LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091216\
Data File : BF090068.D
Acq On : 12 Sep 2016 17:28
Operator : UM/SJ
Sample : H4744-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1B

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-BF083116.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	1.713	9	11	63	rVB	4944578	13317023	100.00%	24.710%
2	4.696	269	272	286	rBV	570821	1018609	7.65%	1.890%
3	5.153	309	312	314	rBV	3647597	4099472	30.78%	7.607%
4	6.227	403	406	408	rBV	3559143	3795697	28.50%	7.043%
5	6.342	413	416	419	rVV	3920055	3916062	29.41%	7.266%
6	6.570	434	436	439	rBV	793087	1048449	7.87%	1.945%
7	6.730	448	450	453	rBV	3272810	3046621	22.88%	5.653%
8	7.142	483	486	489	rBV	1999274	2201475	16.53%	4.085%
9	7.862	547	549	551	rBV	1554029	1378769	10.35%	2.558%
10	8.948	641	644	646	rBV	2827137	4135981	31.06%	7.675%
11	9.336	676	678	681	rBV	982763	1046011	7.85%	1.941%
12	9.610	699	702	704	rBV	1124956	1422960	10.69%	2.640%
13	10.388	767	770	773	rBV	2169716	2198612	16.51%	4.080%
14	10.696	795	797	799	rBV	410982	343323	2.58%	0.637%
15	11.073	828	830	835	rVV2	1324181	1490772	11.19%	2.766%
16	11.325	850	852	857	rBV	365382	387552	2.91%	0.719%
17	12.136	921	923	927	rBV2	141773	219290	1.65%	0.407%
18	12.274	933	935	939	rBV	406105	396689	2.98%	0.736%
19	12.502	952	955	957	rBV	326852	409975	3.08%	0.761%
20	12.662	966	969	971	rBV	3150809	3348343	25.14%	6.213%
21	12.799	979	981	986	rVB	314062	340538	2.56%	0.632%
22	13.565	1046	1048	1052	rVB	180608	202467	1.52%	0.376%
23	13.691	1056	1059	1063	rVV2	1555807	2008515	15.08%	3.727%
24	13.748	1063	1064	1066	rVV	142726	153712	1.15%	0.285%
25	13.908	1076	1078	1083	rVB2	95217	139363	1.05%	0.259%
26	14.468	1125	1127	1130	rBV	179444	301436	2.26%	0.559%
27	14.674	1142	1145	1151	rVB	141583	264219	1.98%	0.490%
28	15.028	1174	1176	1181	rVV	665804	838027	6.29%	1.555%
29	18.366	1464	1468	1476	rVB4	144815	422385	3.17%	0.784%

