

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
 Data File : BF085465.D
 Acq On : 15 Mar 2016 20:25
 Operator : UM/SJ
 Sample : H1774-20
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-06-COMP

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-BF031516.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	3.121	71	73	76	rVB3	29532	57357	1.37%	0.148%
2	4.207	166	168	172	rBV3	55036	52926	1.26%	0.137%
3	5.122	246	248	256	rBV	61257	106194	2.53%	0.275%
4	5.522	280	283	285	rBV	3585801	4187203	99.68%	10.835%
5	6.539	369	372	375	rBV	2968481	3949393	94.02%	10.220%
6	6.676	381	384	387	rBV	3473901	3934404	93.66%	10.181%
7	6.905	402	404	407	rVB	823364	857121	20.40%	2.218%
8	7.065	415	418	420	rBV	3196204	3031610	72.17%	7.845%
9	7.476	451	454	456	rBV	2695446	2880412	68.57%	7.454%
10	7.556	459	461	464	rVB	46404	49994	1.19%	0.129%
11	8.196	514	517	519	rBV	1367268	1217580	28.98%	3.151%
12	9.270	608	611	614	rBV	3767245	4200748	100.00%	10.871%
13	9.659	643	645	647	rBV	530441	667854	15.90%	1.728%
14	9.876	662	664	666	rVB	69916	81268	1.93%	0.210%
15	9.956	668	671	673	rVB	979499	1269551	30.22%	3.285%
16	10.379	707	708	710	rVB	174844	135840	3.23%	0.352%
17	10.596	724	727	731	rBV	53087	103516	2.46%	0.268%
18	10.745	736	740	742	rBV	2800764	3119290	74.26%	8.072%
19	10.848	748	749	756	rVB	112461	205171	4.88%	0.531%
20	11.305	786	789	790	rBV	76436	82879	1.97%	0.214%
21	11.431	798	800	803	rBV2	1159208	1274467	30.34%	3.298%
22	11.499	803	806	809	rVB2	32056	57480	1.37%	0.149%
23	11.956	843	846	853	rBV2	86481	139198	3.31%	0.360%
24	12.745	912	915	918	rBV4	36681	98872	2.35%	0.256%
25	13.019	936	939	942	rVB	3318647	3966346	94.42%	10.264%
26	13.911	1015	1017	1021	rBV	269052	339389	8.08%	0.878%
27	14.071	1028	1031	1034	rVB	1170342	1050691	25.01%	2.719%
28	14.551	1070	1073	1079	rVB3	19208	45434	1.08%	0.118%
29	15.523	1155	1158	1164	rBV	574111	710584	16.92%	1.839%
30	15.808	1180	1183	1186	rBV3	174526	210115	5.00%	0.544%
31	16.037	1200	1203	1205	rBV2	30239	66175	1.58%	0.171%
32	16.174	1212	1215	1218	rVV4	35079	76610	1.82%	0.198%
33	16.243	1218	1221	1223	rVB4	32514	65699	1.56%	0.170%
34	16.391	1233	1234	1237	rVB3	24365	45844	1.09%	0.119%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

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-BF031516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.471	1237	1241	1243	rBV4	26812	84070	2.00%	0.218%
36	17.511	1329	1332	1335	rBV5	60377	127476	3.03%	0.330%
37	17.728	1350	1351	1355	rVB2	75938	94744	2.26%	0.245%

