

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
 Data File : BF086965.D
 Acq On : 13 May 2016 10:06
 Operator : UM/SJ
 Sample : H2916-05
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VITALE-FILL-CSPH3-5K

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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	1.633	3	4	12	rVB	521138	783142	14.10%	1.596%
2	1.747	12	14	50	rVB	2074158	5060844	91.11%	10.315%
3	4.764	276	278	290	rBV	432236	751148	13.52%	1.531%
4	5.221	315	318	320	rBV	4486429	5048345	90.88%	10.289%
5	5.621	351	353	358	rVB	54234	84205	1.52%	0.172%
6	6.296	408	412	414	rBV	4100156	5554688	100.00%	11.321%
7	6.399	418	421	423	rBV	4856869	5061870	91.13%	10.317%
8	6.616	438	440	443	rBV	692105	919560	16.55%	1.874%
9	6.776	452	454	457	rBV	3502992	3464561	62.37%	7.061%
10	7.199	488	491	493	rBV	3237249	3401984	61.25%	6.934%
11	7.325	500	502	508	rVB	63408	99650	1.79%	0.203%
12	7.907	551	553	556	rBV	1244765	1115050	20.07%	2.273%
13	8.993	645	648	650	rBV	4266943	4673023	84.13%	9.524%
14	9.119	657	659	661	rBV	115011	110315	1.99%	0.225%
15	9.393	680	683	685	rBV	756375	839221	15.11%	1.710%
16	9.599	699	701	703	rBV	98753	94703	1.70%	0.193%
17	9.656	703	706	708	rVV	1155665	1040918	18.74%	2.122%
18	10.102	743	745	746	rVB	169735	132820	2.39%	0.271%
19	10.319	761	764	767	rBV	55268	80363	1.45%	0.164%
20	10.445	772	775	778	rBV	2452914	2375579	42.77%	4.842%