Sum of corrected areas: 53892347

LSC Report - Integrated Chromatogram

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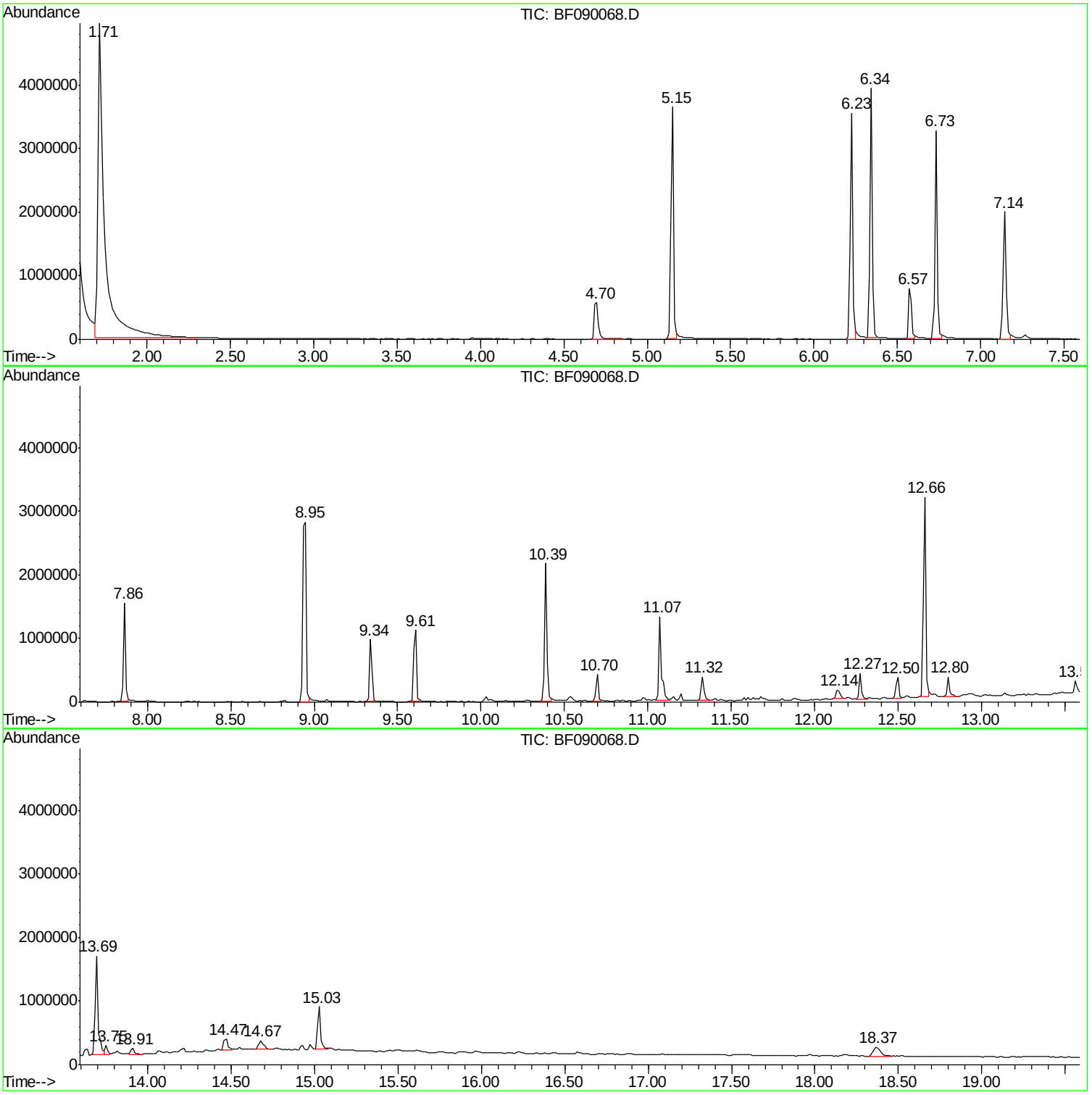
Data File : BF090068.D
Acq On : 12 Sep 2016 17:28
Operator : UM/SJ
Sample : H4744-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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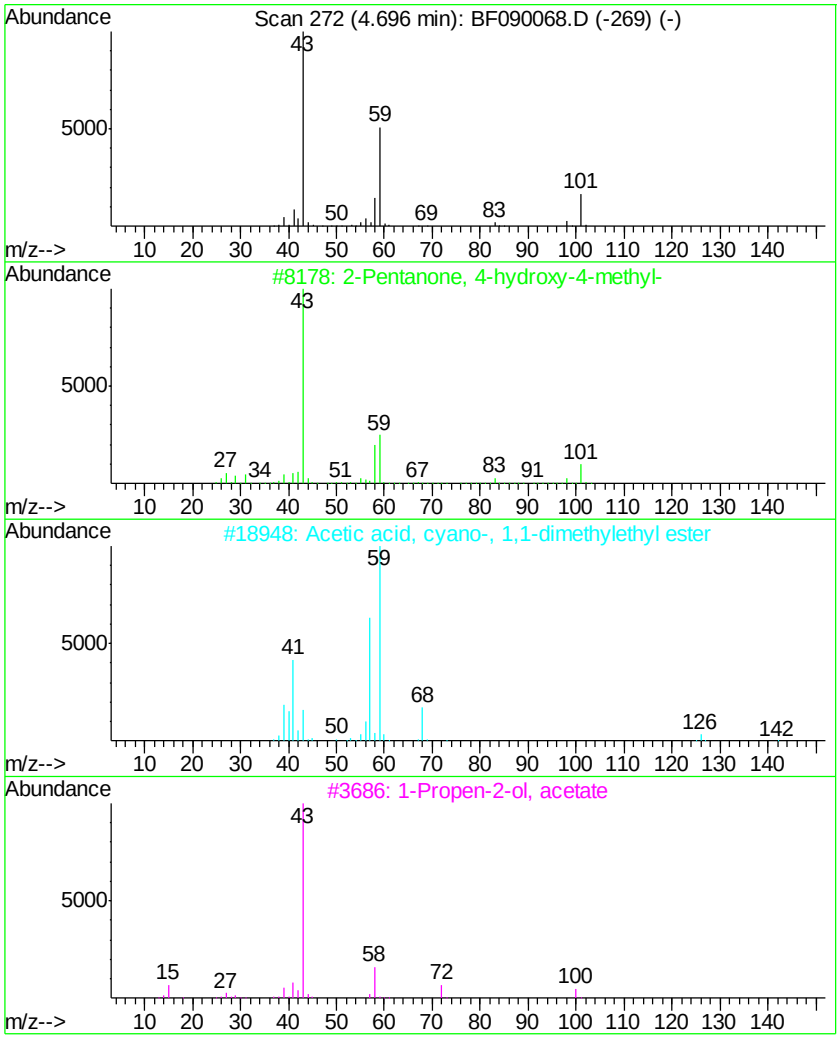
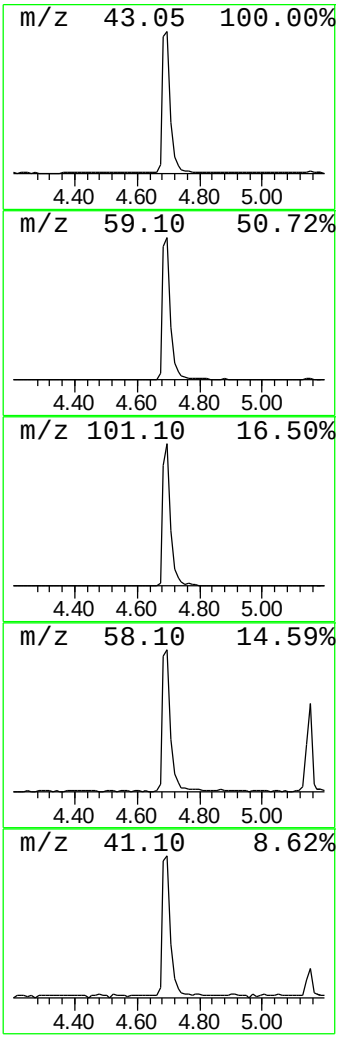
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	19.43 ng	1018610	1,4-Dichlorobenzene-d4	6.57

