LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040216\
Data File : BF085993.D
Acq On : 2 Apr 2016 6:25
Operator : UM/SJ
Sample : H2079-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-NE-14

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-BF040216.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	5.367	284	287	310	rBV	1174971	1298386	36.60%	5.344%
2	6.407	376	378	387	rBV	882801	882783	24.89%	3.633%
3	6.533	387	389	392	rBV	1652071	2291745	64.61%	9.432%
4	6.773	408	410	416	rBV	733890	657975	18.55%	2.708%
5	6.922	421	423	426	rBV	1654890	2251195	63.46%	9.265%
6	7.345	457	460	462	rBV	1773888	1992058	56.16%	8.199%
7	8.053	520	522	525	rBV	843937	858603	24.20%	3.534%
8	9.139	614	617	619	rBV	2650883	3547314	100.00%	14.600%
9	9.528	649	651	654	rBV3	42513	53720	1.51%	0.221%
10	9.802	673	675	678	rBV	695509	950544	26.80%	3.912%
11	9.882	680	682	687	rVB	40012	49199	1.39%	0.202%
12	10.602	742	745	747	rBV	1882723	2189229	61.72%	9.010%
13	10.716	753	755	759	rVB	38422	53781	1.52%	0.221%
14	11.162	789	794	798	rBV2	56608	105861	2.98%	0.436%
15	11.288	803	805	808	rBV	1103124	1031091	29.07%	4.244%
16	11.825	850	852	858	rBV2	220097	274735	7.74%	1.131%
17	12.534	910	914	918	rBV2	33333	88905	2.51%	0.366%
18	12.614	918	921	927	rVV	230619	344348	9.71%	1.417%
19	12.694	927	928	932	rVB2	25713	42772	1.21%	0.176%
20	12.877	941	944	946	rBV	3296414	3221488	90.81%	13.259%
21	13.791	1020	1024	1032	rBV	52005	117734	3.32%	0.485%
22	13.928	1033	1036	1038	rBV	908677	992608	27.98%	4.085%
23	14.500	1084	1086	1089	rBV	159610	159427	4.49%	0.656%
24	14.682	1098	1102	1105	rBV2	30427	54566	1.54%	0.225%
25	15.334	1156	1159	1169	rVB	540505	786915	22.18%	3.239%