21	10.571	784	786	793	rVB	181605	228354	4.11%	0.465%
22	11.016	823	825	826	rBV	98356	81422	1.47%	0.166%
23	11.131	833	835	838	rBV	925365	809271	14.57%	1.649%
24	11.382	854	857	861	rBV	241704	499765	9.00%	1.019%
25	11.439	861	862	865	rVB	66129	66088	1.19%	0.135%
26	11.679	881	883	889	rBV	112096	153497	2.76%	0.313%
27	12.194	926	928	934	rBV	699067	1118357	20.13%	2.279%
28	12.548	957	959	962	rBV	61048	76755	1.38%	0.156%
29	12.719	971	974	976	rBV	3519541	3267551	58.83%	6.660%
30	13.074	1003	1005	1008	rBV	64292	104681	1.88%	0.213%
31	13.177	1011	1014	1016	rBV	78342	118967	2.14%	0.242%
32	13.257	1019	1021	1023	rBV2	55709	72044	1.30%	0.147%
33	13.634	1051	1054	1061	rVB	80954	188994	3.40%	0.385%
34	13.759	1062	1065	1067	rBV	937901	869762	15.66%	1.773%

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35	15.120	1182	1184	1186	rBV	588533	660033	11.88%	1.345%
36	16.617	1313	1315	1320	rVB3	30502	56707	1.02%	0.116%

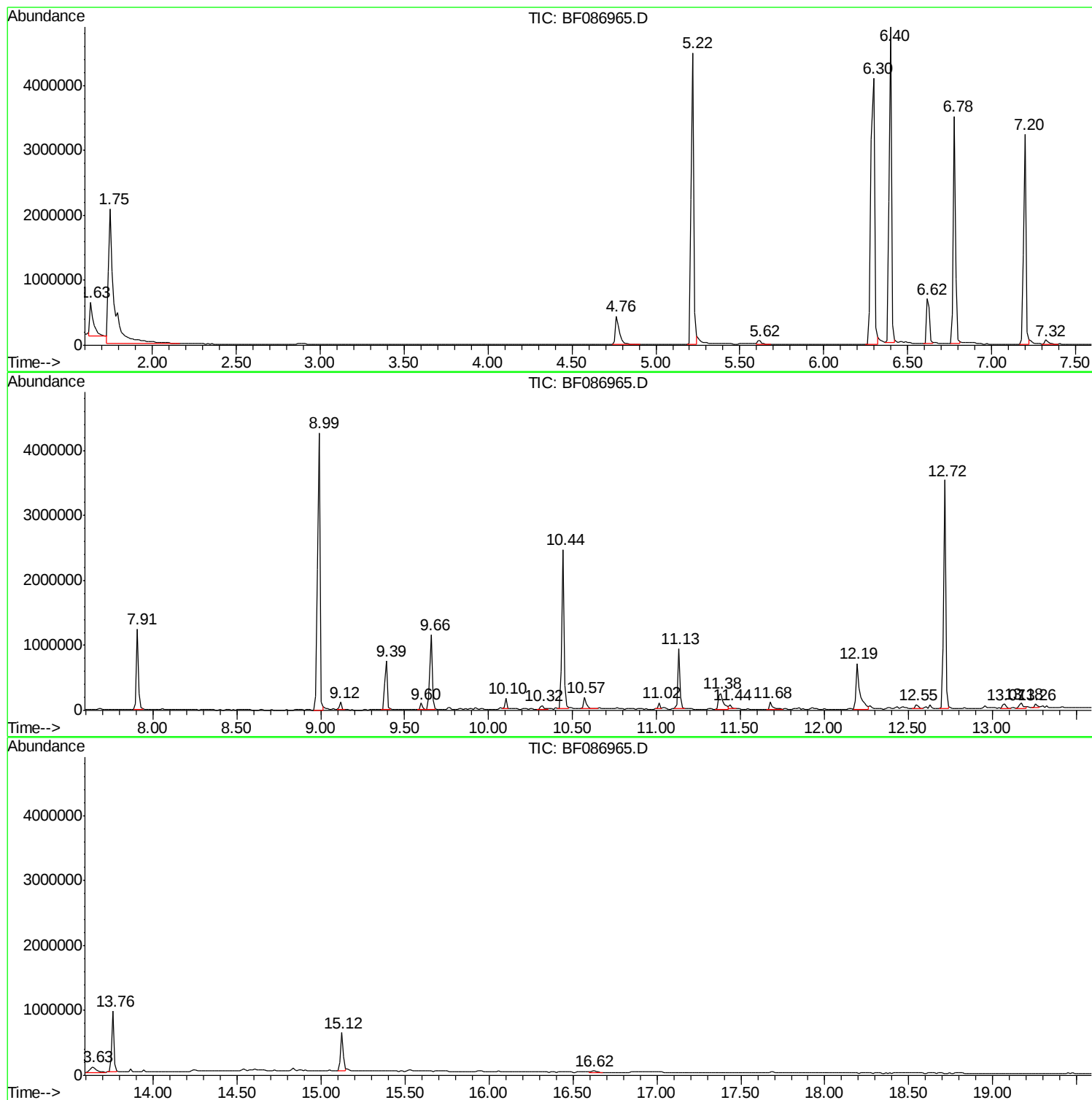
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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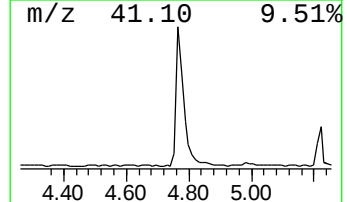
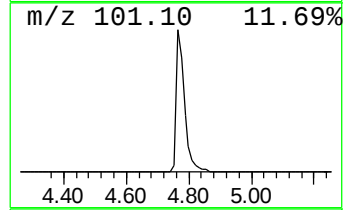
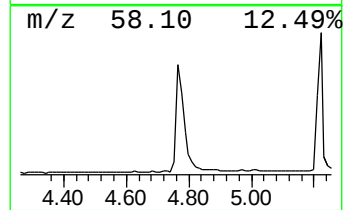
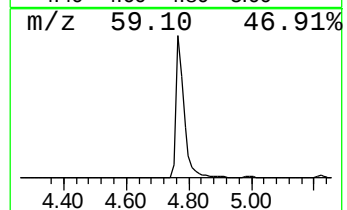
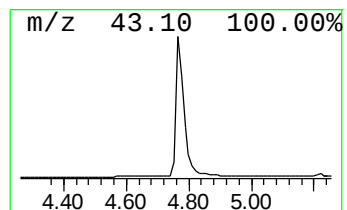
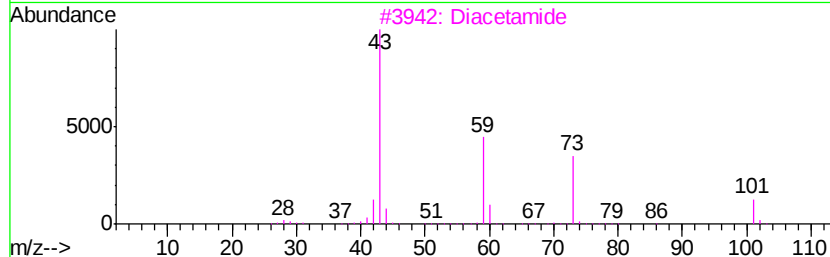
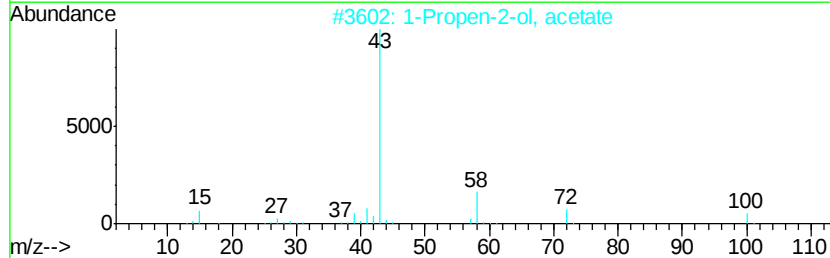