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Sample : H4744-04
Misc :
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Instrument : BNA_F
ClientSampleId : SP-1B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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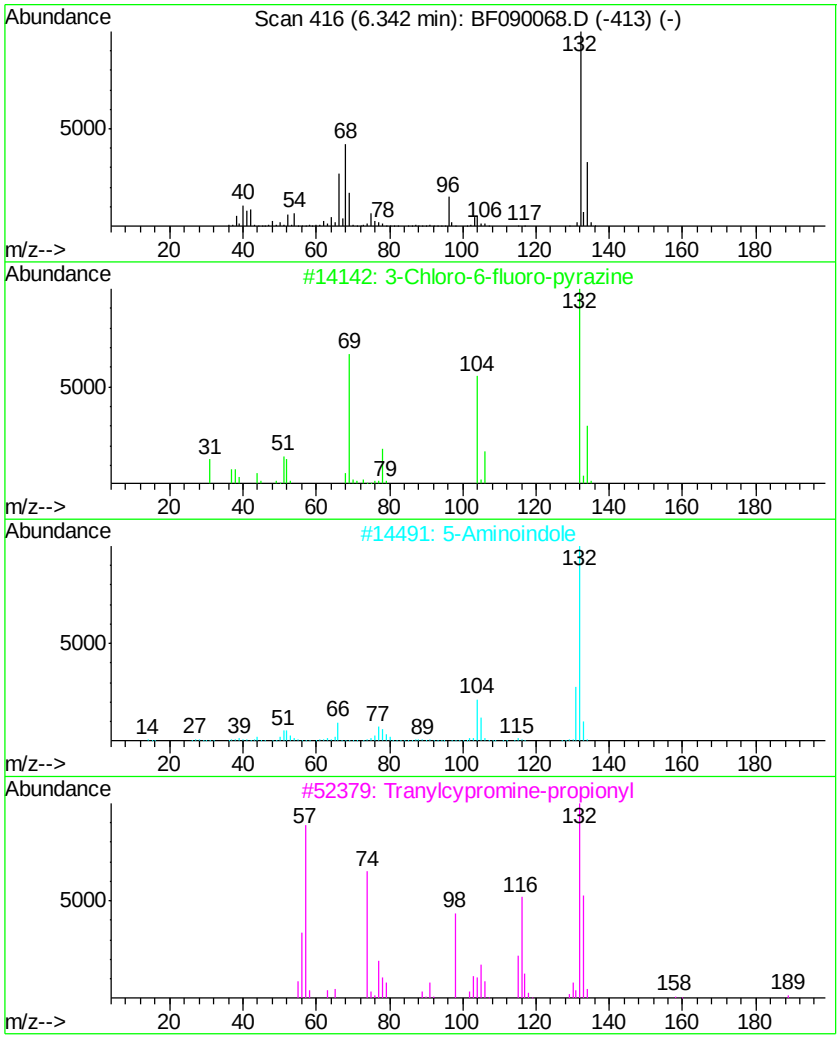
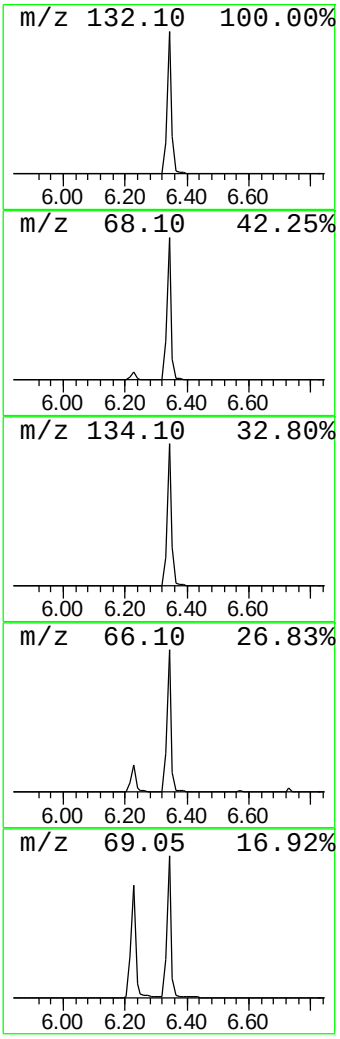
Peak Number 3 unknown6.34 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	74.70 ng	3916060	1,4-Dichlorobenzene-d4	6.57

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Misc :
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Instrument : BNA_F
ClientSampleId : SP-1B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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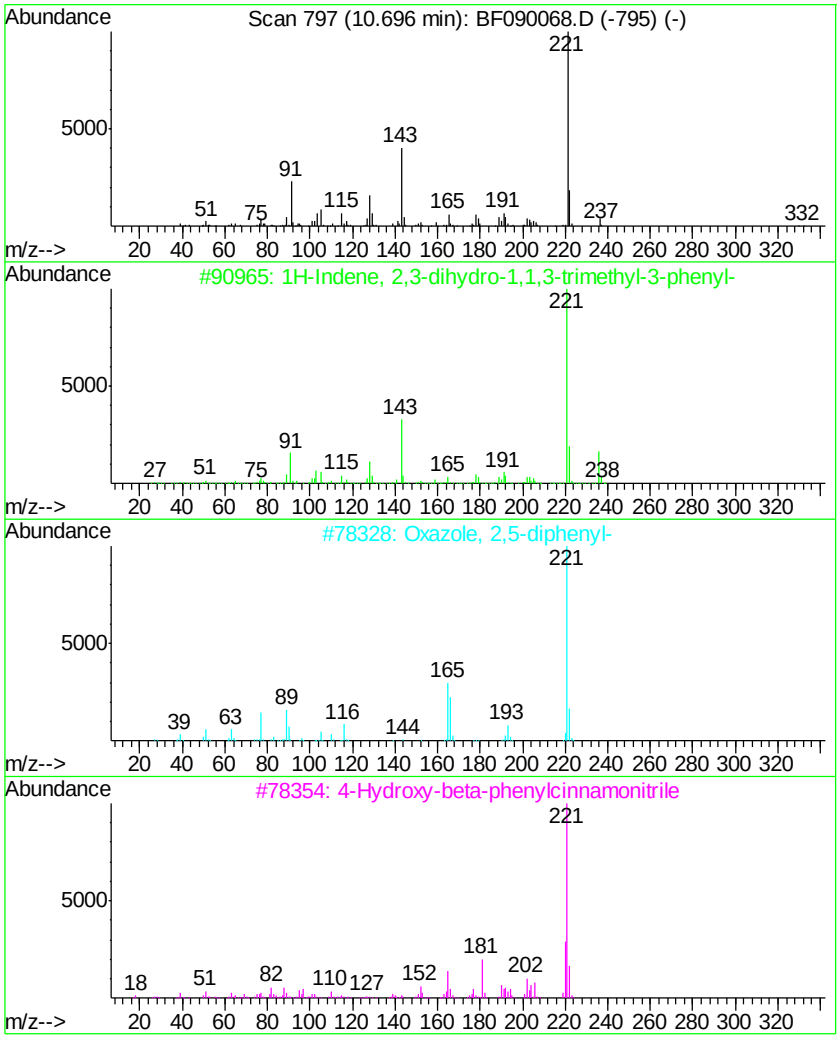
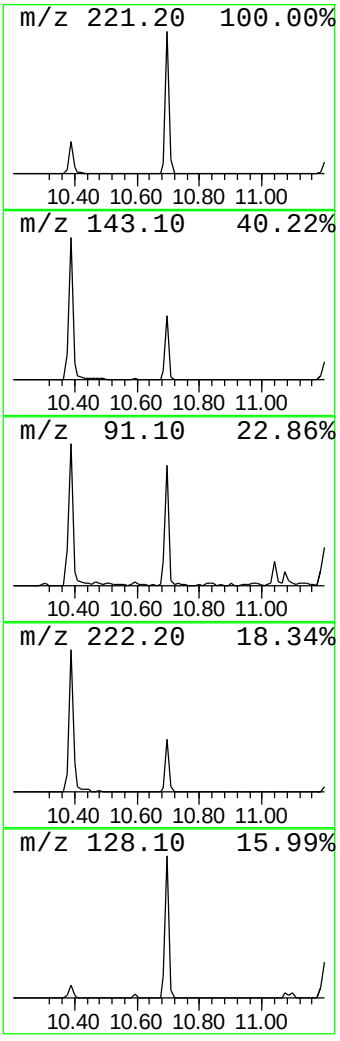
Peak Number 5 1H-Indene, 2,3-dihydro-1,1,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	4.61 ng	343323	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	90
2	Oxazole, 2,5-diphenyl-	221	C15H11NO	000092-71-7	43
3	4-Hydroxy-beta-phenylcinnamonitrile	221	C15H11NO	016281-90-6	43
4	Benzene, 1-methoxy-4-[(4-pentylp...	278	C20H22O	039969-28-3	37
5	4,6-Dimethyl-2-thioxo-1,2-dihydr...	278	C14H22N2SSi	1000332-68-8	37





