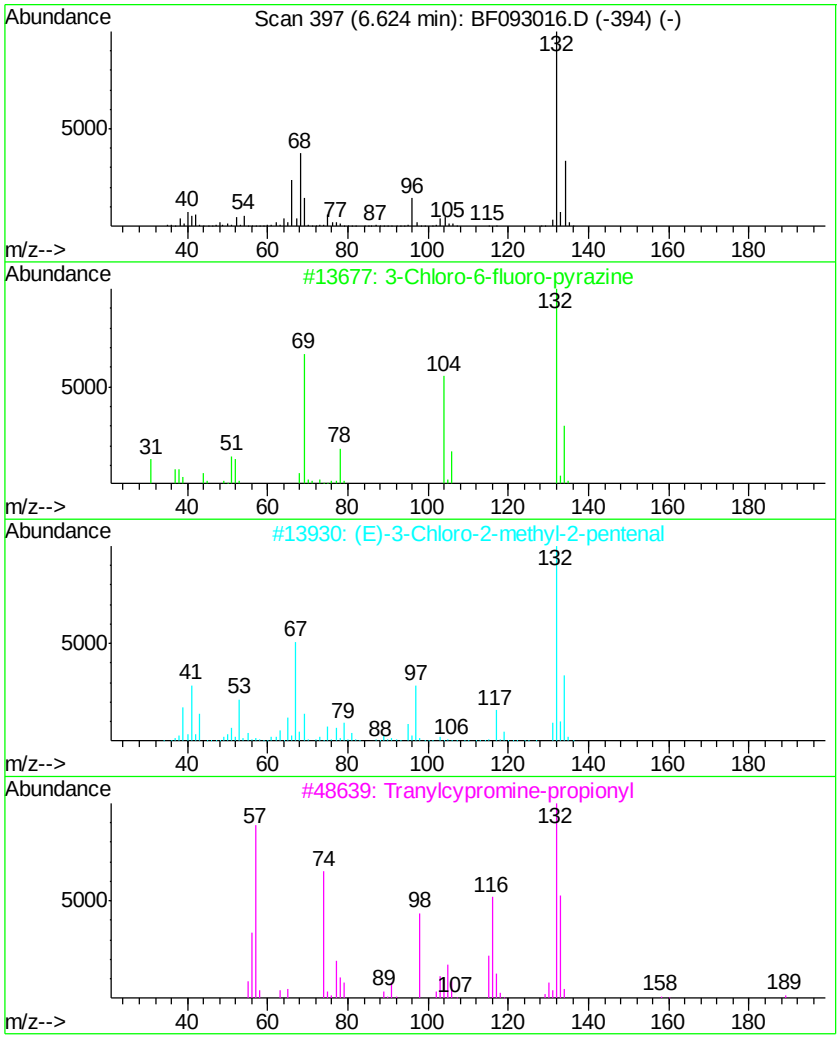
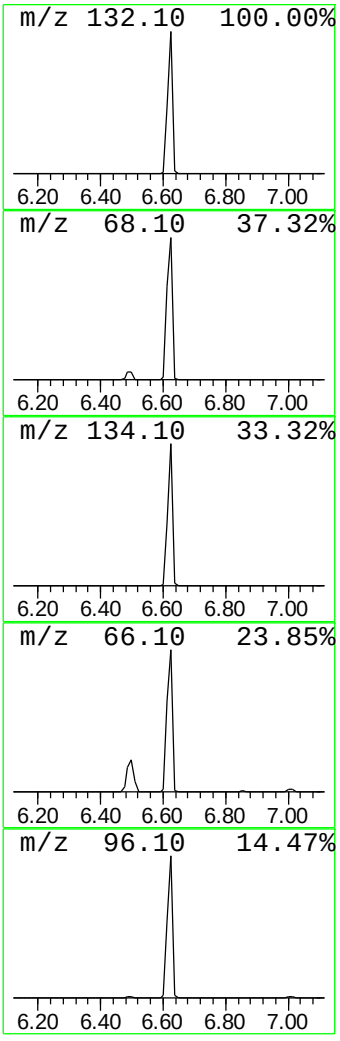
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	75.39 ng	3614440	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	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

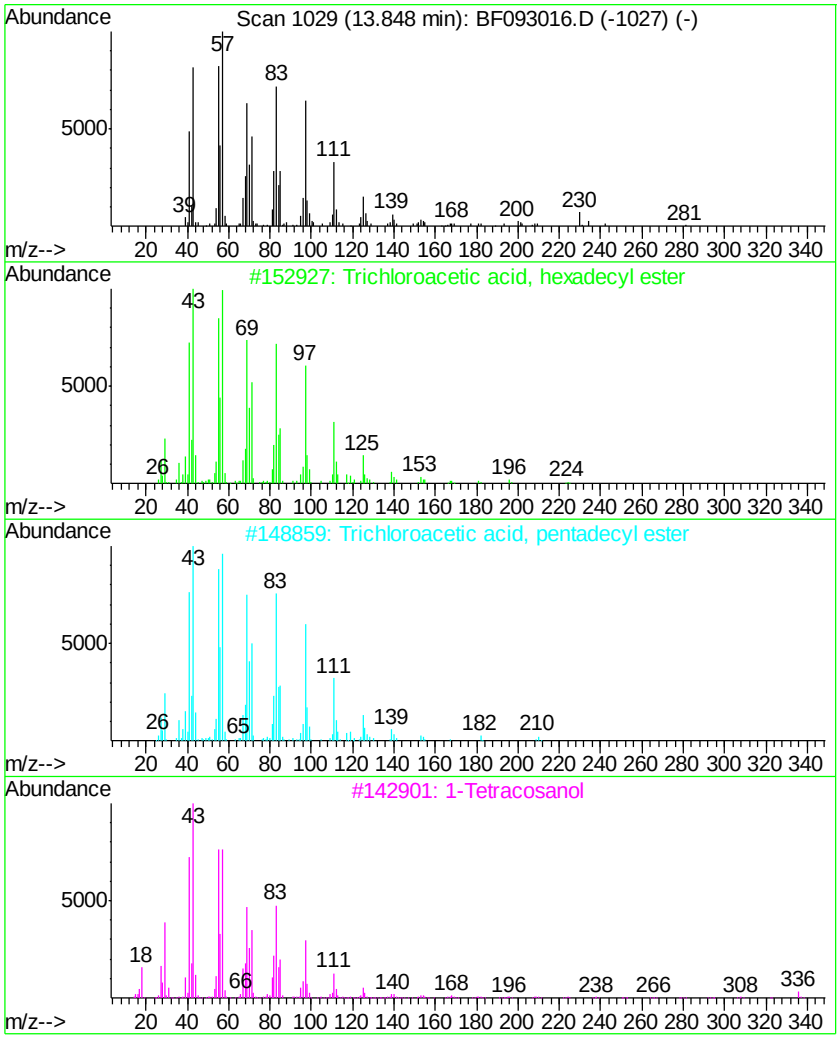
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

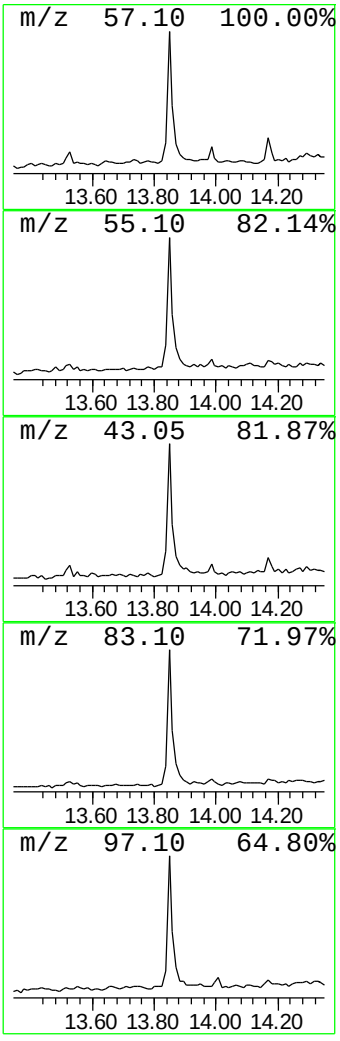
****

Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.40 ng	354512	