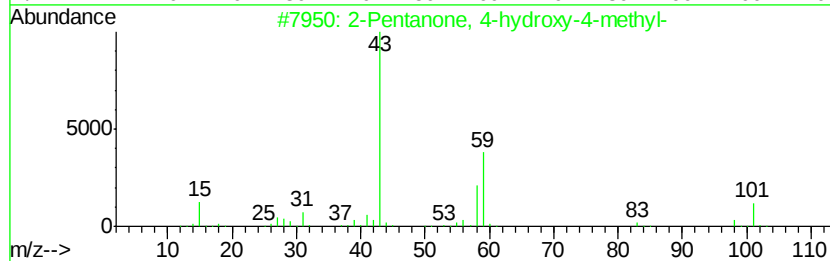
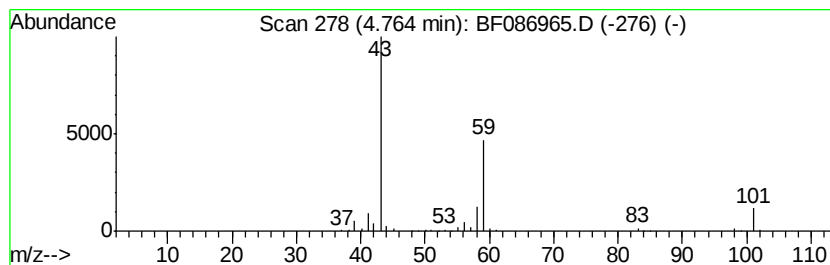
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	16.34 ng	751148	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Diacetamide	101	C4H7NO2	000625-77-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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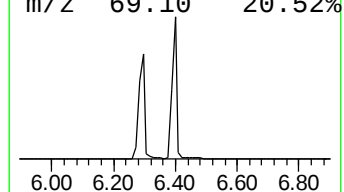
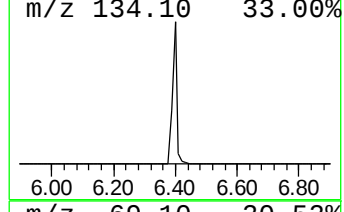
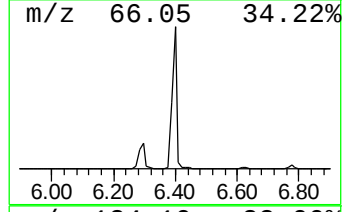
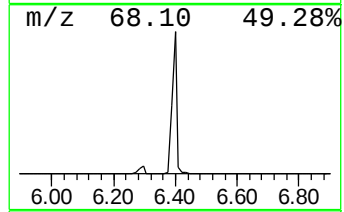
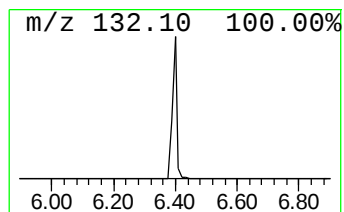
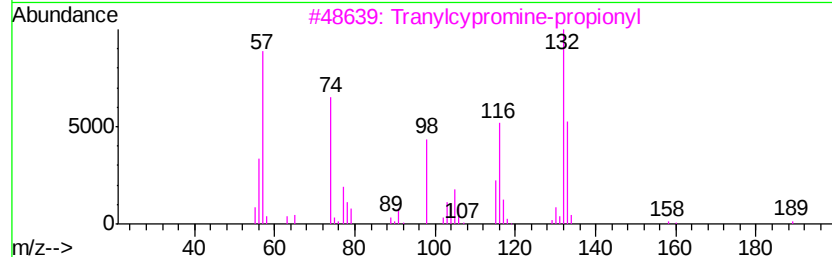
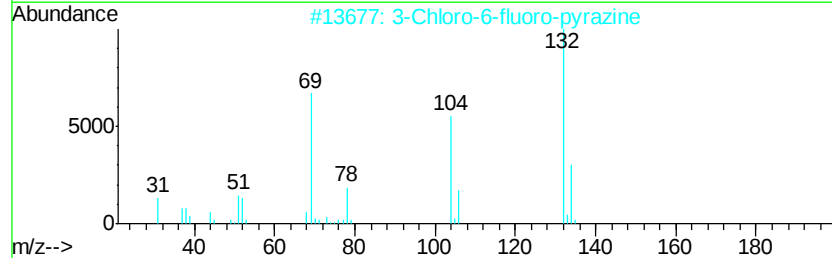
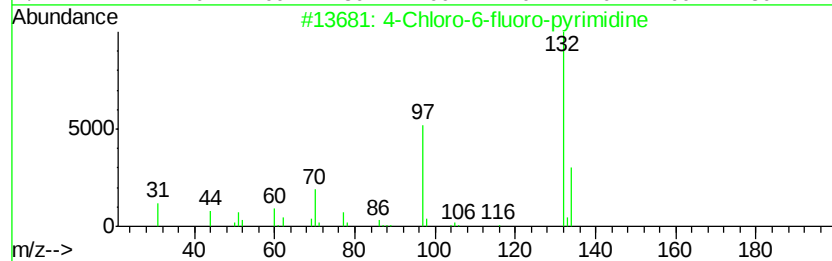
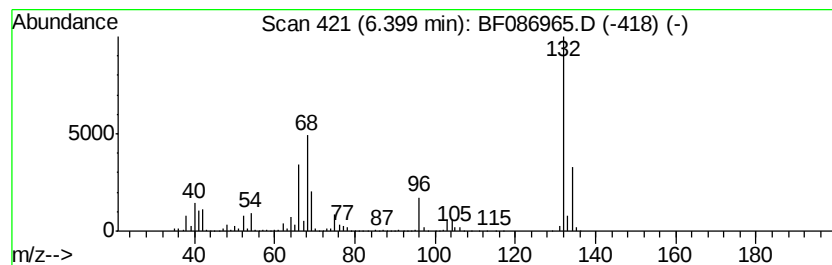
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	110.09 ng	5061870	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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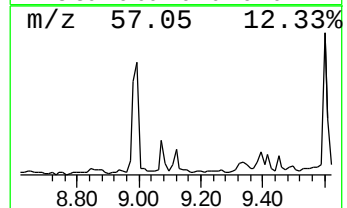
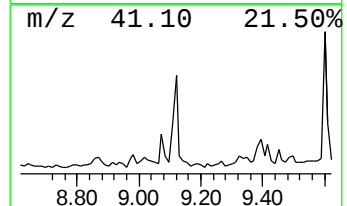
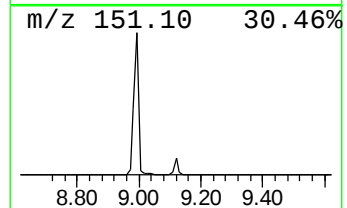
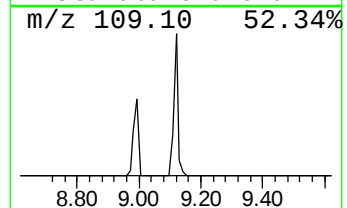
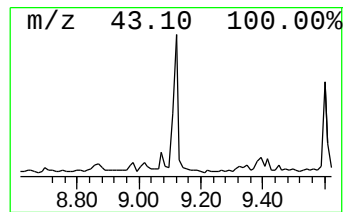
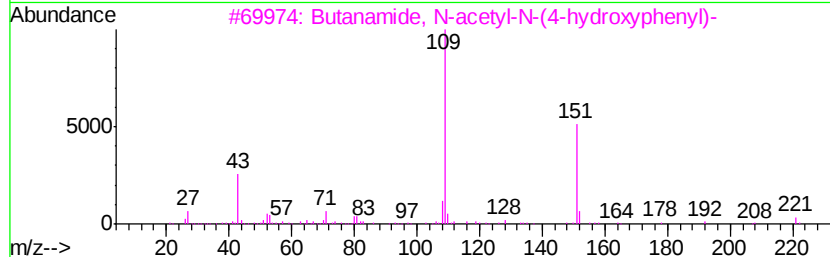
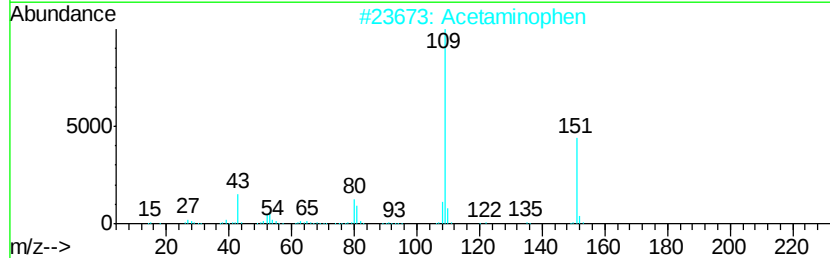
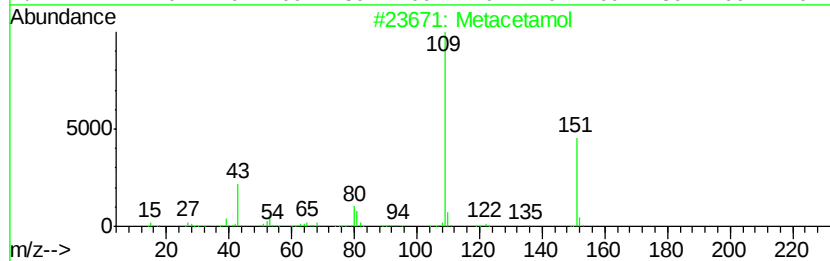
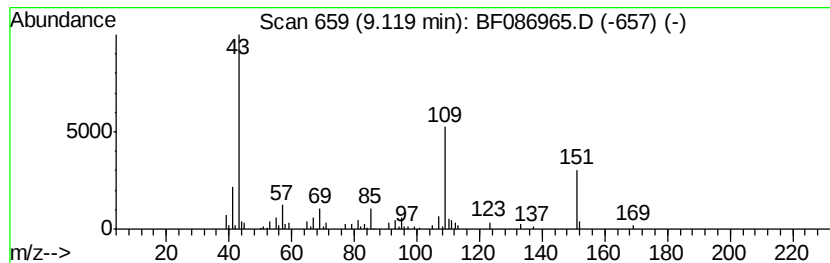