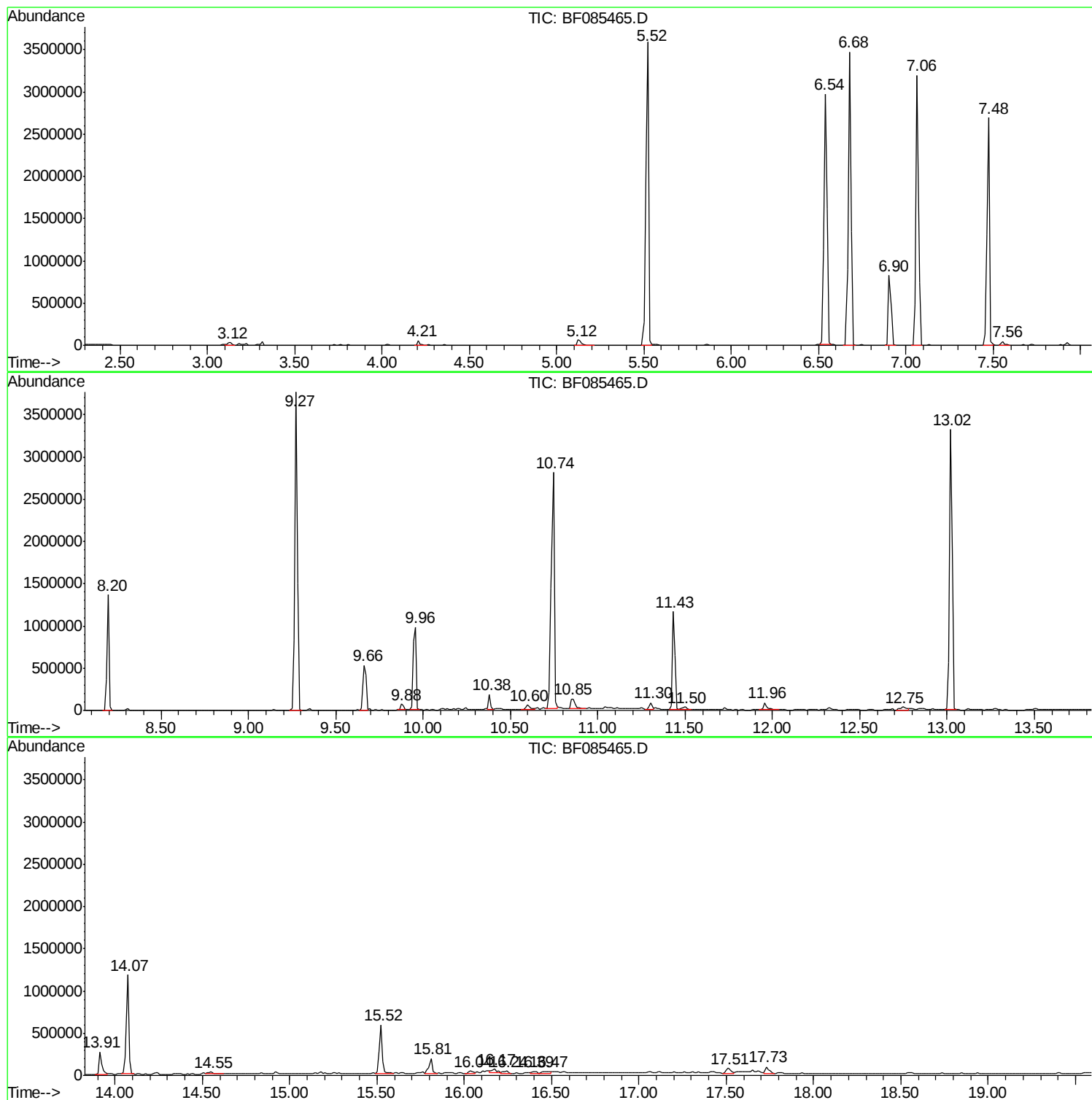
Sum of corrected areas: 38643505

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

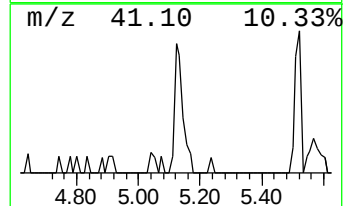
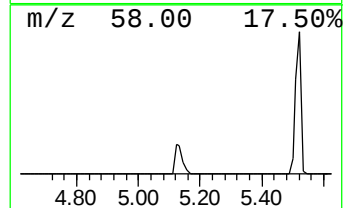
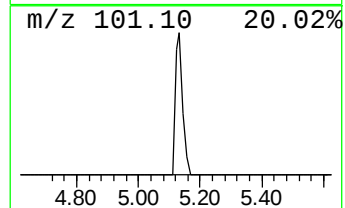
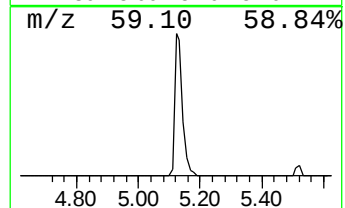
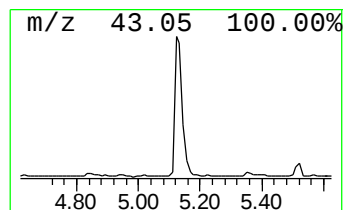
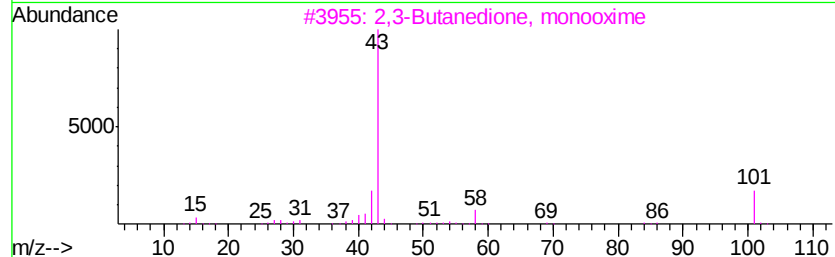
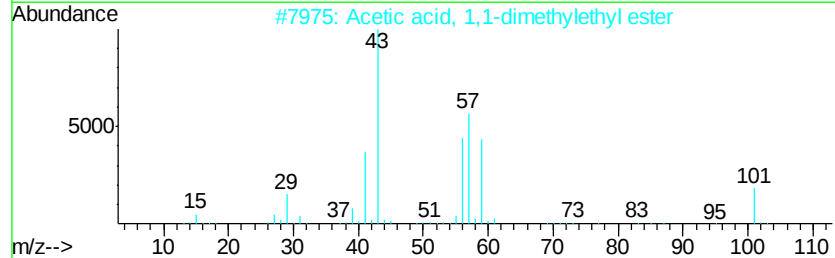
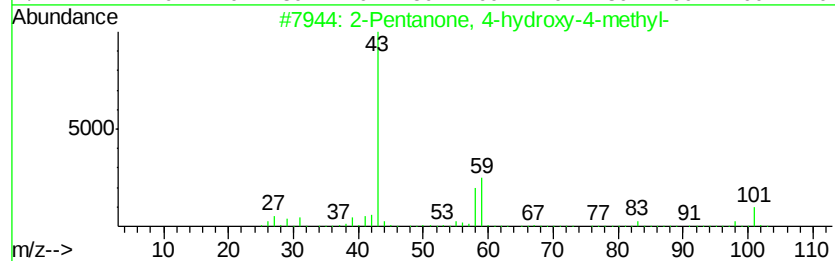
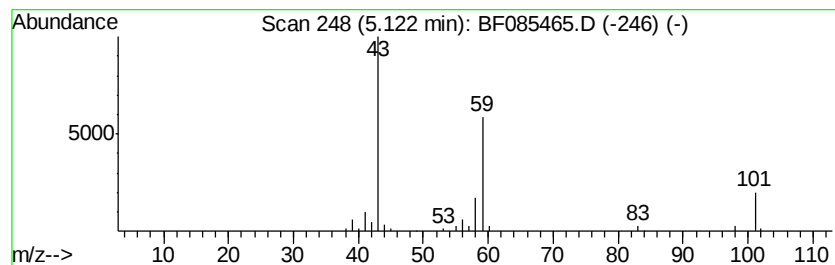
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.48 ng	106194	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			2-Nonanone	142	C9H18O	000821-55-6	12
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