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	1-Tetracosanol	354	C24H50O	000506-51-4	91
4	1-Docosene	308	C22H44	001599-67-3	90
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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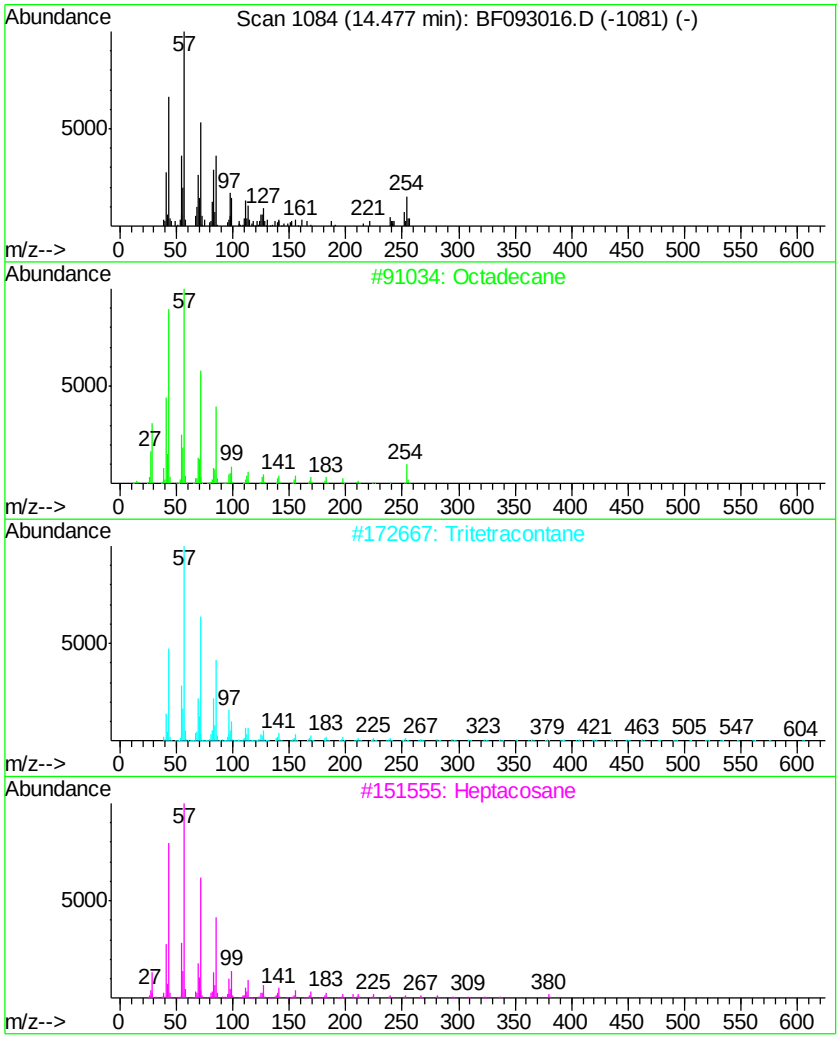
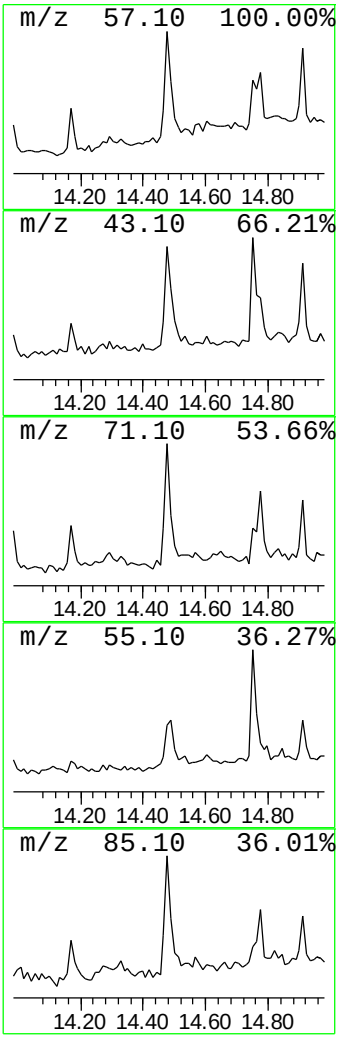
Peak Number 5 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	2.10 ng	169212	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	86