Sum of corrected areas: 24296982

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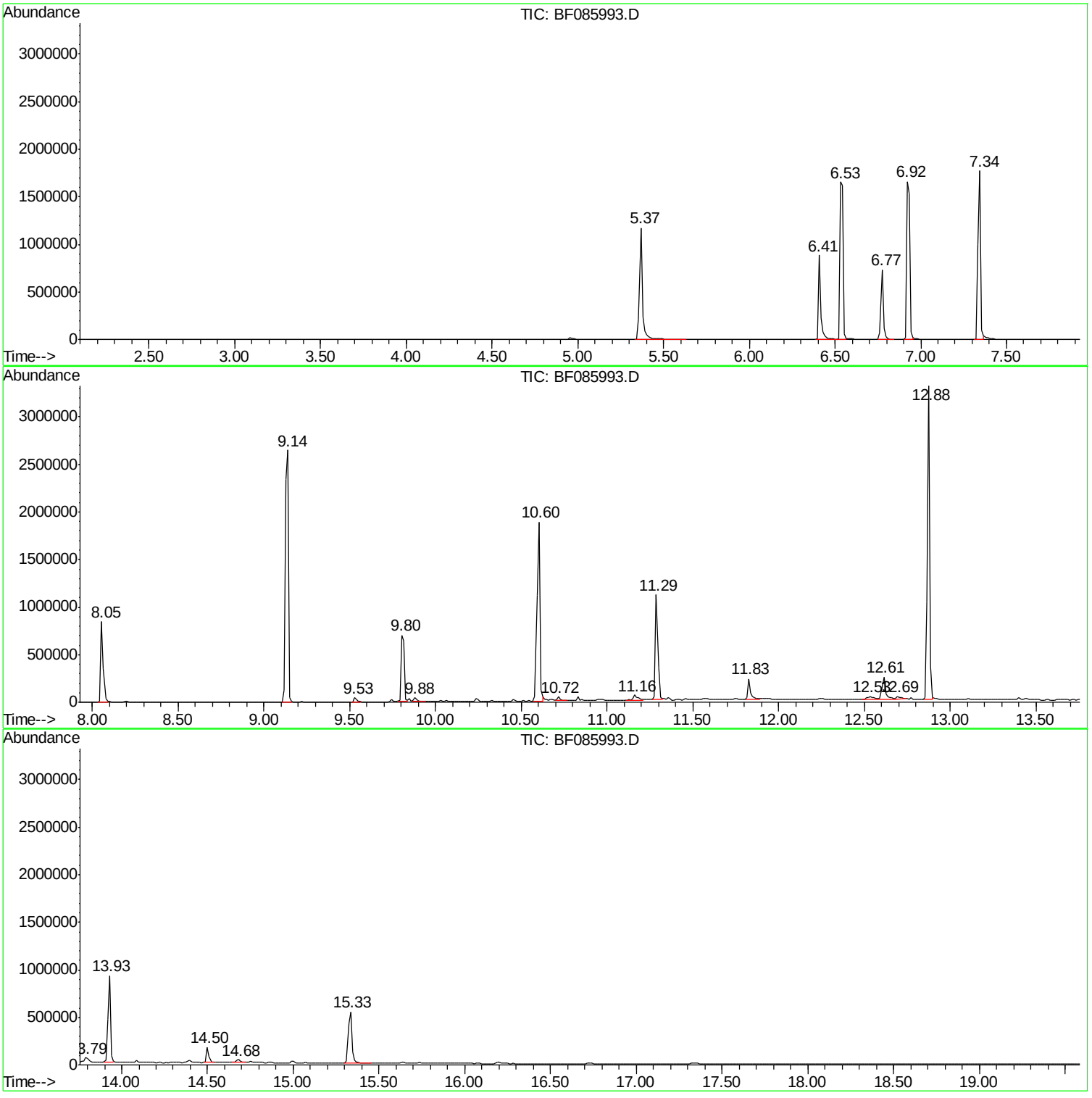
BNA_F
ClientSampleId :
DB-NE-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