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Peak Number 6 unknown9.12 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.12	2.12 ng	110315	Acenaphthene-d10	9.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Metacetamol	151	C8H9NO2	000621-42-1	49
2		Acetaminophen	151	C8H9NO2	000103-90-2	47
3		Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	47
4		(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	45
5		2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	40



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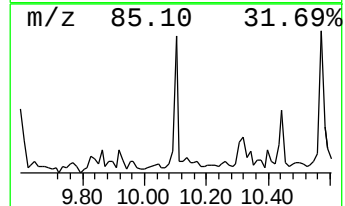
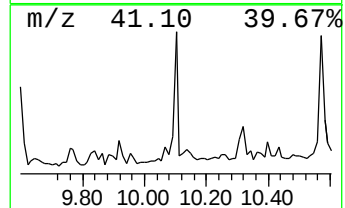
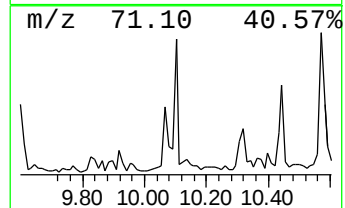
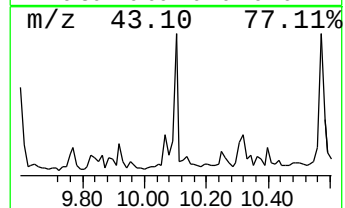
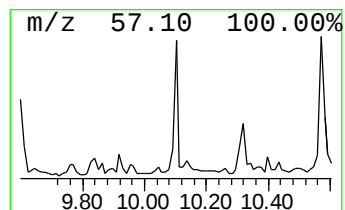
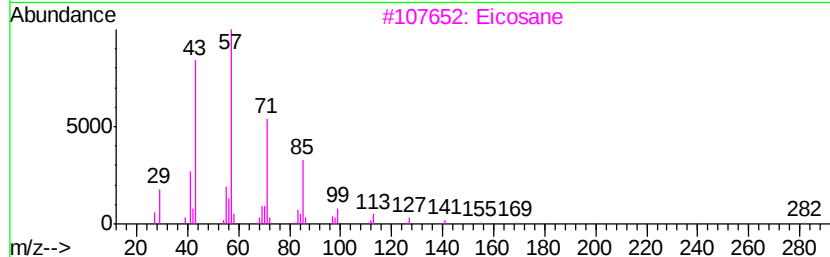
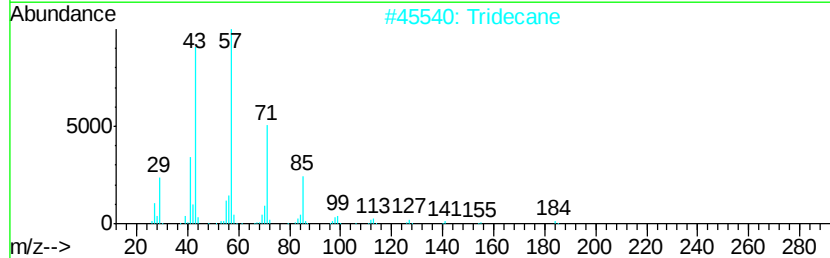
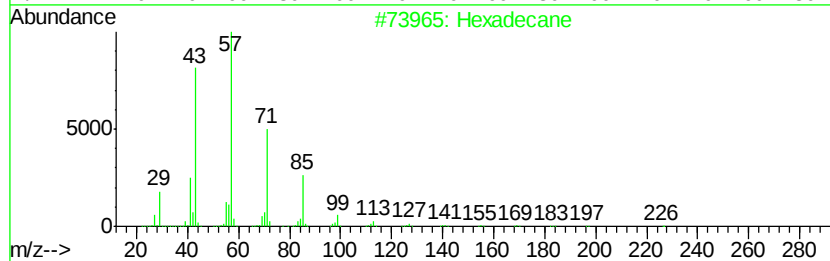
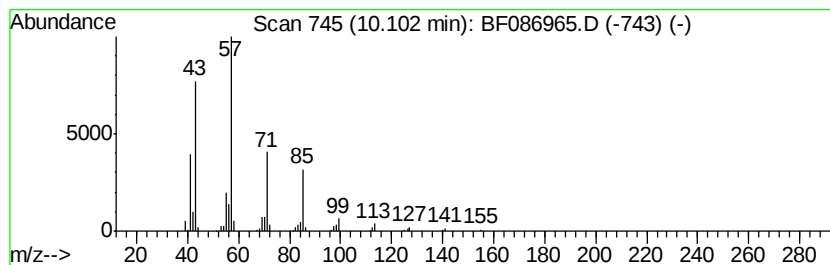
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Peak Number 7 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	2.55 ng	132820	Acenaphthene-d10	9.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Tridecane	184	C13H28	000629-50-5	90
3		Eicosane	282	C20H42	000112-95-8	90
4		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
5		Tetradecane	198	C14H30	000629-59-4	80



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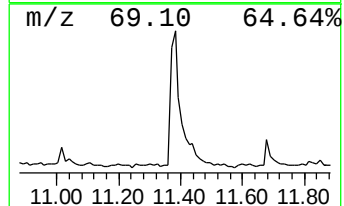
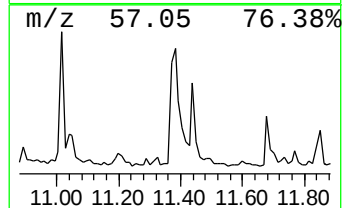