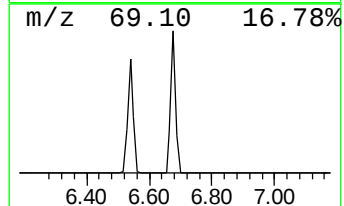
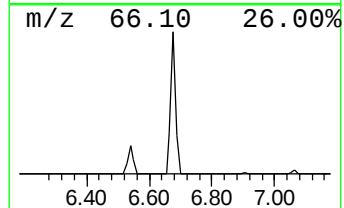
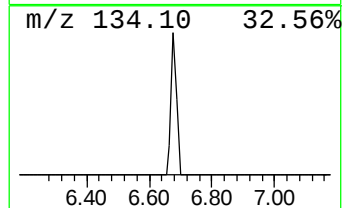
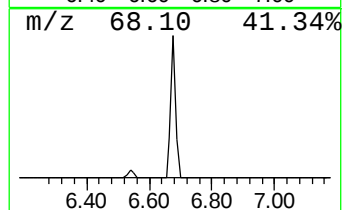
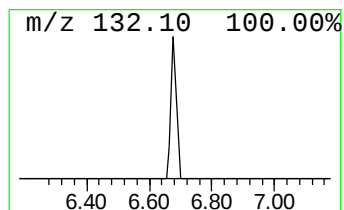
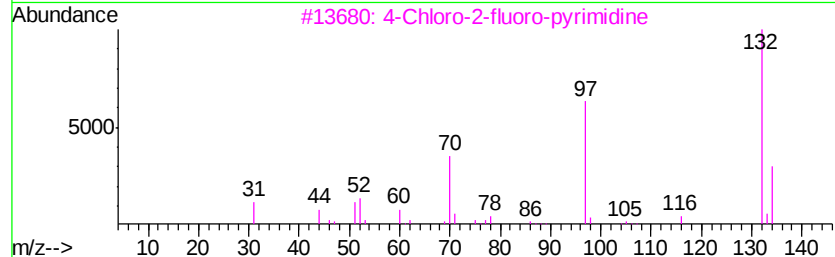
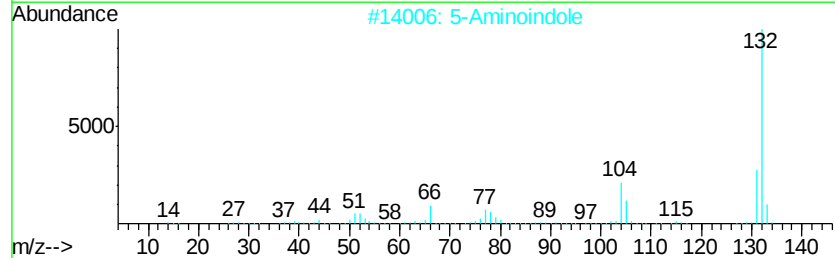
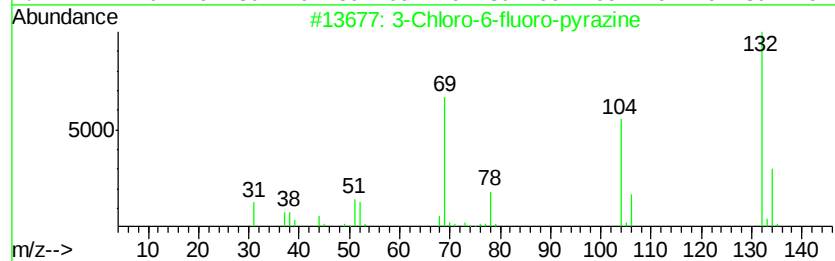
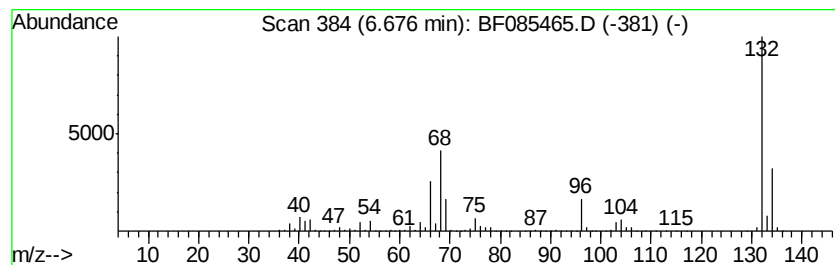
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	91.81 ng	3934400	1,4-Dichlorobenzene-d4	6.90

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	1-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine			132	C8H8N2	064608-60-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

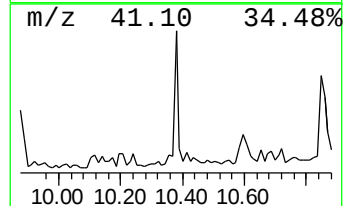
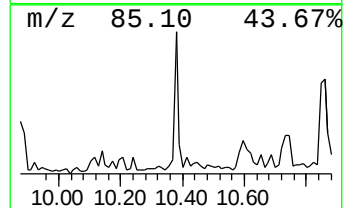
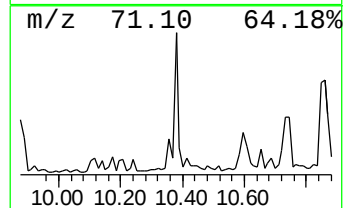
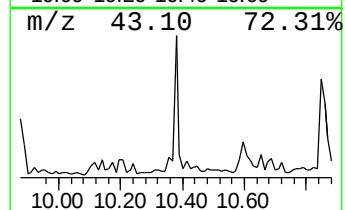
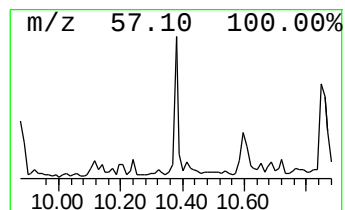
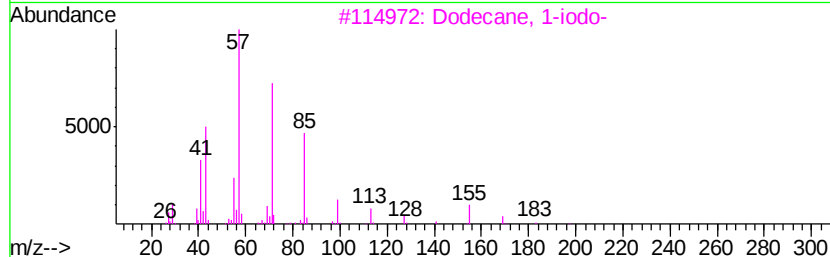
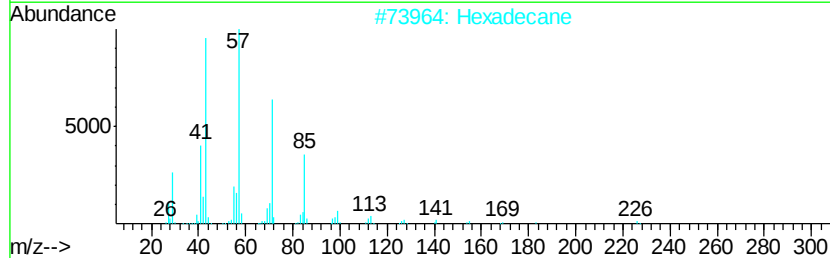
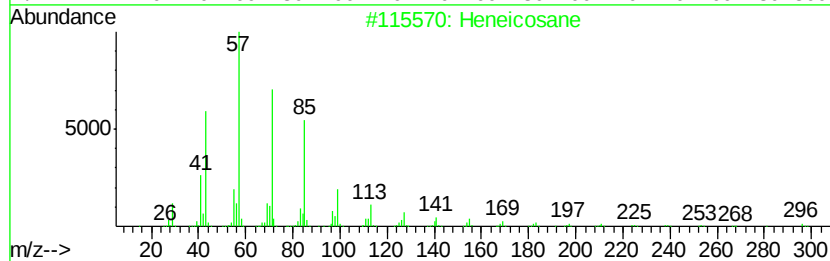
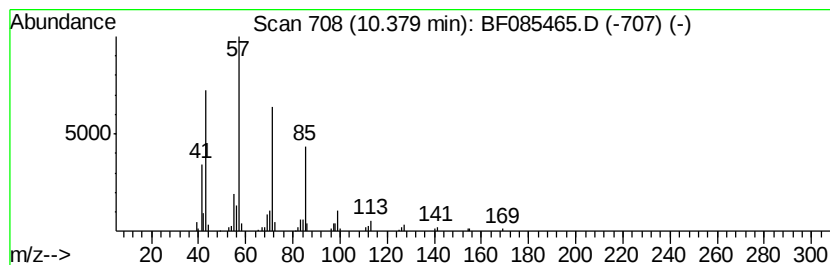
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.14 ng	135840	Acenaphthene-d10	9.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Hexadecane		226	C16H34	000544-76-3	86
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
4	Eicosane		282	C20H42	000112-95-8	83
5	Decane, 3-bromo-		220	C10H21Br	030571-71-2	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