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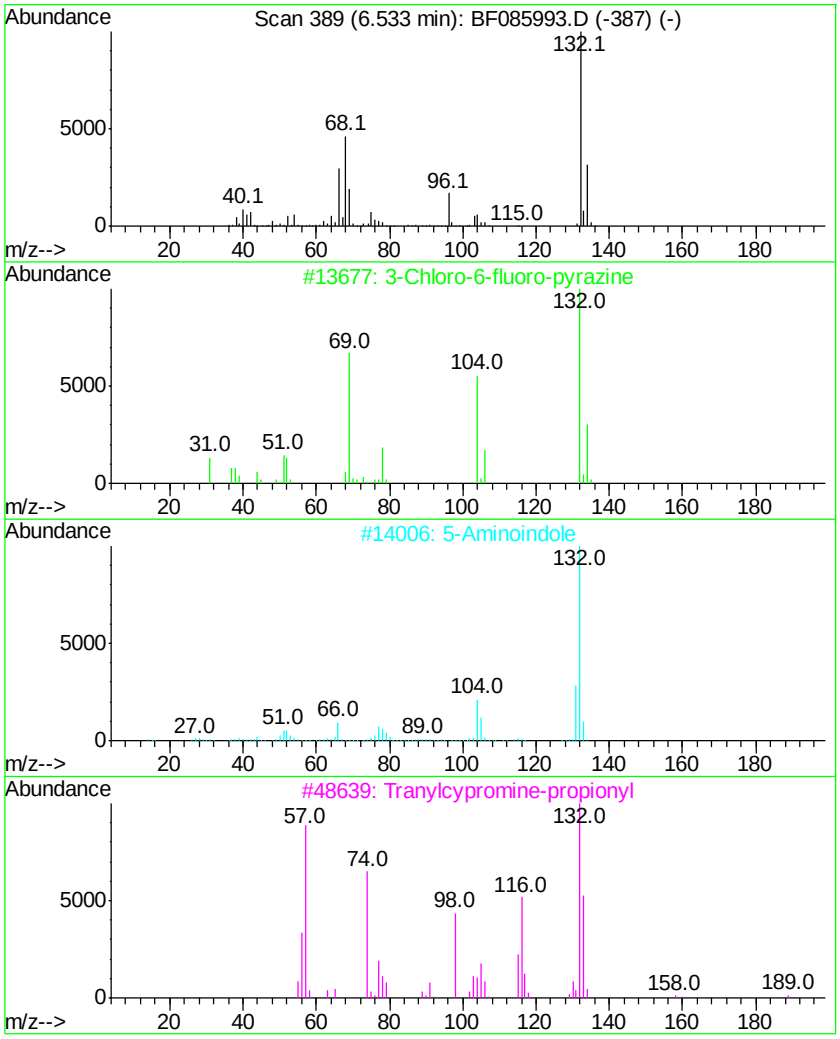
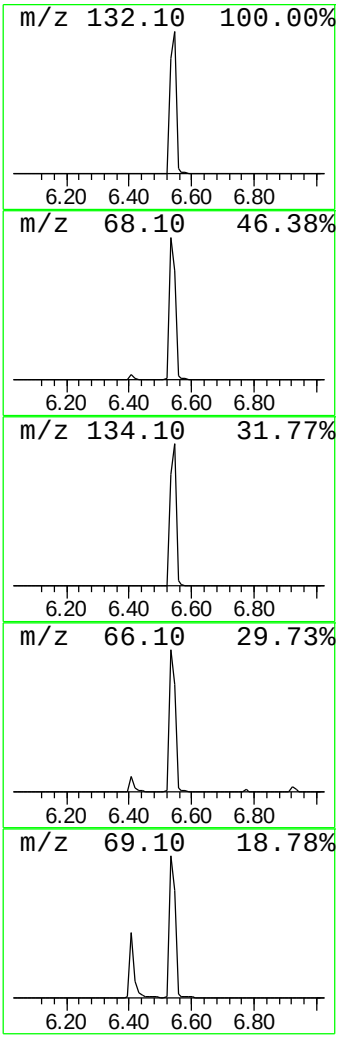
Peak Number 1 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	69.66 ng	2291750	1,4-Dichlorobenzene-d4	6.77