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Sample : H4744-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

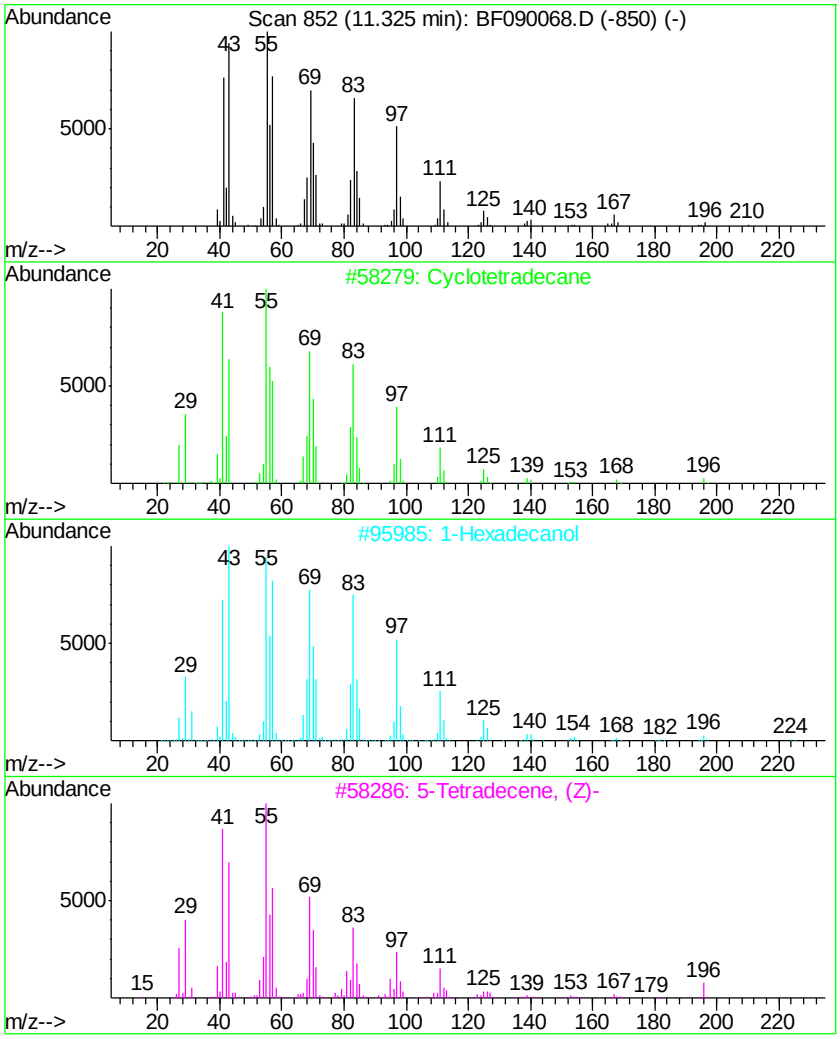
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

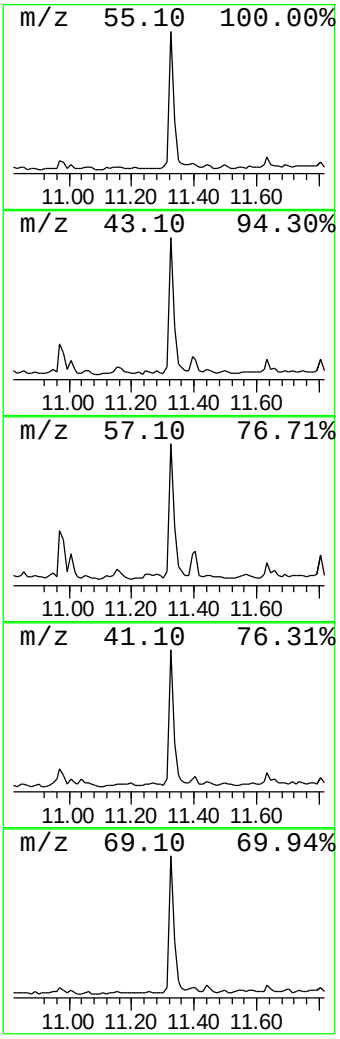
****

Peak Number 6 Cyclotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.32	5.20 ng	387552	Phenanthrene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	95
2	1-Hexadecanol	242	C16H34O	036653-82-4	95
3	5-Tetradecene, (Z)-	196	C14H28	041446-62-2	91
4	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
5	n-Pentadecanol	228	C15H32O	000629-76-5	91