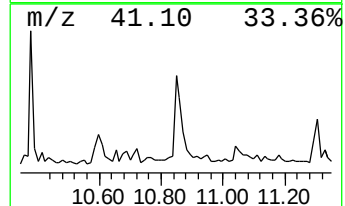
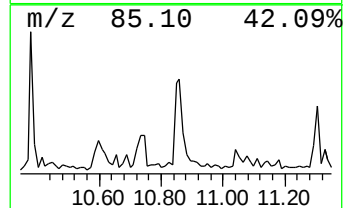
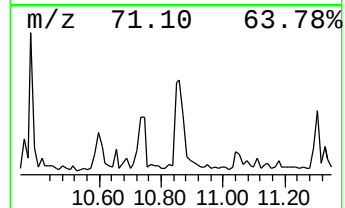
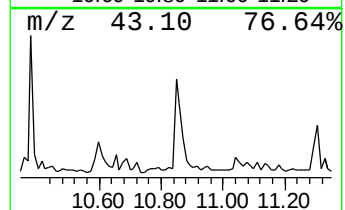
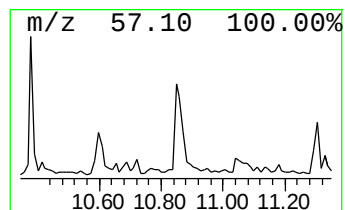
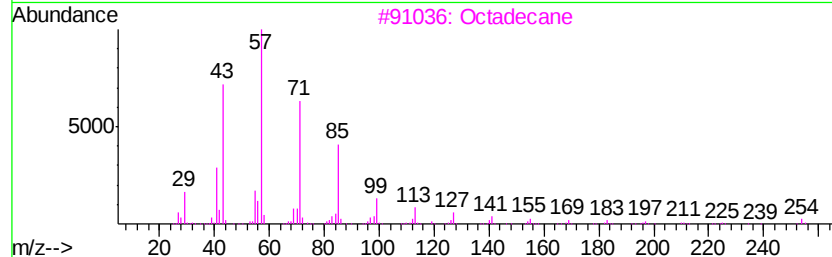
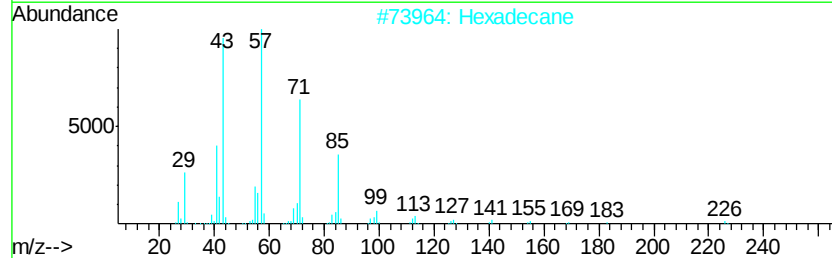
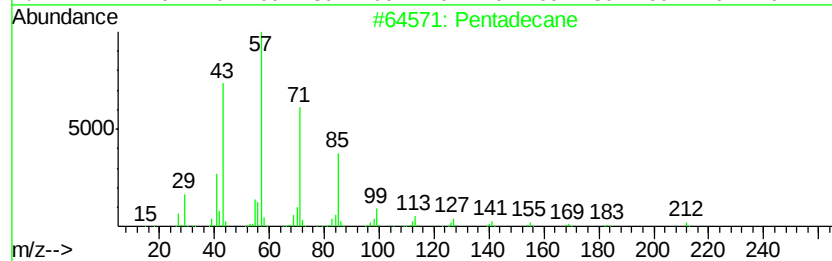
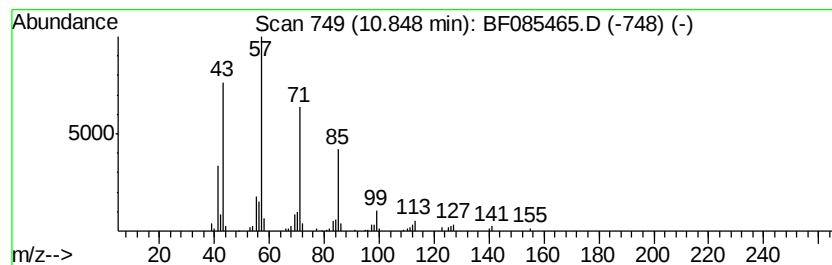
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	3.22 ng	205171	Phenanthrene-d10	11.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	86
2	Hexadecane		226	C16H34	000544-76-3	78
3	Octadecane		254	C18H38	000593-45-3	78
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	78
5	Eicosane		282	C20H42	000112-95-8	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