2	Tritetracontane	605	C43H88	007098-21-7	74
3	Heptacosane	380	C27H56	000593-49-7	72
4	Tetratetracontane	619	C44H90	007098-22-8	72
5	Heptadecane	240	C17H36	000629-78-7	60





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

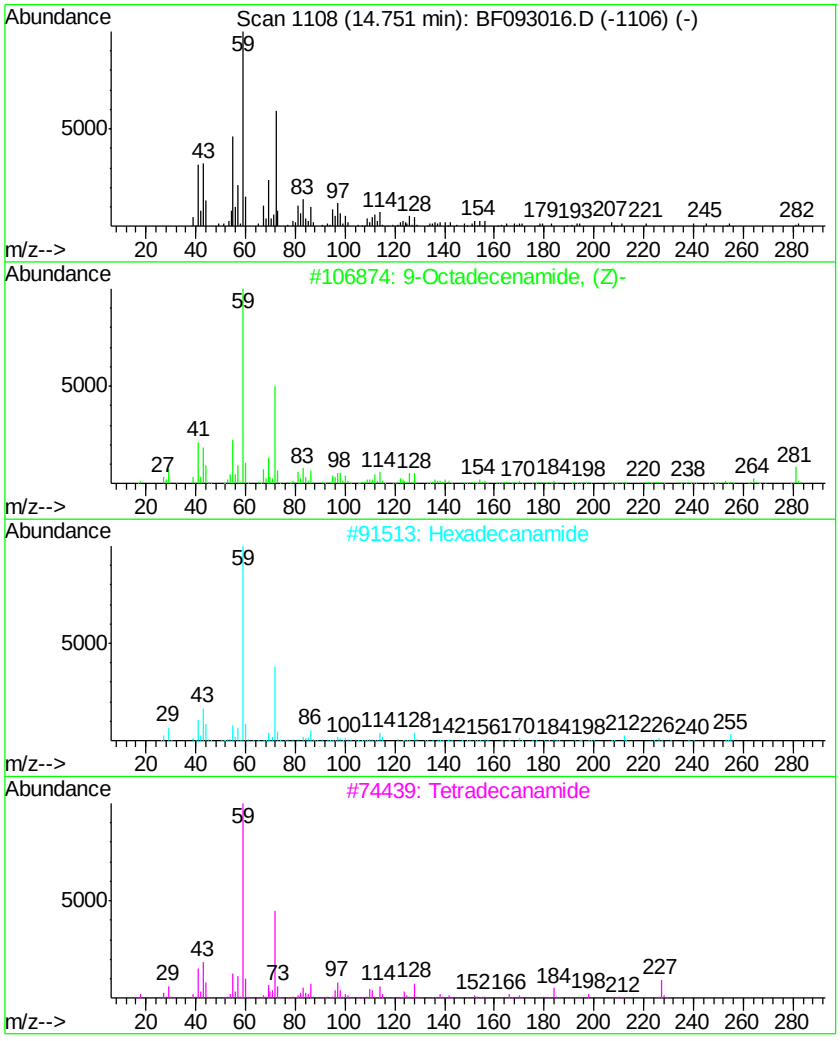
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

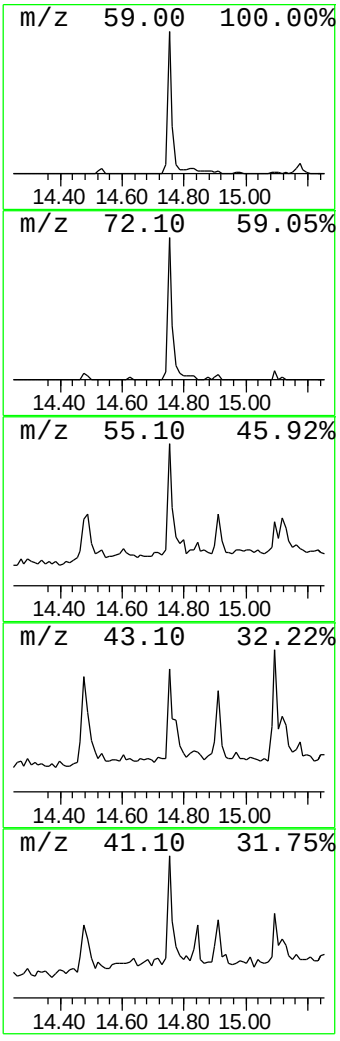
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	3.87 ng	209108	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	Hexadecanamide	255	C16H33NO	000629-54-9	78