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
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TIC Library : C:\DATABASE\NIST02.L
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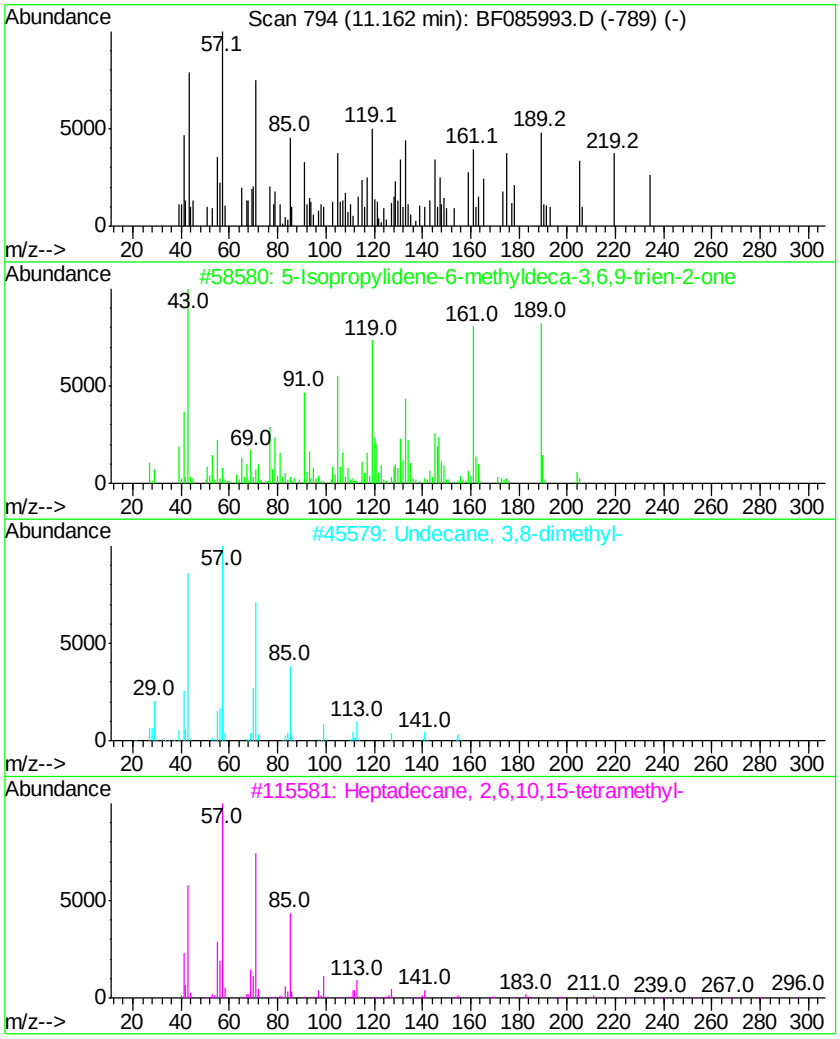
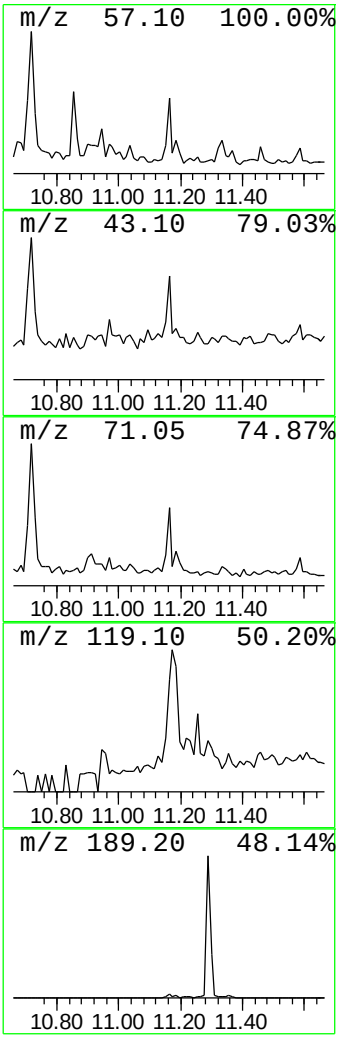
Peak Number 3 unknown11.16 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	2.05 ng	105861	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Isopropylidene-6-methyldeca-3,...	204	C14H20O	1000197-84-7	27
2	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	25
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	25
4	1-Octanol, 2,2-dimethyl-	158	C10H22O	002370-14-1	22
5	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	22