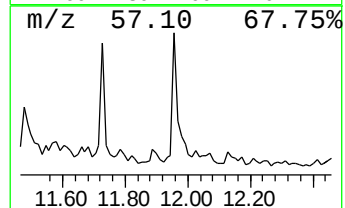
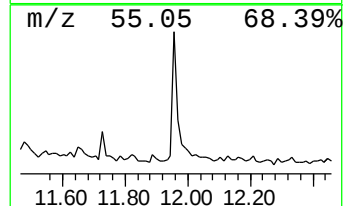
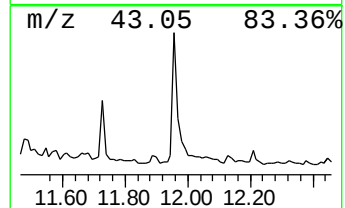
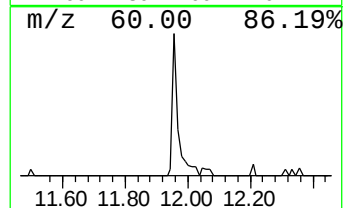
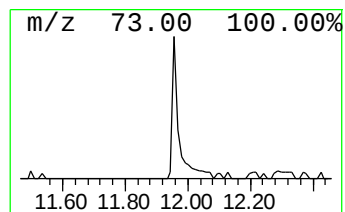
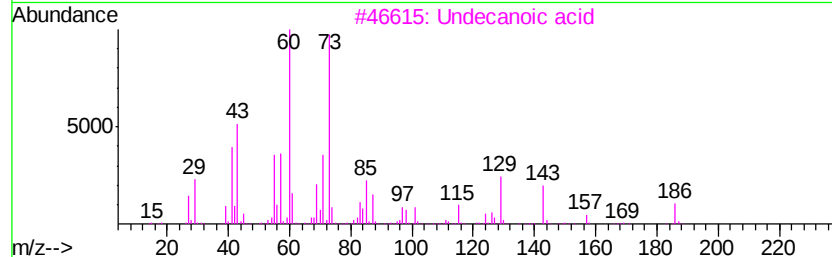
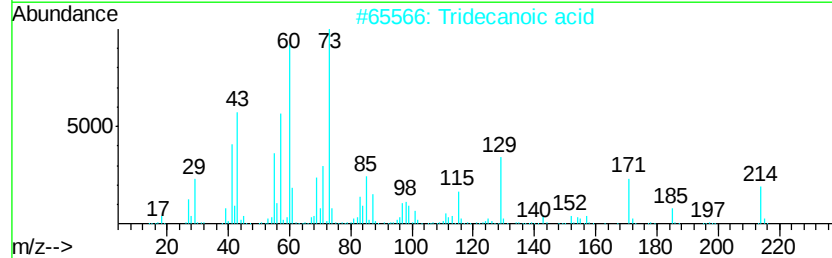
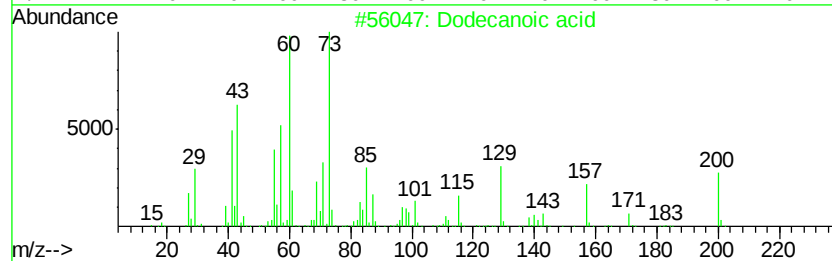
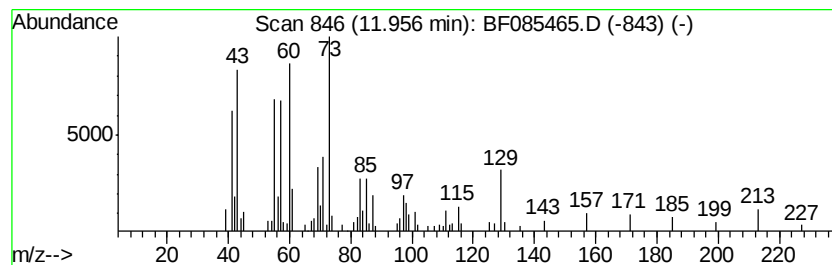
Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.96	2.18 ng	139198	Phenanthrene-d10		11.43	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid		200	C12H24O2	000143-07-7	86
2	Tridecanoic acid		214	C13H26O2	000638-53-9	80
3	Undecanoic acid		186	C11H22O2	000112-37-8	43
4	tert-Hexadecanethiol		258	C16H34S	025360-09-2	11
5	1-Nonadecanol		284	C19H40O	001454-84-8	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