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Sample : H4744-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1B

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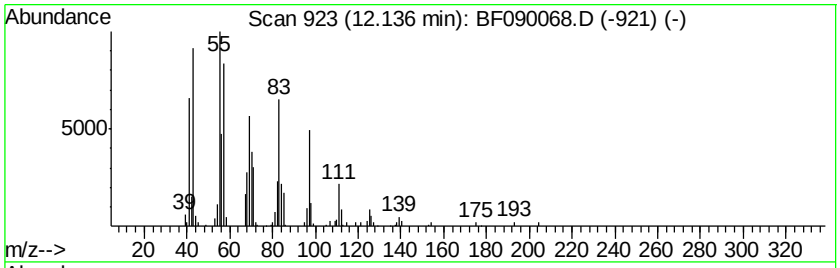
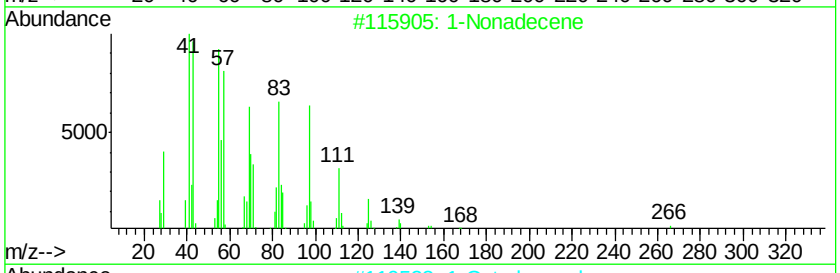
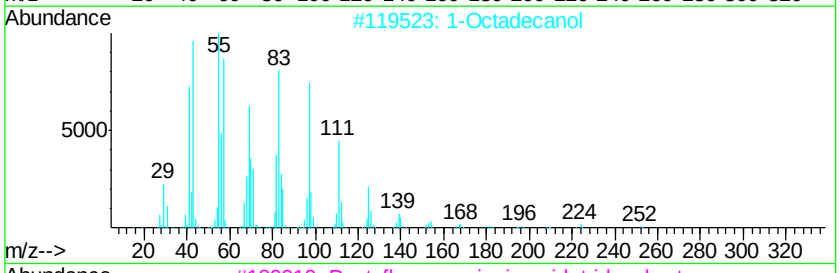
Peak Number 7 1-Nonadecene Concentration Rank 10

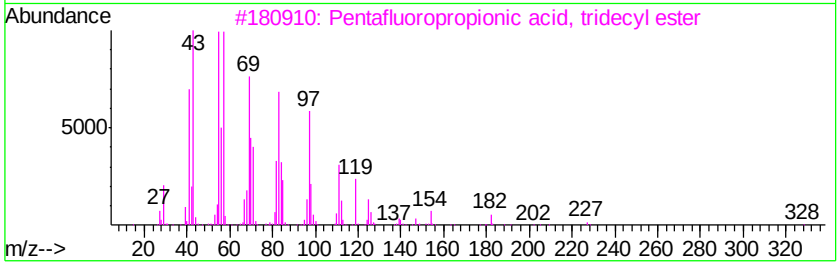
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	2.94 ng	219290	Phenanthrene-d10	11.07

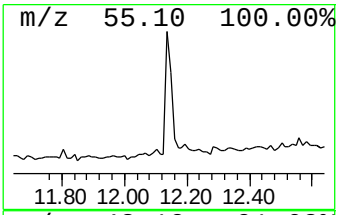
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	1-Octadecanol	270	C18H38O	000112-92-5	91
3	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91

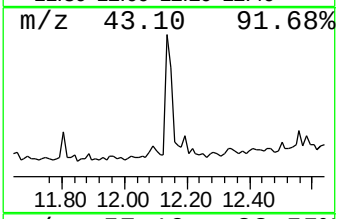


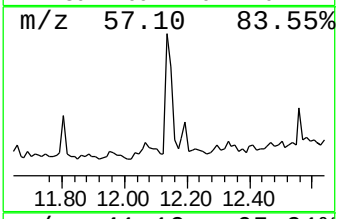


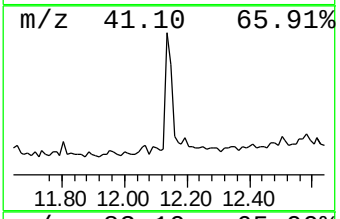


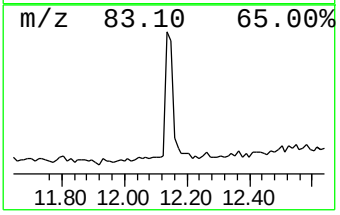












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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