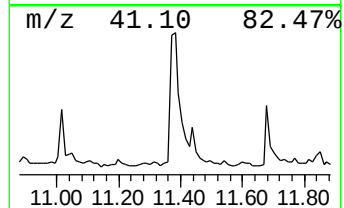
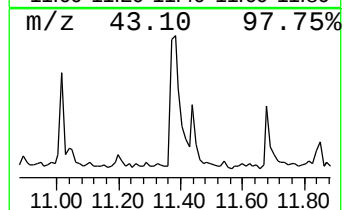
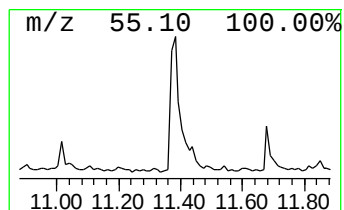
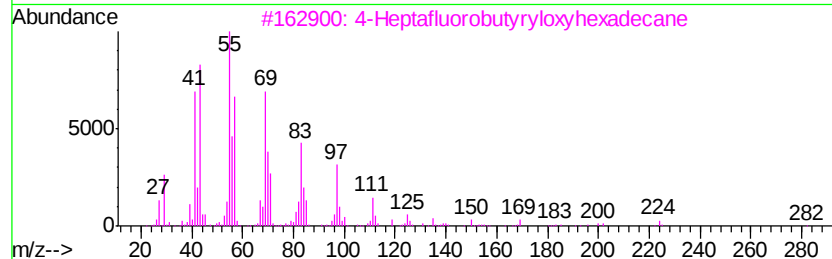
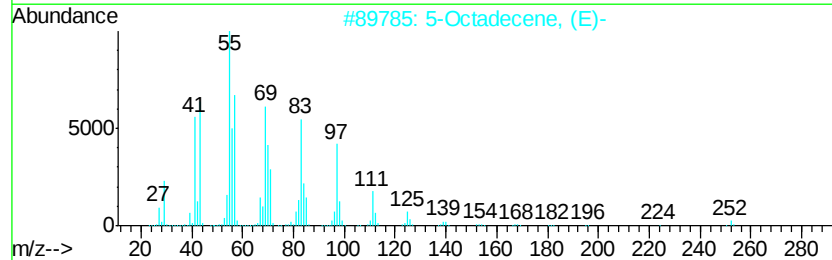
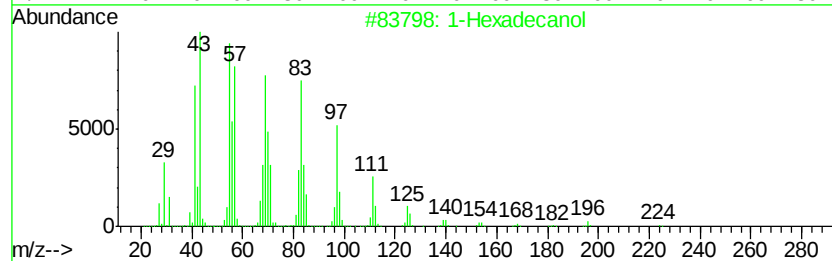
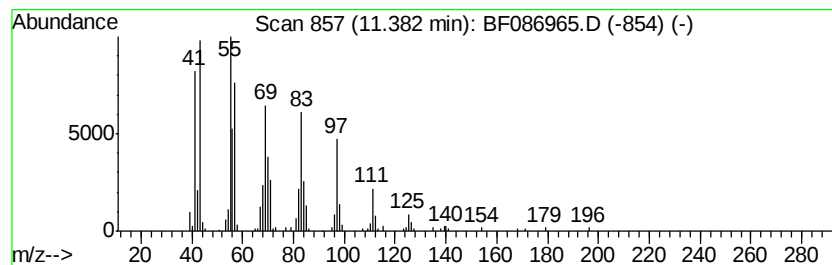
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Peak Number 10 1-Hexadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.38	12.35 ng	499765	Phenanthrene-d10	11.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexadecanol	242	C16H34O	036653-82-4	95
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
3		4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
4		1-Hexadecene	224	C16H32	000629-73-2	91
5		Cyclotetradecane	196	C14H28	000295-17-0	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086965.D
Acq On : 13 May 2016 10:06
Operator : UM/SJ
Sample : H2916-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-5K

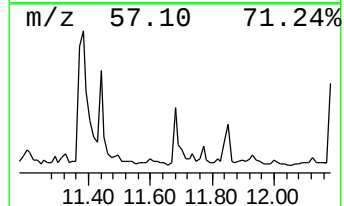
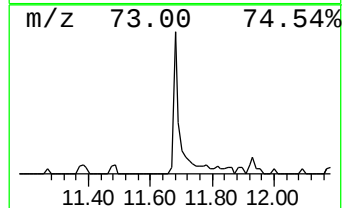
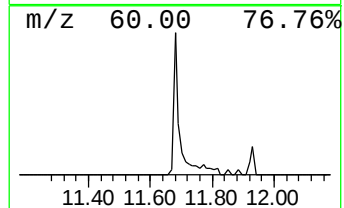
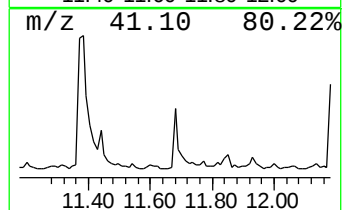
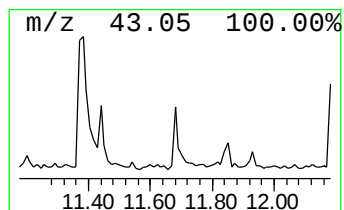
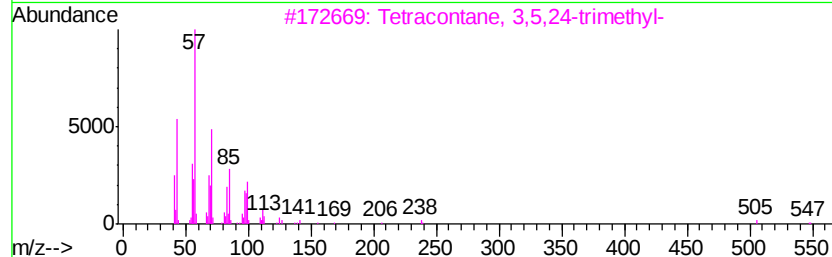
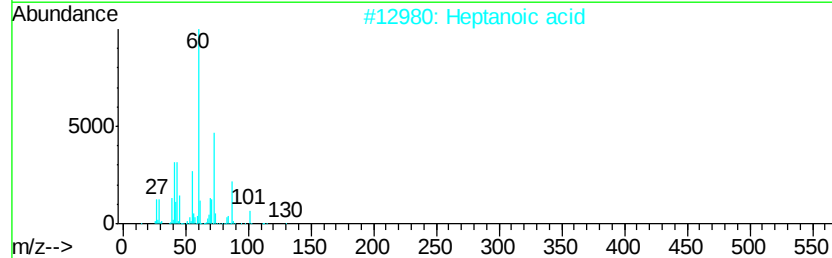
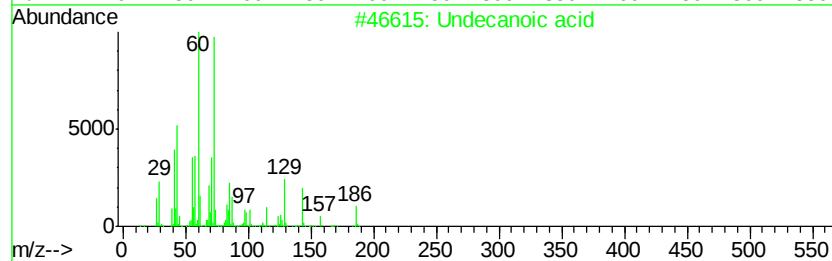
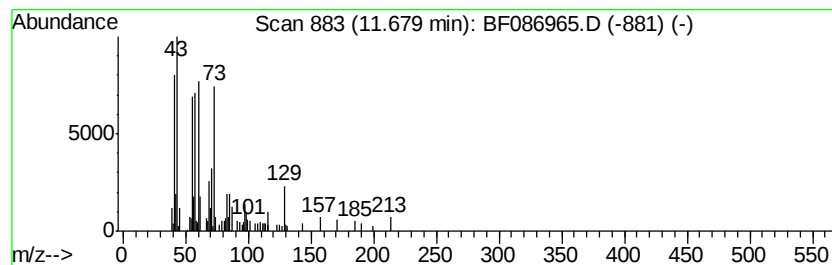