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Data File : BF085993.D
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Operator : UM/SJ
Sample : H2079-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-NE-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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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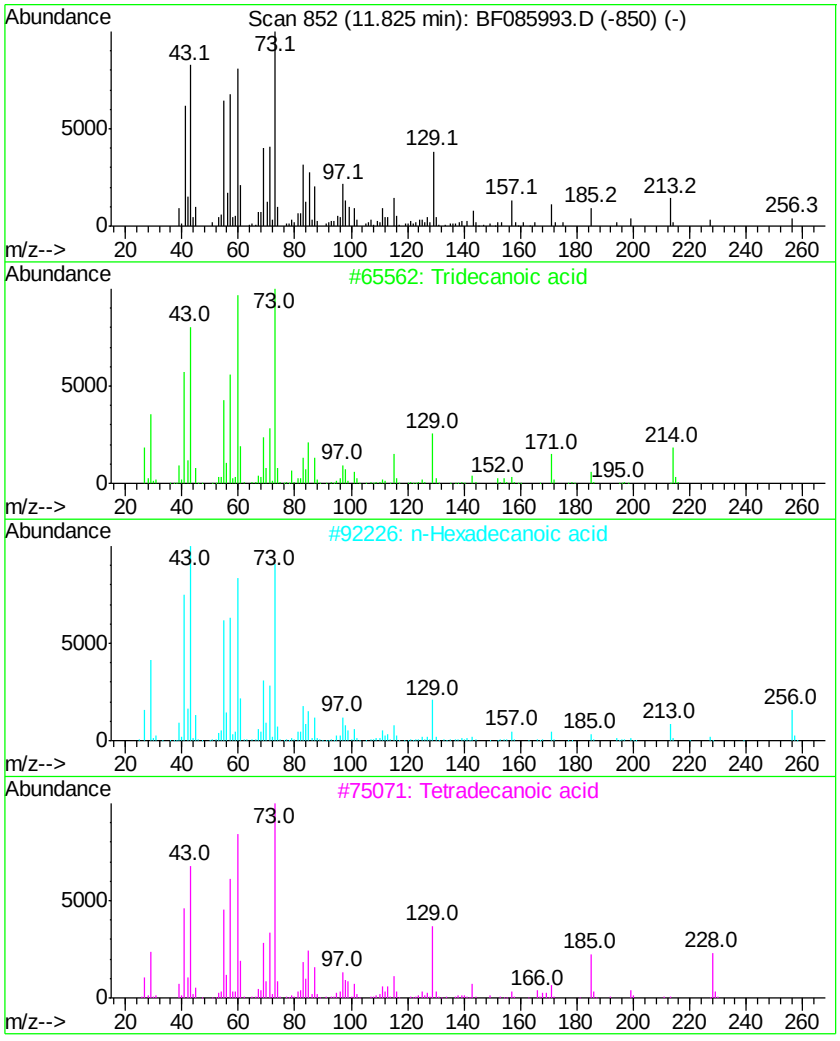
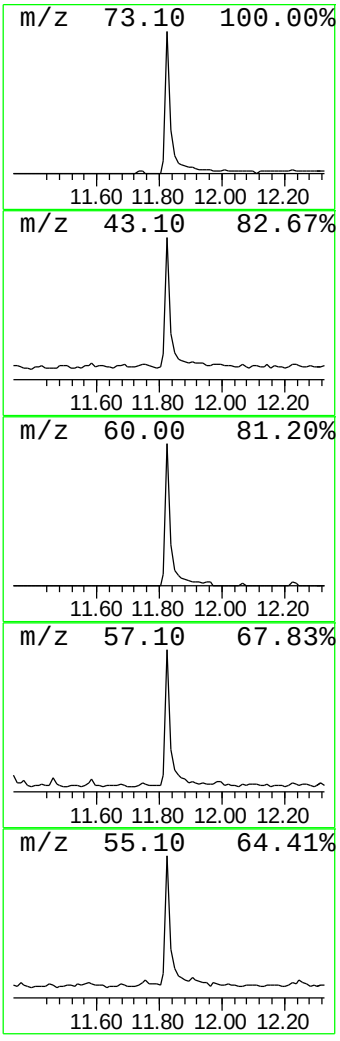
Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	5.33 ng	274735	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040216\