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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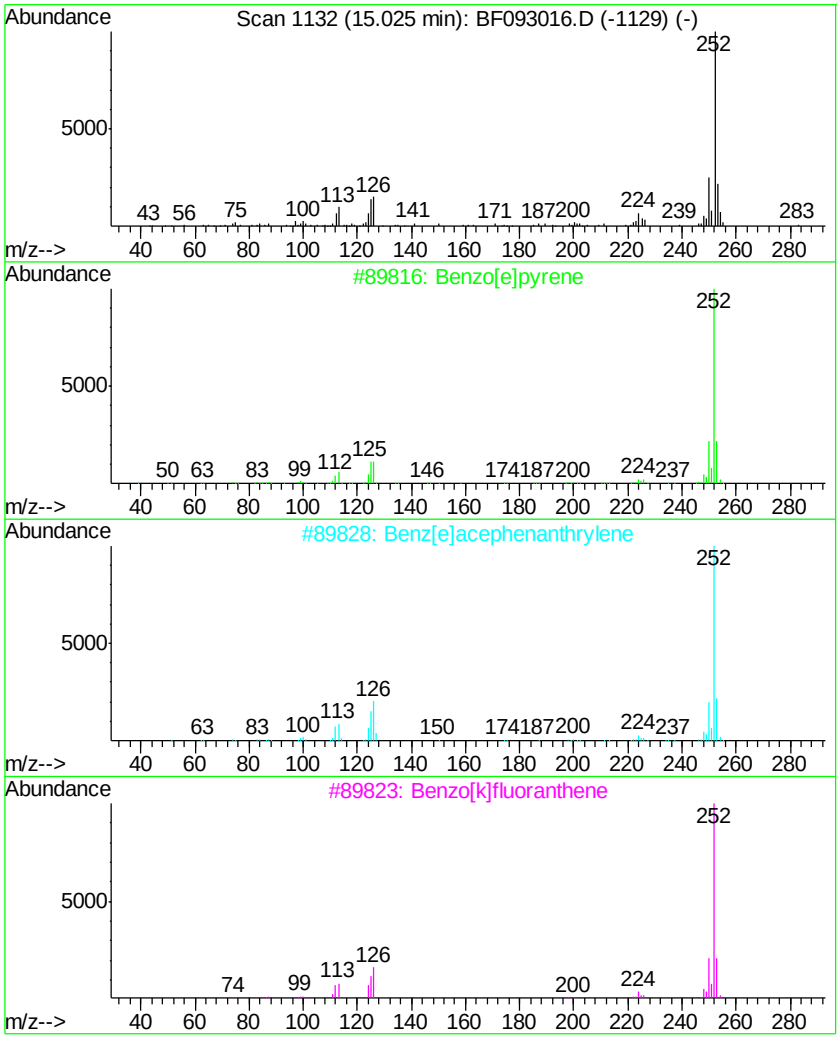
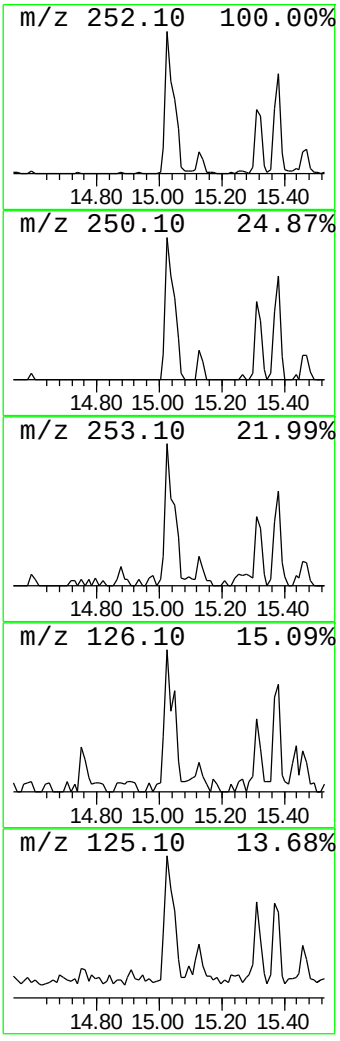
Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	3.51 ng	189349	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Perylene	252	C20H12	000198-55-0	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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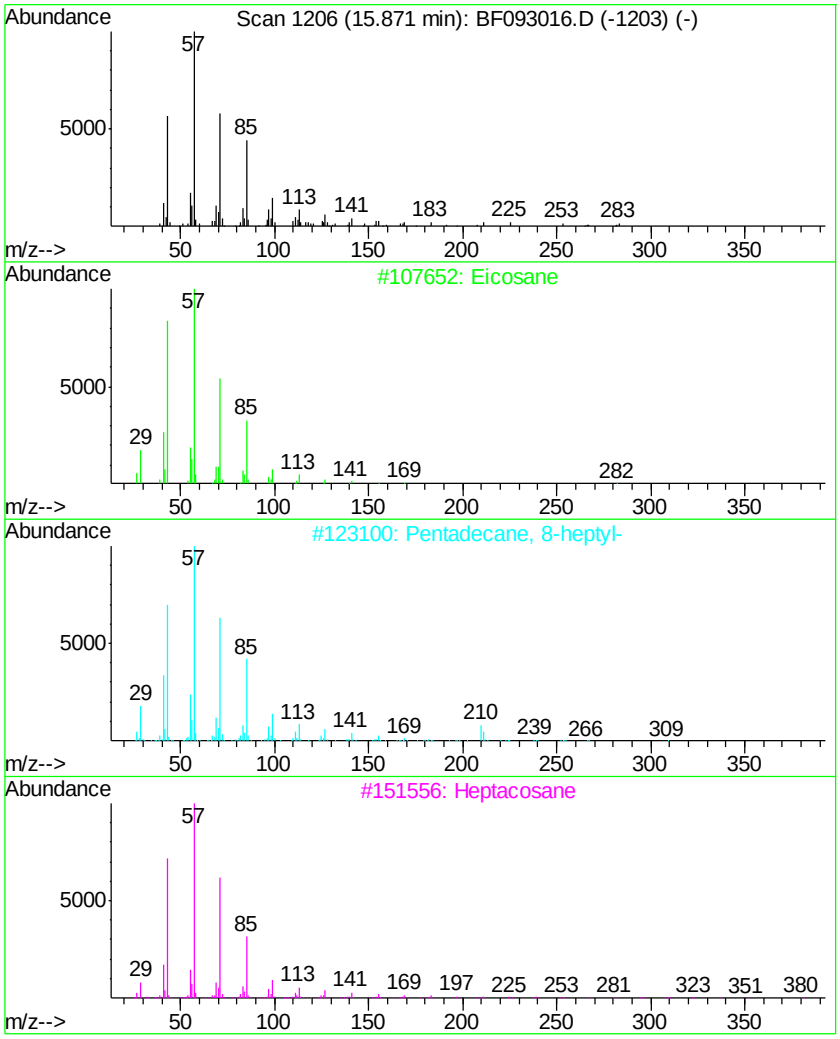