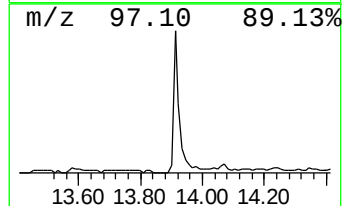
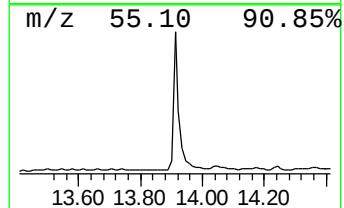
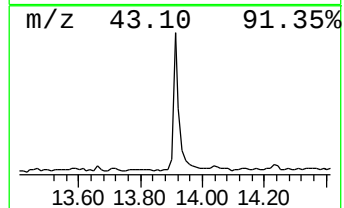
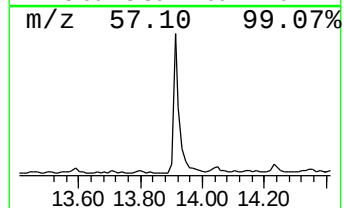
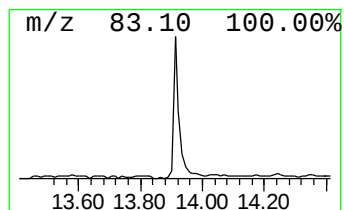
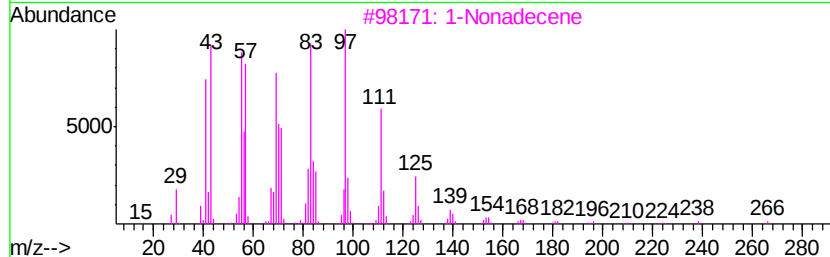
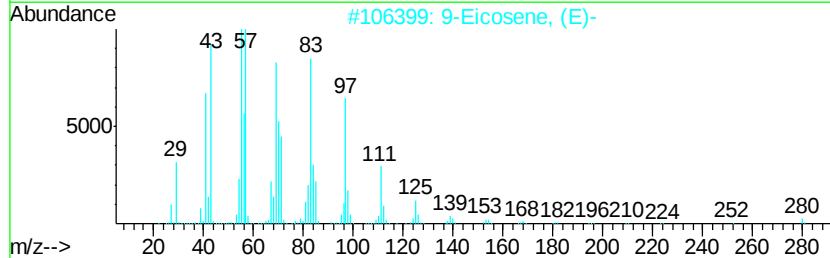
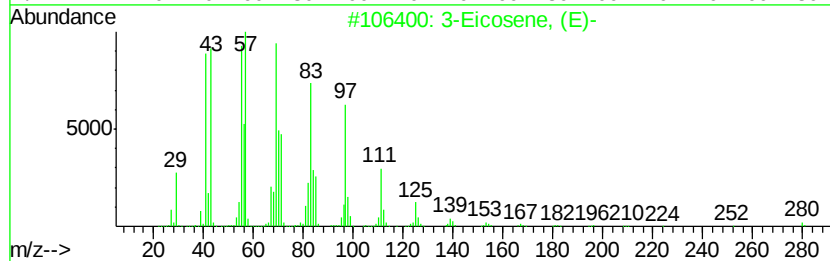
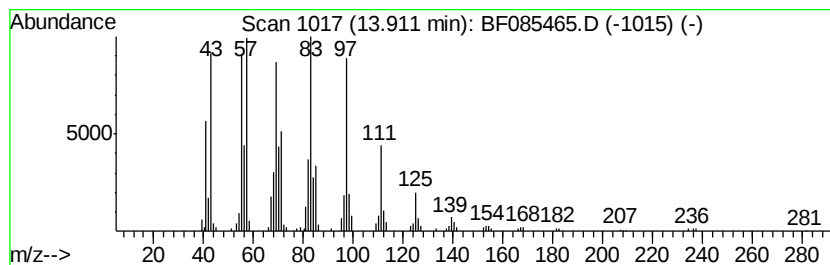
Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.91	6.46 ng	339389	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5	Cyclopentadecane	210	C15H30	000295-48-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

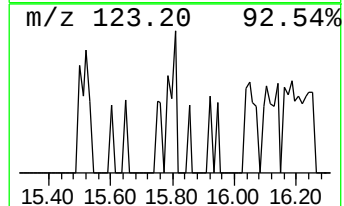
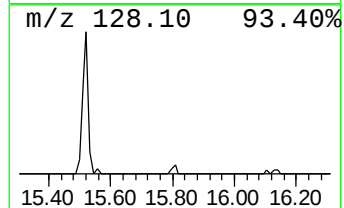
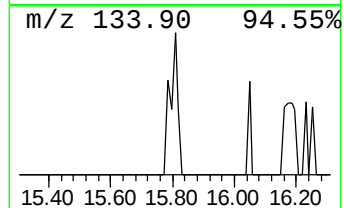
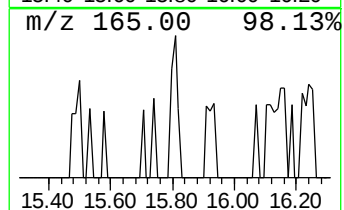
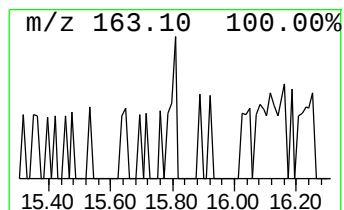
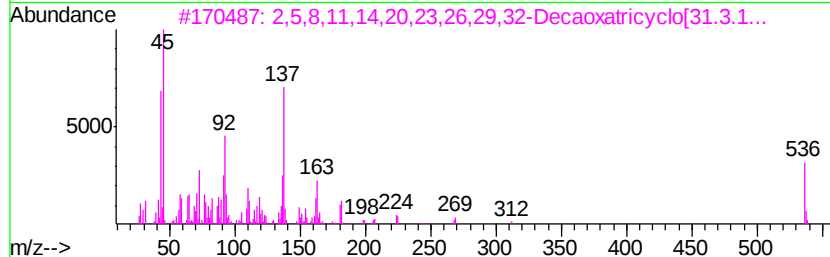
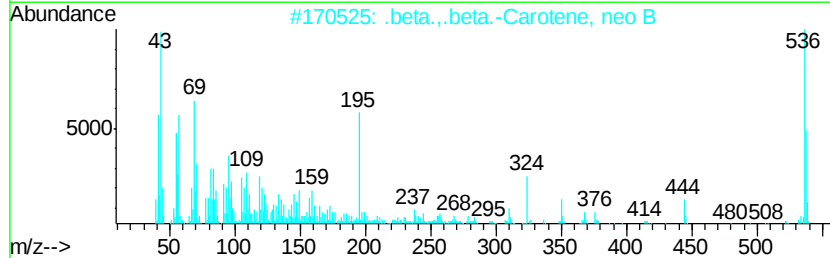
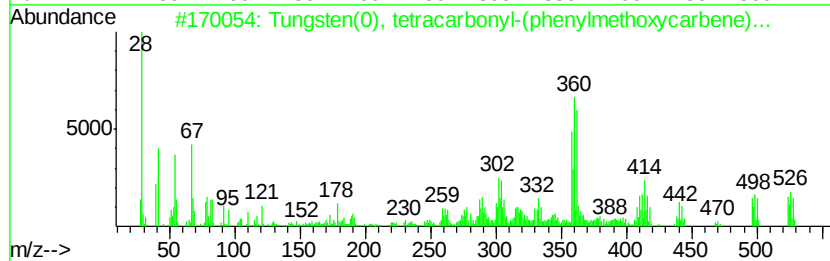
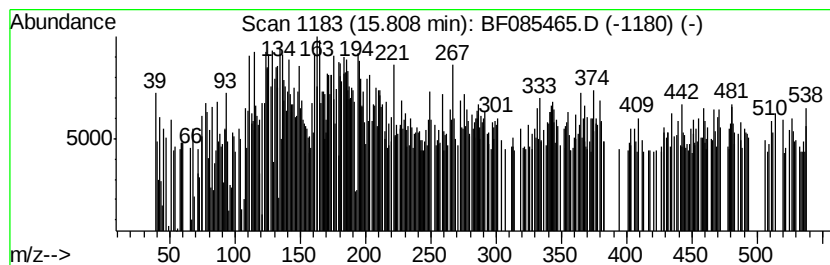
Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.81 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	5.91 ng	210115	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tungsten(0), tetracarbonyl-(phen...	526 C20H22O5W	1000154-58-9 20
2		.beta.,.beta.-Carotene, neo B	536 C40H56	006811-73-0 18
3		2,5,8,11,14,20,23,26,29,32-Decao...	536 C28H40O10	064739-07-7 10
4		Spiro(pyrano[2,3-b]naphthalene)-...	528 C32H48O6	1000187-84-8 10
5		Hexa-2,4-dien-2,5-zirconium-3,4-...	526 C26H26MoZr	1000154-45-6 10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