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Undecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	3.79 ng	153497	Phenanthrene-d10	11.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecanoic acid	186	C11H22O2	000112-37-8	80
2		Heptanoic acid	130	C7H14O2	000111-14-8	43
3		Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	18
4		Tetratetracontane	619	C44H90	007098-22-8	14
5		Decane	142	C10H22	000124-18-5	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086965.D
Acq On : 13 May 2016 10:06
Operator : UM/SJ
Sample : H2916-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-5K

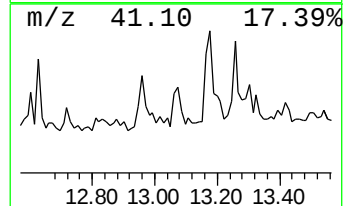
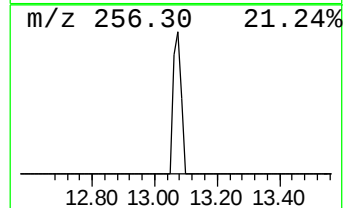
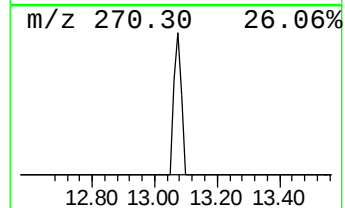
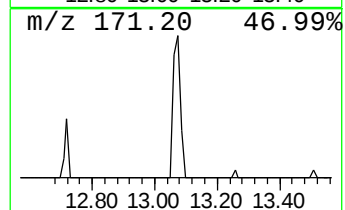
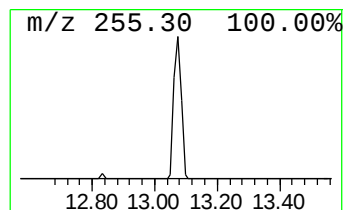
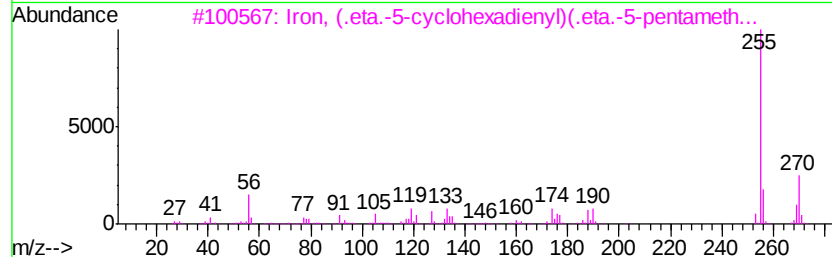
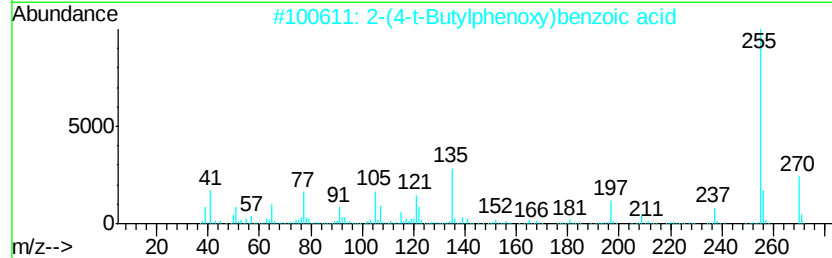
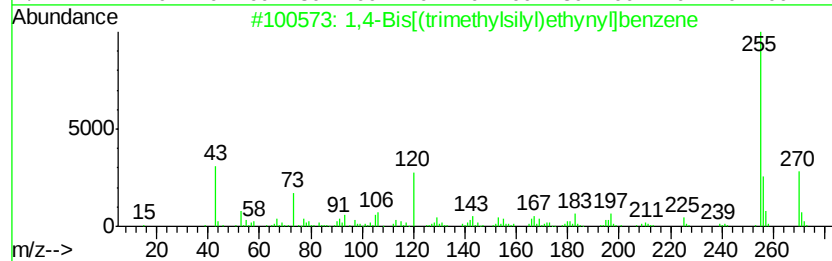
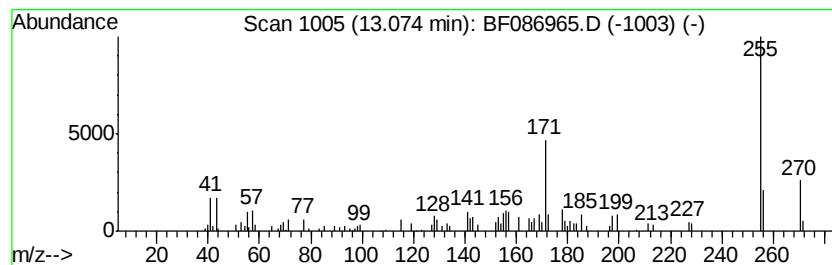
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown13.07 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.07	2.41 ng	104681	Chrysene-d12	13.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Bis[(trimethylsilyl)ethynyl]...	270	C16H22Si2	073392-23-1	43
2		2-(4-t-Butylphenoxy)benzoic acid	270	C17H18O3	069737-65-1	43
3		Iron, (.eta.-5-cyclohexadienyl)(...	270	C16H22Fe	1000162-99-3	43
4		2-Sec-butyl-6-[1-hydroxy-1-cyclo...	283	C19H25NO	035871-05-7	37