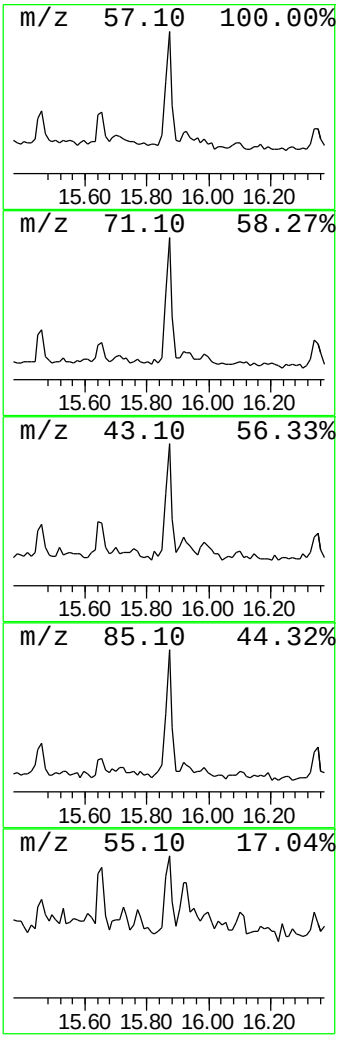
Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.32 ng	125444	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Nonacosane	408	C29H60	000630-03-5	90
5	Tetracosane	338	C24H50	000646-31-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021717\
Data File : BF093016.D
Acq On : 17 Feb 2017 17:52
Operator : SJ/MA
Sample : I1879-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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
2-Pentanone, 4-hy...	5.02	31.9	ng	1527290	1	6.85	958829	20.0
unknown6.62	6.62	75.4	ng	3614440	1	6.85	958829	20.0
Trichloroacetic a...	13.85	4.4	ng	354512	5	14.01	1610890	20.0
Octadecane	14.48	2.1	ng	169212	5	14.01	1610890	20.0
9-Octadecenamide,...	14.75	3.9	ng	209108	6	15.44	1080230	20.0
Benzo[e]pyrene	15.03	3.5	ng	189349	6	15.44	1080230	20.0
Eicosane	15.87	2.3	ng	125444	6	15.44	1080230	20.0