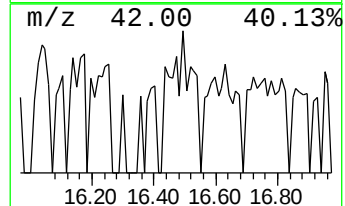
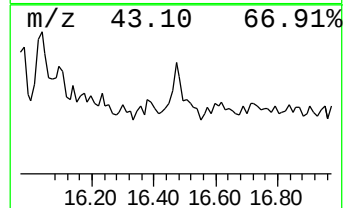
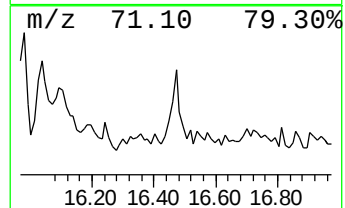
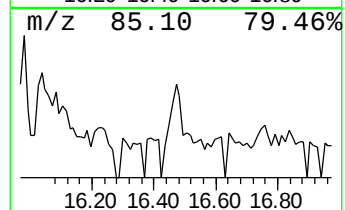
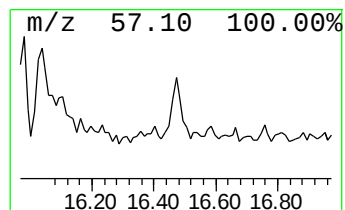
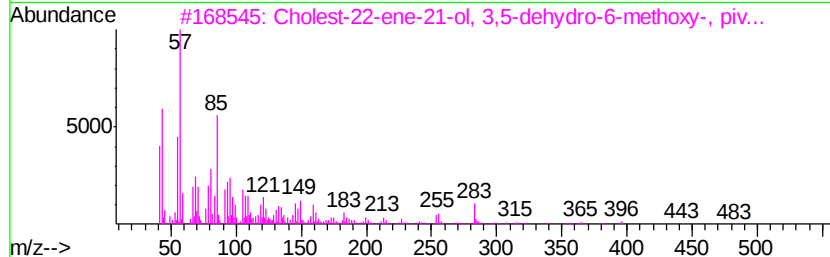
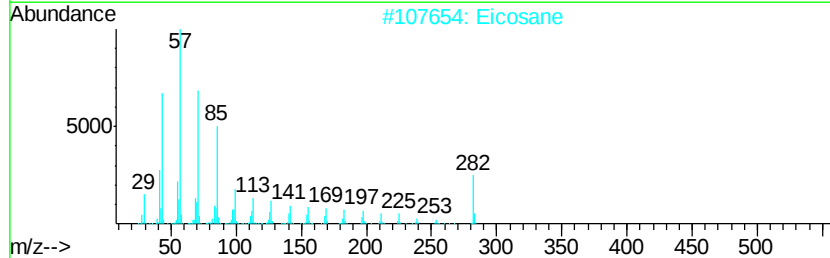
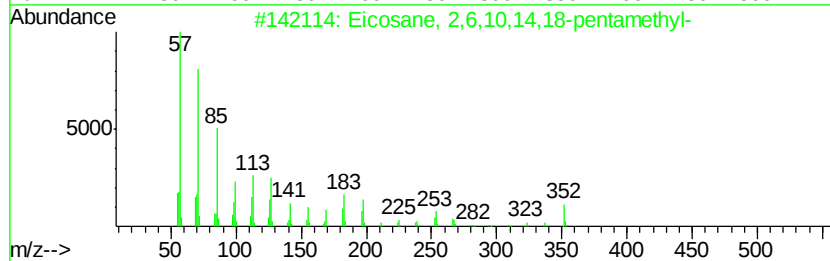
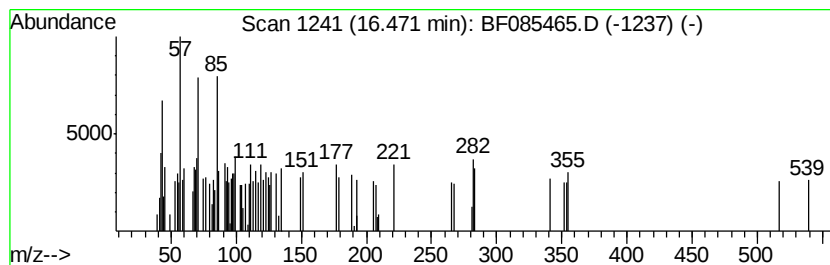
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.47 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.37 ng	84070	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 2,6,10,14,18-pentamethyl-	352	C25H52	051794-16-2	22
2		Eicosane	282	C20H42	000112-95-8	22
3		Cholest-22-ene-21-ol, 3,5-dehydr...	498	C33H54O3	1000124-60-2	10
4		13,17,21-Trimethylheptatriacontane	563	C40H82	058668-40-9	10
5		Pentacosane	352	C25H52	000629-99-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