5		2-Phenylacenaphtheno[5,5a,6-b,c]...	255	C19H13N	202264-22-0	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086965.D
Acq On : 13 May 2016 10:06
Operator : UM/SJ
Sample : H2916-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-5K

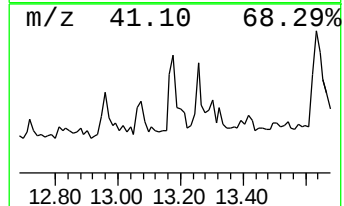
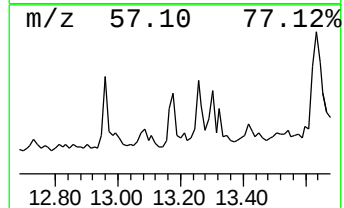
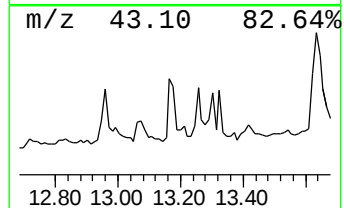
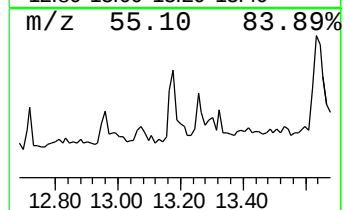
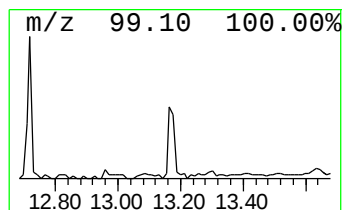
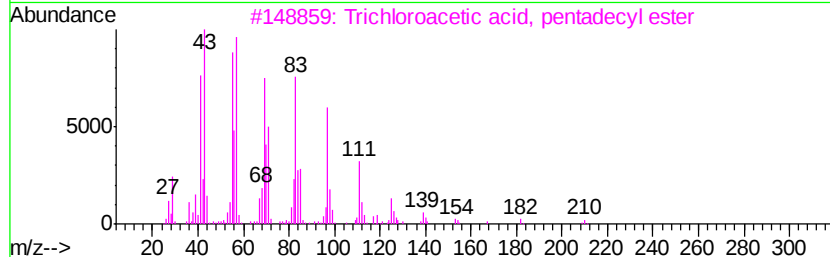
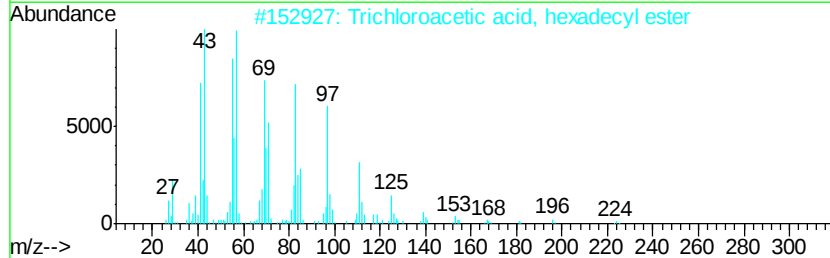
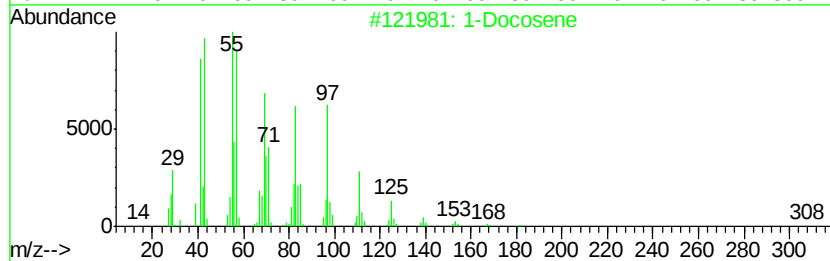
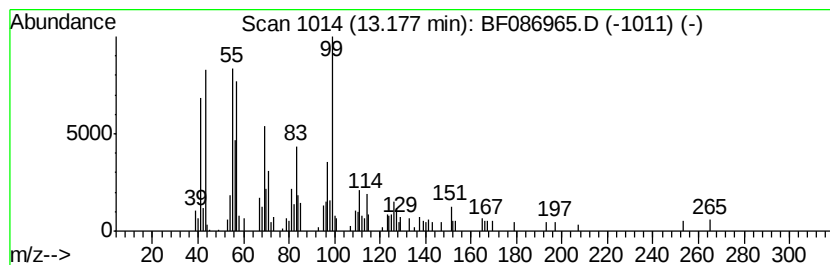
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown13.18 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	2.74 ng	118967	Chrysene-d12	13.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	42
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	42
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	42
4			3-Octadecene, (E)-	252	C18H36	007206-19-1	41
5			5-Octadecene, (E)-	252	C18H36	007206-21-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086965.D
Acq On : 13 May 2016 10:06
Operator : UM/SJ
Sample : H2916-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

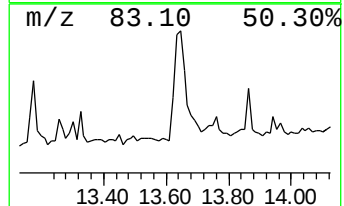
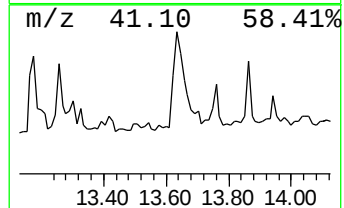
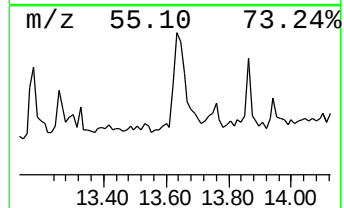
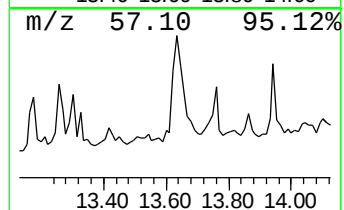