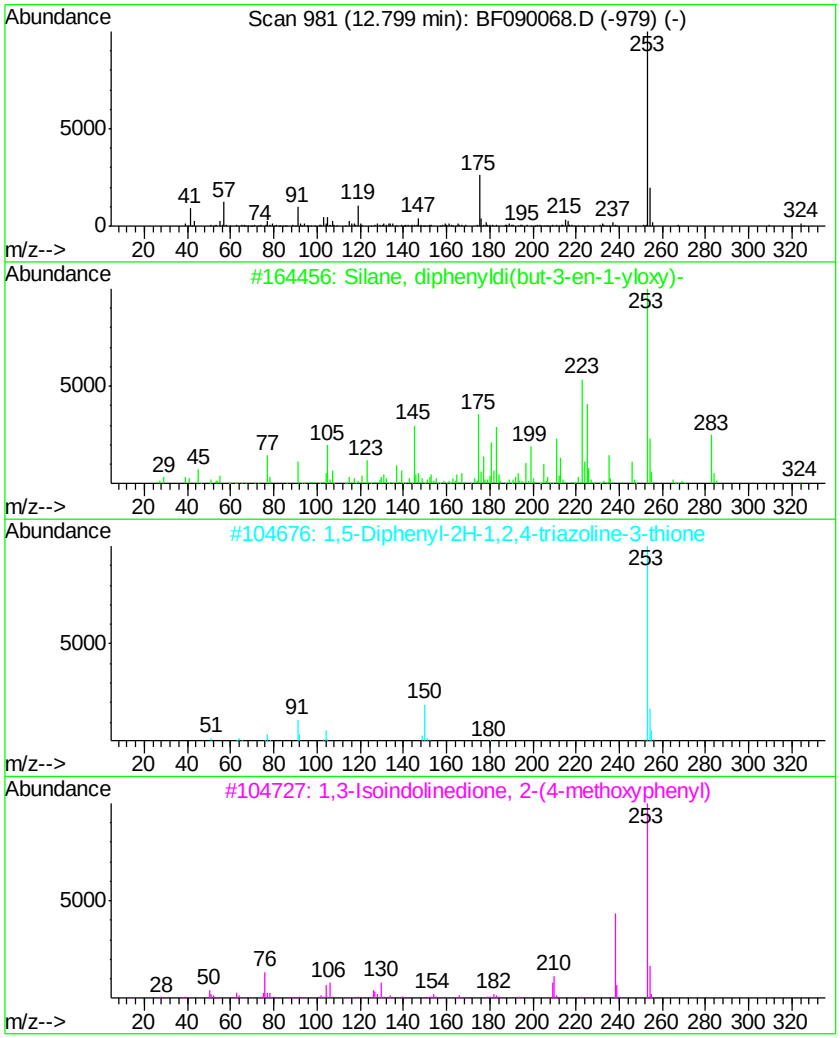
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

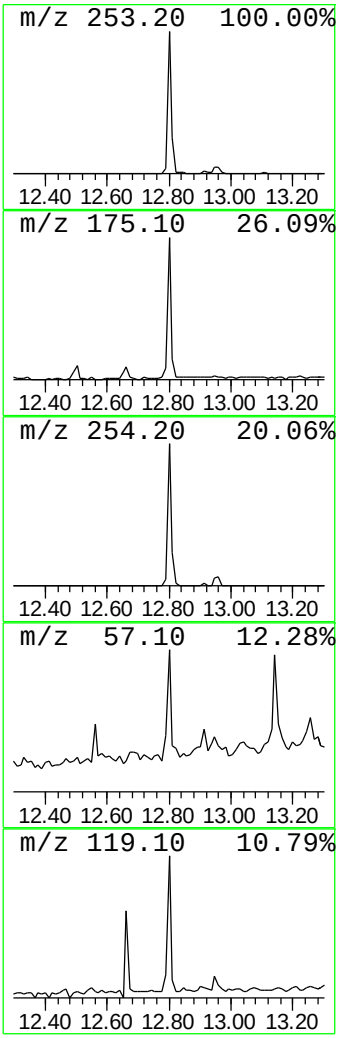
****

Peak Number 8 Silane, diphenyldi(but-3-en... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	3.39 ng	340538	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, diphenyldi(but-3-en-1-yl...	324	C20H24O2Si	1000367-84-9	50
2	1,5-Diphenyl-2H-1,2,4-triazoline...	253	C14H11N3S	005055-74-3	50
3	1,3-Isoindolinedione, 2-(4-metho...	253	C15H11NO3	002142-04-3	40
4	Phthalic acid, di(3-ethylphenyl)...	374	C24H22O4	1000357-08-4	40
5	Phthalic acid, di(2,3-dimethylph...	374	C24H22O4	1000357-09-2	40





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TIC Library : C:\Database\NIST11.L
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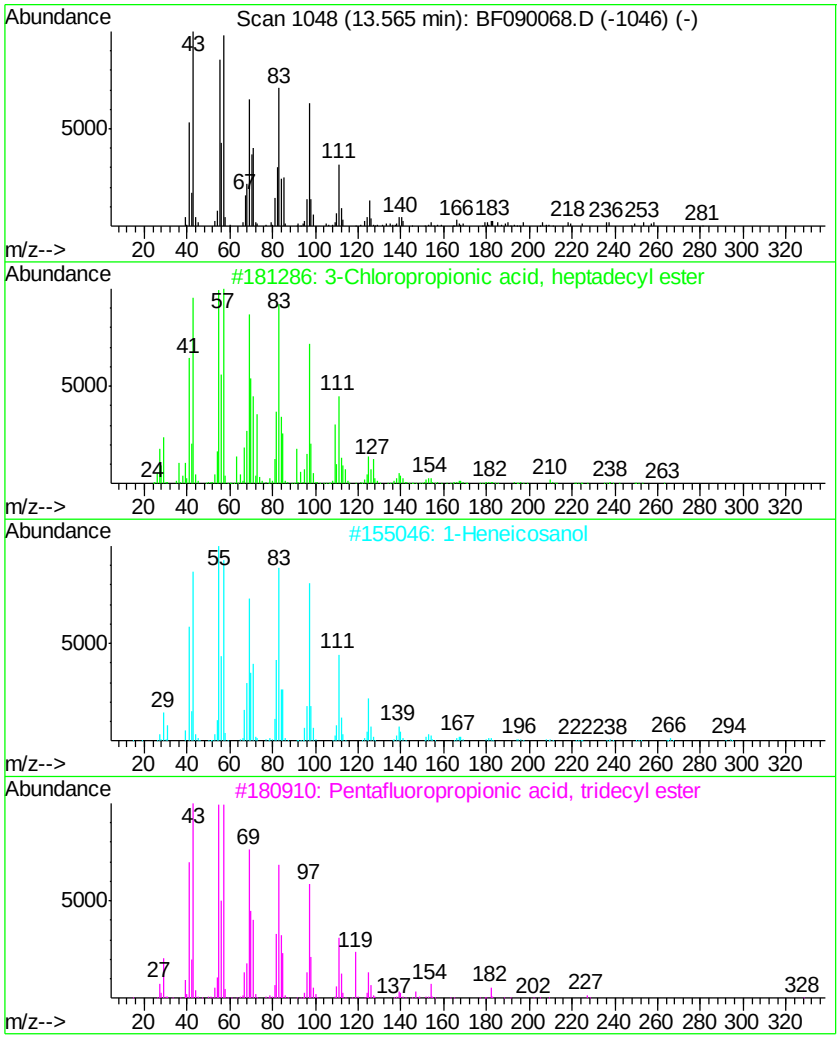
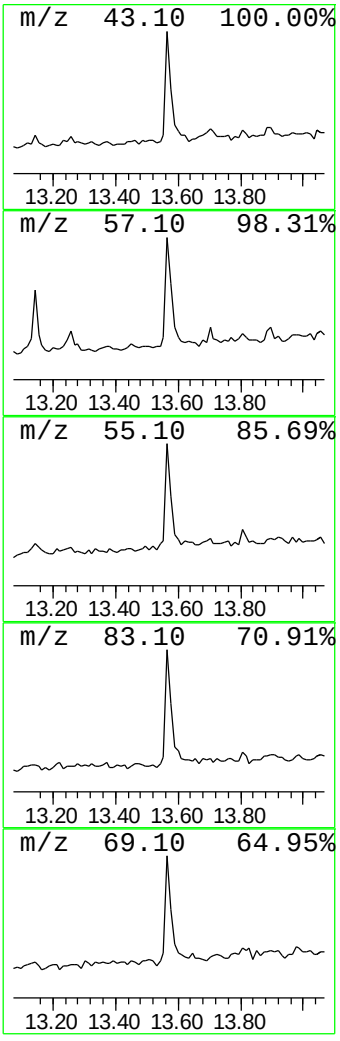
Peak Number 9 3-Chloropropionic acid, hep... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	2.02 ng	202467	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94