Data File : BF085993.D
Acq On : 2 Apr 2016 6:25
Operator : UM/SJ
Sample : H2079-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-NE-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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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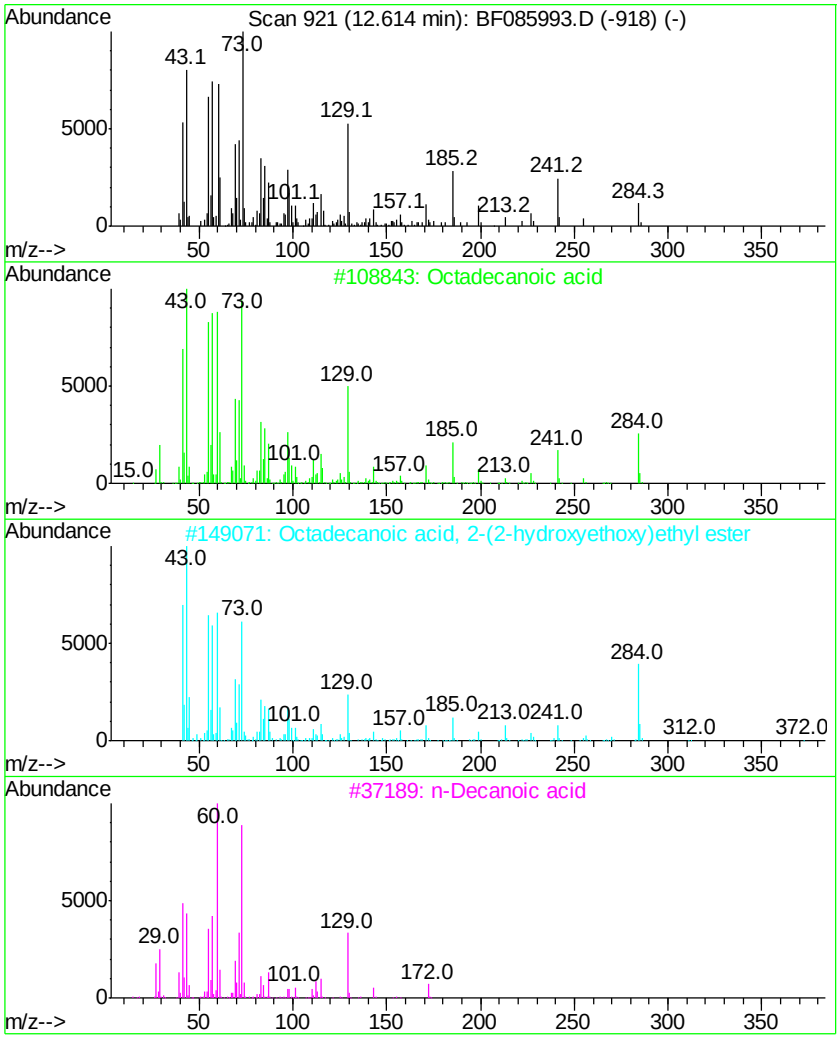
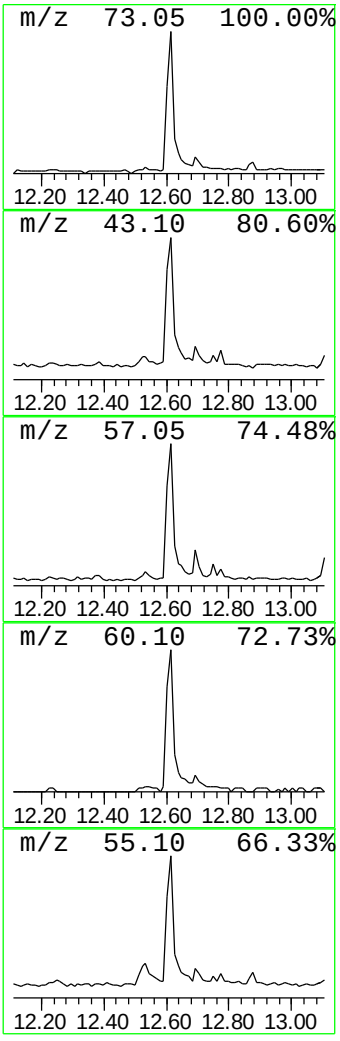
Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	6.94 ng	344348	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	30