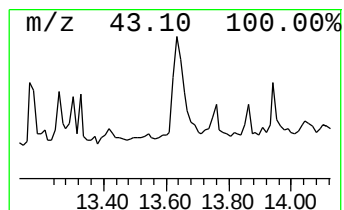
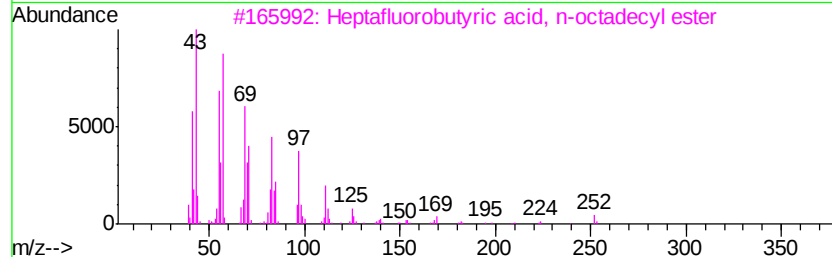
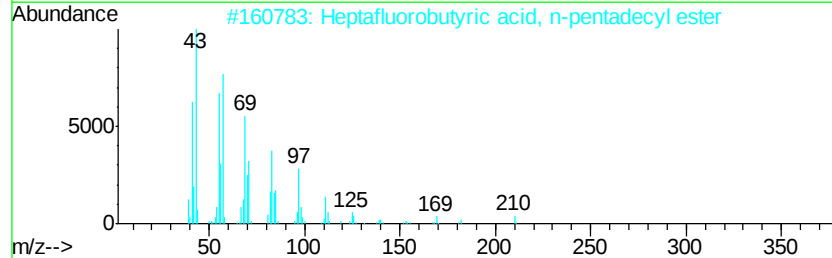
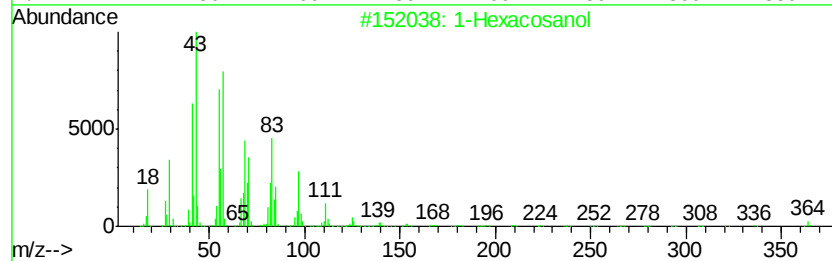
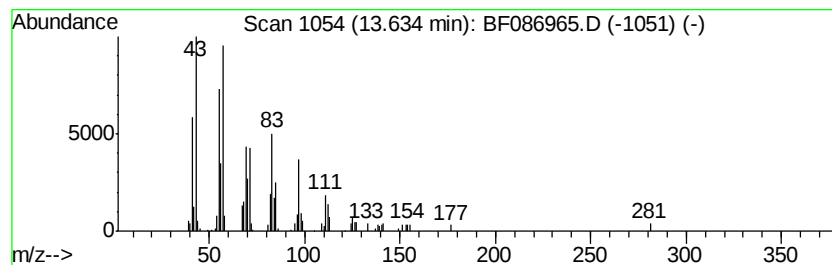
Instrument :
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ClientSampleId :
VITALE-FILL-CSPH3-5K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Hexacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.63	4.35 ng	188994	Chrysene-d12	13.76		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexacosanol	382	C26H54O	000506-52-5	91
2		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
3		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87



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Acq On : 13 May 2016 10:06
Operator : UM/SJ
Sample : H2916-05
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VITALE-FILL-CSPH3-5K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.76	16.3	ng	751148	1	6.63	919560	20.0
unknown6.40	6.40	110.1	ng	5061870	1	6.63	919560	20.0
unknown9.12	9.12	2.1	ng	110315	3	9.66	1040920	20.0
Hexadecane	10.10	2.5	ng	132820	3	9.66	1040920	20.0
1-Hexadecanol	11.38	12.4	ng	499765	4	11.13	809271	20.0
Undecanoic acid	11.68	3.8	ng	153497	4	11.13	809271	20.0
unknown13.07	13.07	2.4	ng	104681	5	13.76	869762	20.0
unknown13.18	13.18	2.7	ng	118967	5	13.76	869762	20.0
1-Hexacosanol	13.63	4.3	ng	188994	5	13.76	869762	20.0