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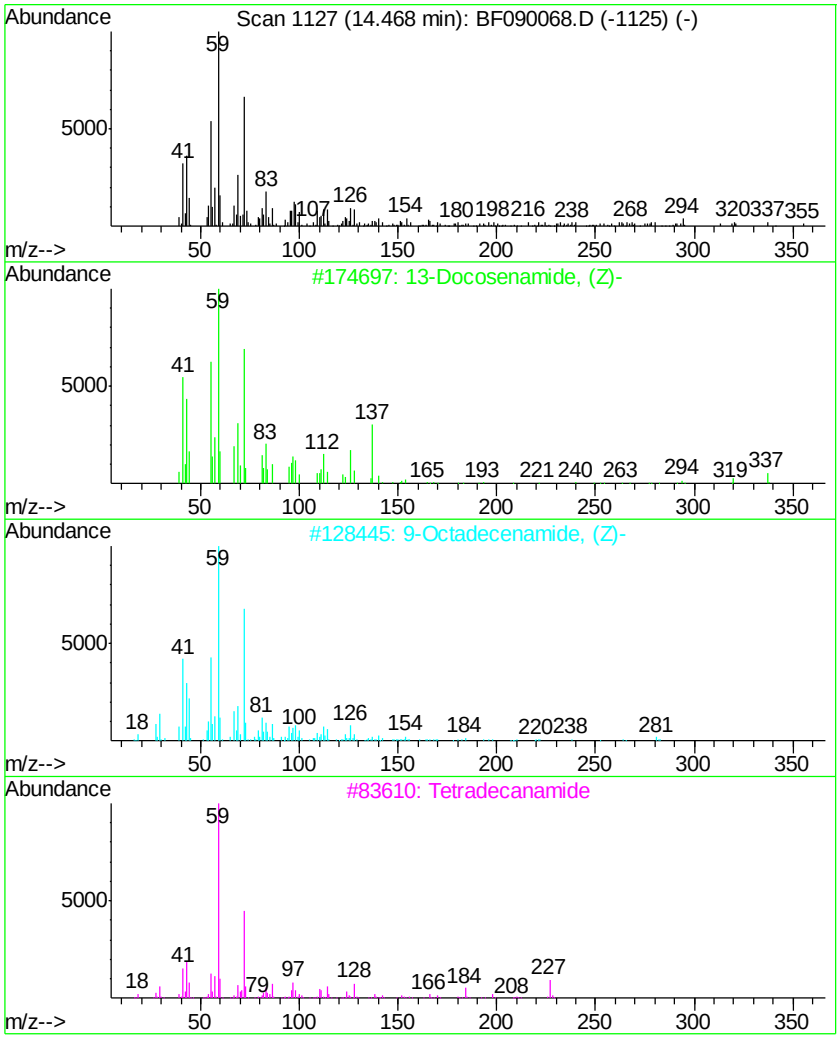
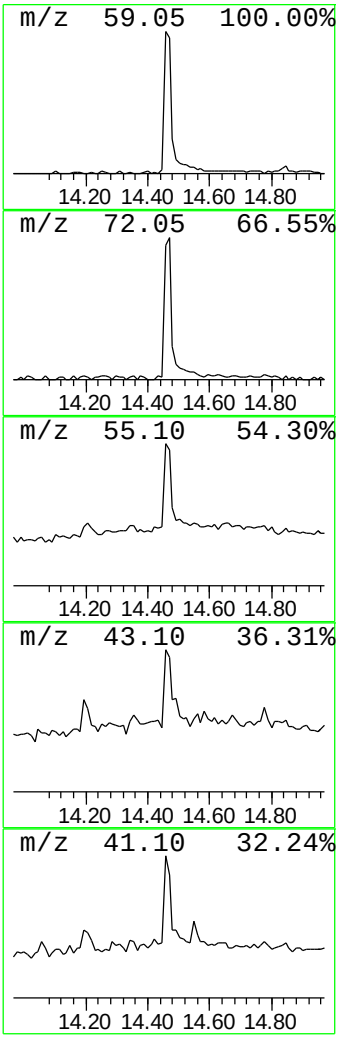
****