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040216\
Data File : BF085993.D
Acq On : 2 Apr 2016 6:25
Operator : UM/SJ
Sample : H2079-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-NE-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.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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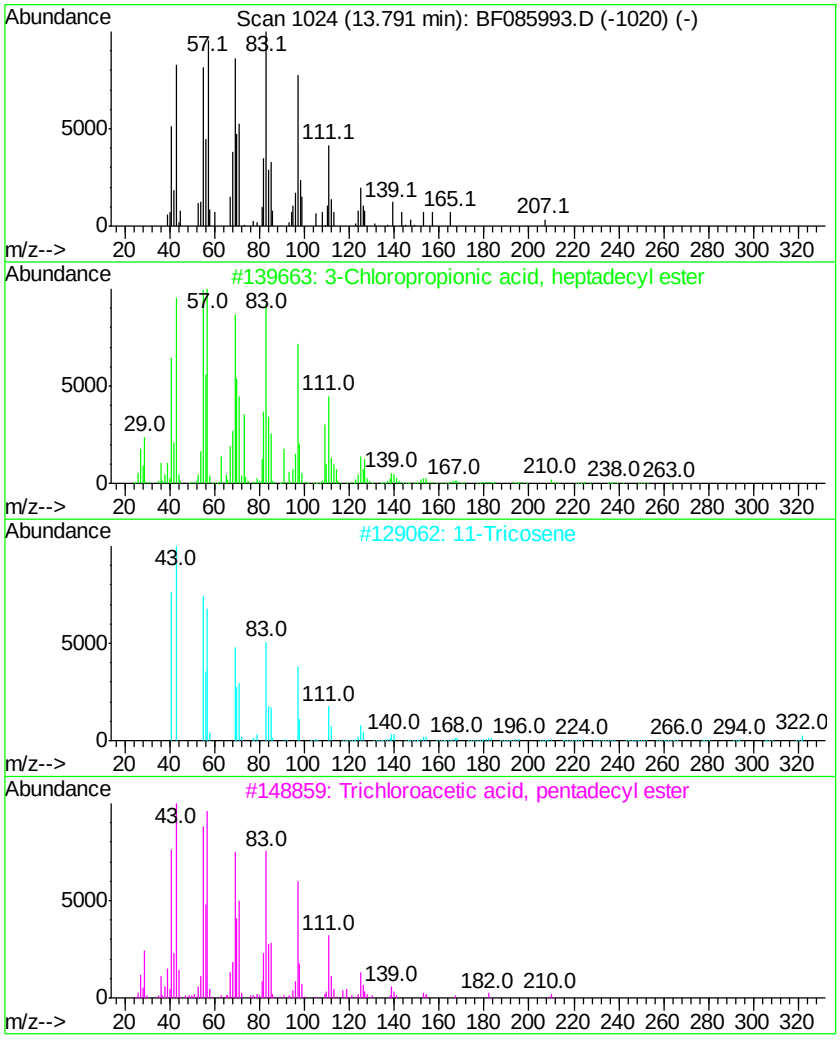
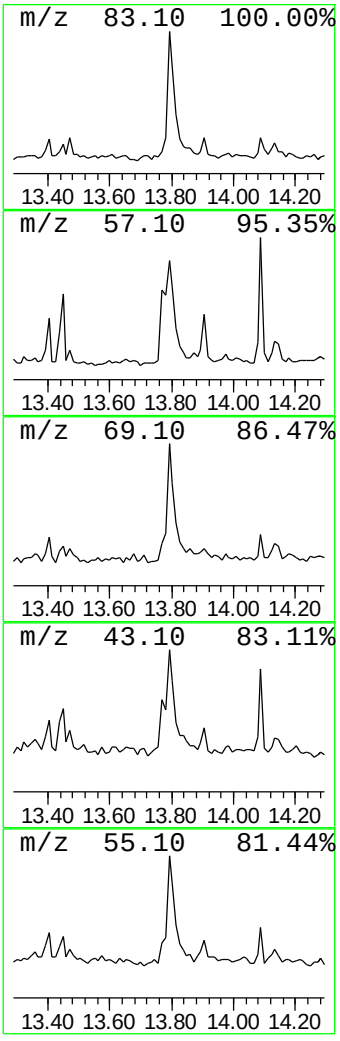
Peak Number 6 3-Chloropropionic acid, hep... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.37 ng	117734	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2	11-Tricosene	322	C23H46	052078-56-5	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Sample : H2079-01
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-NE-14