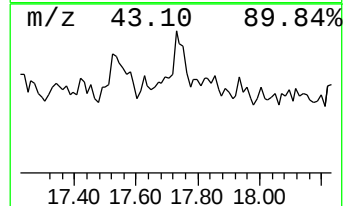
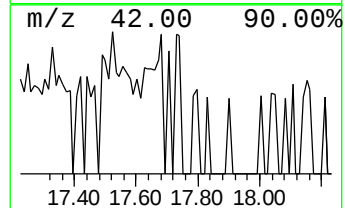
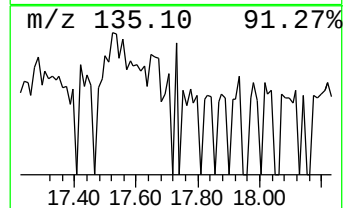
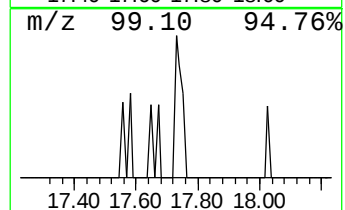
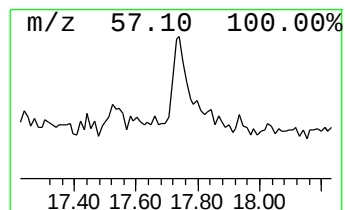
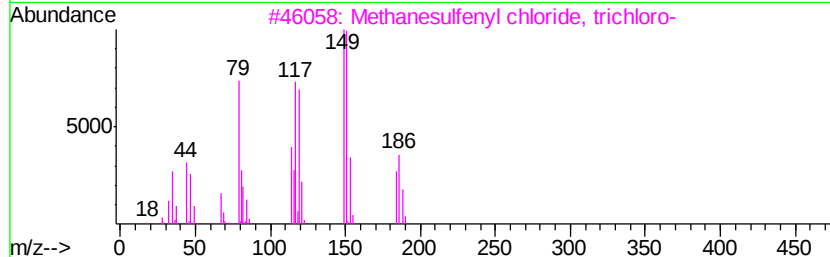
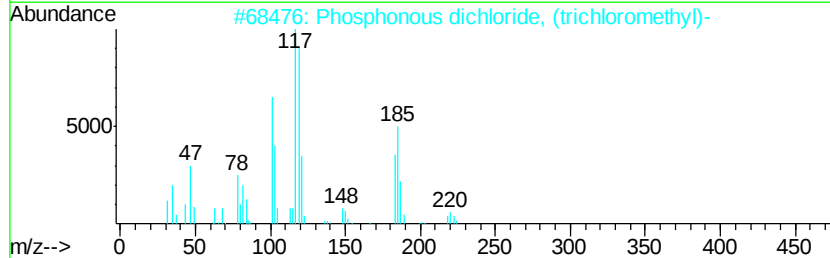
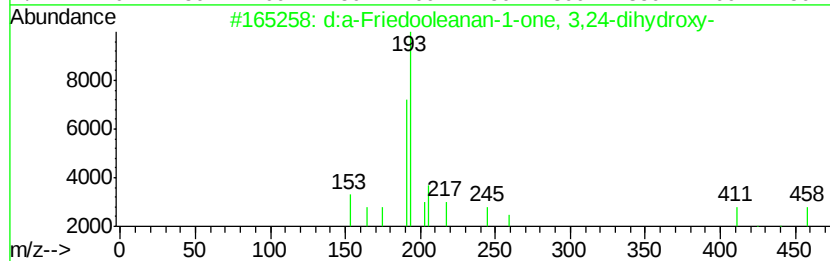
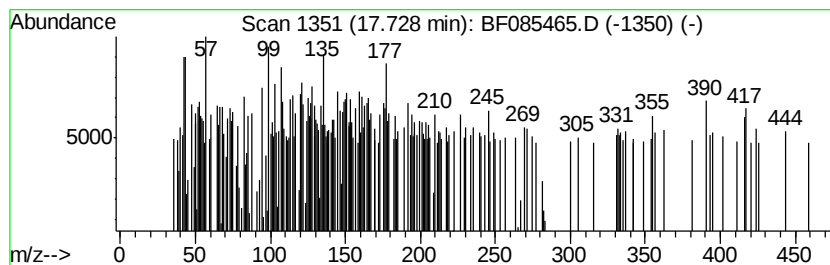
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.73	2.67 ng	94744	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	d:a-Friedooleanan-1-one, 3,24-di...	458	C30H50O3	056816-61-6	35
2		Phosphonous dichloride, (trichlo...	218	CCl5P	003582-11-4	10
3		Methanesulphenyl chloride, trichl...	184	CCl4S	000594-42-3	10
4		1-Propene, 1,1,2,3,3,3-hexachloro-	246	C3Cl6	001888-71-7	10
5		Dimethyl-tetraselenafulvalene	424	C8H8Se4	1000149-11-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031516\
Data File : BF085465.D
Acq On : 15 Mar 2016 20:25
Operator : UM/SJ
Sample : H1774-20
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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...	5.12	2.5	ng	106194	1	6.90	857121	20.0
unknown6.68	6.68	91.8	ng	3934400	1	6.90	857121	20.0
Heneicosane	10.38	2.1	ng	135840	3	9.96	1269550	20.0
Pentadecane	10.85	3.2	ng	205171	4	11.43	1274470	20.0
Dodecanoic acid	11.96	2.2	ng	139198	4	11.43	1274470	20.0
3-Eicosene, (E)-	13.91	6.5	ng	339389	5	14.07	1050690	20.0
unknown15.81	15.81	5.9	ng	210115	6	15.52	710584	20.0
unknown16.47	16.47	2.4	ng	84070	6	15.52	710584	20.0
unknown17.73	17.73	2.7	ng	94744	6	15.52	710584	20.0