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	7.19 ng	301436	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Tetradecanamide	227	C14H29NO	000638-58-4	72
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	58
5	Octadecanamide	283	C18H37NO	000124-26-5	53





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091216\
Data File : BF090068.D
Acq On : 12 Sep 2016 17:28
Operator : UM/SJ
Sample : H4744-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

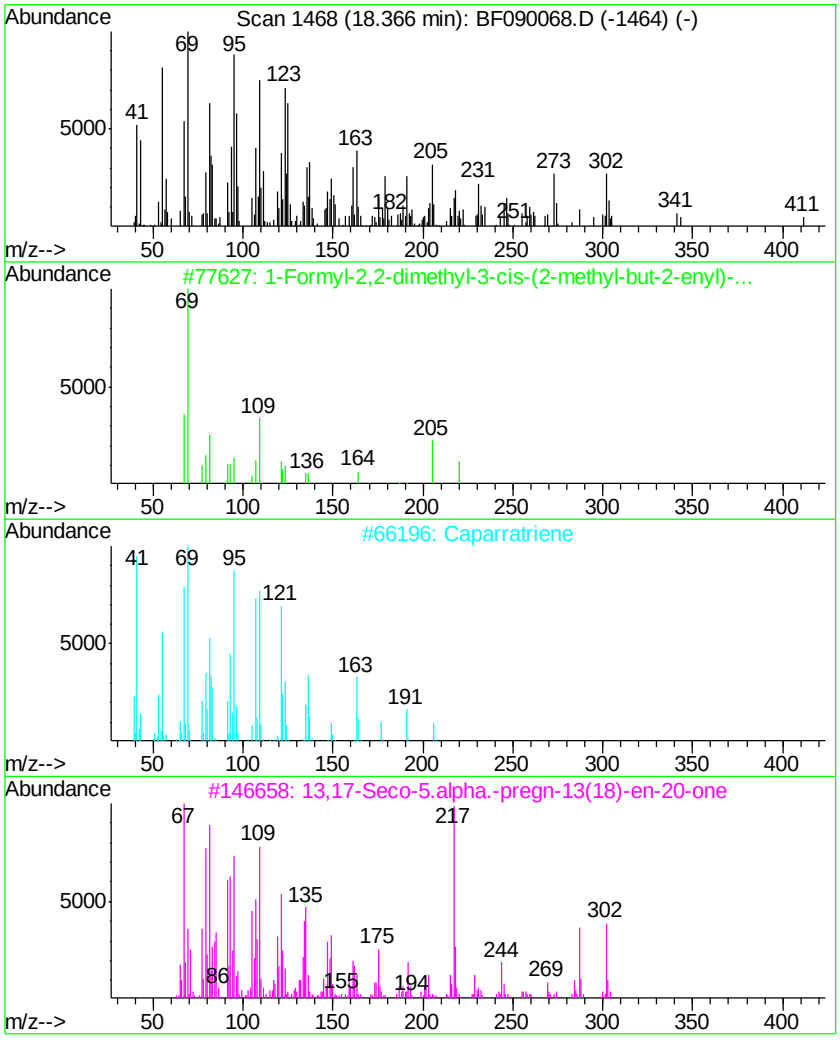
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

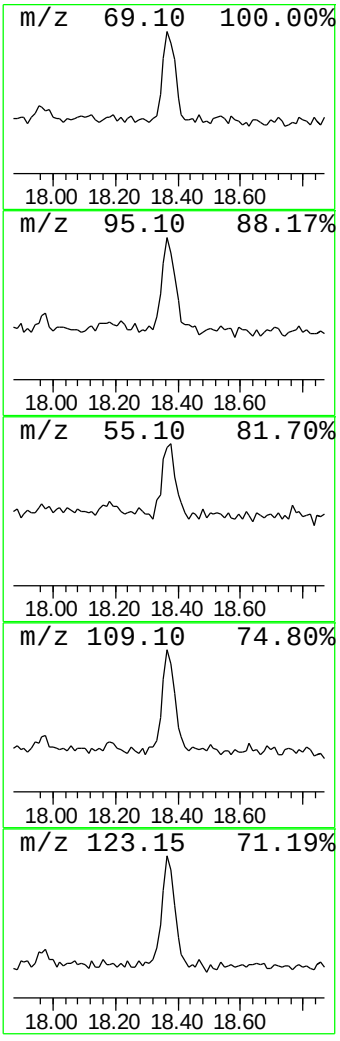
****

Peak Number 11 1-Formyl-2,2-dimethyl-3-cis... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	10.08 ng	422385	Perylene-d12	15.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Formyl-2,2-dimethyl-3-cis-(2-m...	220	C15H24O	1000144-10-0	50
2	Caparratriene	206	C15H26	1000374-08-7	49
3	13,17-Seco-5.alpha.-pregn-13(18)...	302	C21H34O	031239-27-7	45
4	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	40
5	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091216\
Data File : BF090068.D
Acq On : 12 Sep 2016 17:28
Operator : UM/SJ
Sample : H4744-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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...	4.70	19.4	ng	1018610	1	6.57	1048450	20.0
unknown6.34	6.34	74.7	ng	3916060	1	6.57	1048450	20.0
1H-Indene, 2,3-di...	10.70	4.6	ng	343323	4	11.07	1490770	20.0
Cyclotetradecane	11.32	5.2	ng	387552	4	11.07	1490770	20.0
1-Nonadecene	12.14	2.9	ng	219290	4	11.07	1490770	20.0
Silane, diphenyld...	12.80	3.4	ng	340538	5	13.69	2008520	20.0
3-Chloropropionic...	13.57	2.0	ng	202467	5	13.69	2008520	20.0
13-Docosenamide, ...	14.47	7.2	ng	301436	6	15.03	838027	20.0
1-Formyl-2,2-dime...	18.37	10.1	ng	422385	6	15.03	838027	20.0