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

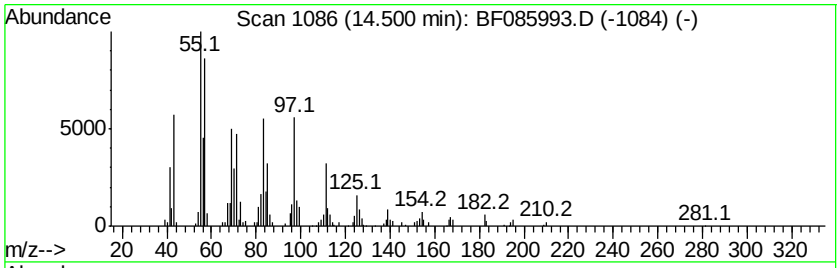
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

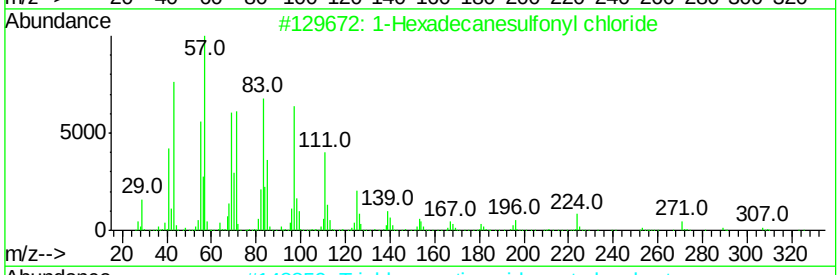
****

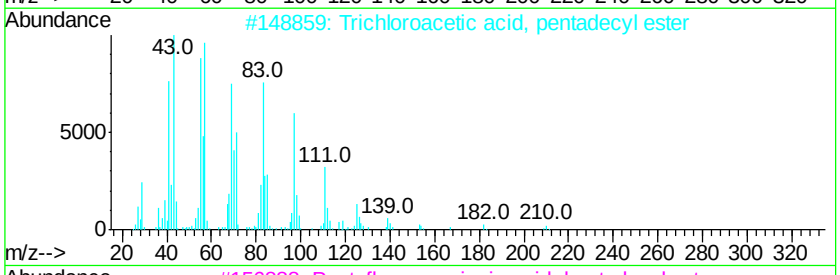
Peak Number 7 1-Hexadecanesulfonyl chloride Concentration Rank 5

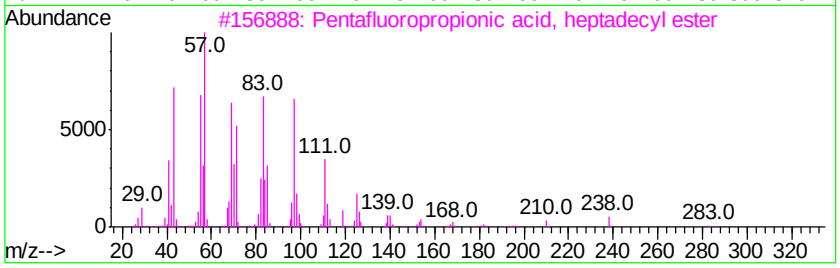
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	3.21 ng	159427	Chrysene-d12	13.93

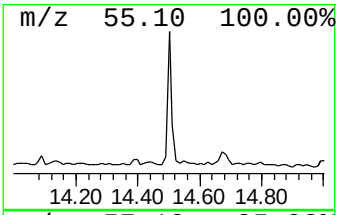
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	87
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	83
5	1-Docosene	308	C22H44	001599-67-3	83

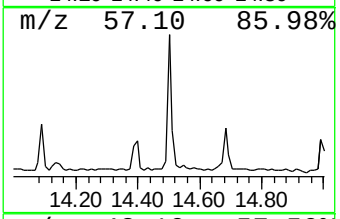


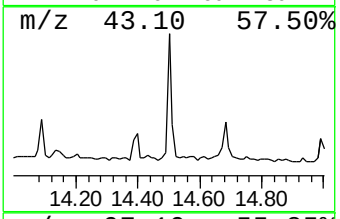


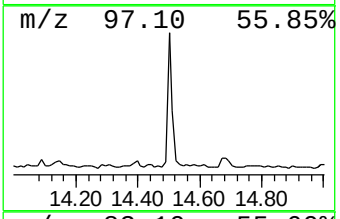


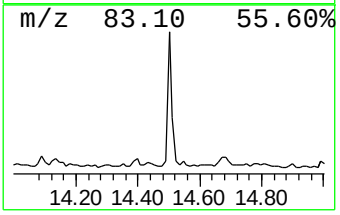












Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.53	6.53	69.7	ng	2291750	1	6.77	657975	20.0
unknown11.16	11.16	2.0	ng	105861	4	11.29	1031090	20.0
Tridecanoic acid	11.83	5.3	ng	274735	4	11.29	1031090	20.0
Octadecanoic acid	12.61	6.9	ng	344348	5	13.93	992608	20.0
3-Chloropropionic...	13.79	2.4	ng	117734	5	13.93	992608	20.0
1-Hexadecanesulfo...	14.50	3.2	ng	159427	5	13.93	992608	20.0