

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
 Data File : BF084828.D
 Acq On : 4 Feb 2016 11:37
 Operator : SJ/IZ
 Sample : H1322-12
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B014(25-27)

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-BF020116.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	4.144	177	180	185	rBV	60046	83531	1.52%	0.169%
2	4.841	239	241	253	rVB	1225749	2173895	39.67%	4.411%
3	5.287	277	280	282	rBV	5090587	5480463	100.00%	11.119%
4	5.687	313	315	318	rBV	76385	68837	1.26%	0.140%
5	6.339	369	372	375	rBV	4312549	4915027	89.68%	9.972%
6	6.453	379	382	385	rVV	4420373	5126403	93.54%	10.401%
7	6.681	400	402	404	rBV	1379620	1193784	21.78%	2.422%
8	6.841	413	416	418	rBV	4455815	3910608	71.36%	7.934%
9	7.253	449	452	455	rBV	2557865	3353818	61.20%	6.804%
10	7.379	459	463	467	rBV2	78896	119040	2.17%	0.242%
11	7.973	512	515	517	rBV	1877364	1660427	30.30%	3.369%
12	9.059	606	610	612	rBV	3567807	4837542	88.27%	9.815%
13	9.447	642	644	646	rBV	819910	782672	14.28%	1.588%
14	9.665	661	663	666	rBV	80497	84904	1.55%	0.172%
15	9.722	666	668	671	rVB	1890278	1646489	30.04%	3.341%
16	10.168	706	707	709	rVB	145217	103401	1.89%	0.210%
17	10.385	724	726	729	rBV	42021	64442	1.18%	0.131%
18	10.510	734	737	740	rBV	3292428	3272788	59.72%	6.640%
19	10.636	746	748	755	rVB	140681	176650	3.22%	0.358%
20	11.082	785	787	789	rBV	88150	88683	1.62%	0.180%
21	11.196	795	797	800	rVB2	1299167	1400035	25.55%	2.840%
22	11.745	843	845	849	rBV3	35203	56382	1.03%	0.114%
23	11.916	856	860	863	rBV3	40291	83864	1.53%	0.170%
24	11.996	863	867	871	rVB3	30556	65043	1.19%	0.132%
25	12.305	891	894	896	rVV	212130	181561	3.31%	0.368%
26	12.625	919	922	924	rBV2	279488	268679	4.90%	0.545%
27	12.785	934	936	939	rBV	3020431	2914632	53.18%	5.913%
28	13.025	955	957	960	rBV	178565	247434	4.51%	0.502%
29	13.322	981	983	985	rBV	134038	155231	2.83%	0.315%
30	13.368	985	987	991	rVB	41543	65546	1.20%	0.133%
31	13.654	1010	1012	1014	rBV	46332	58281	1.06%	0.118%
32	13.699	1014	1016	1025	rBV	619376	974967	17.79%	1.978%
33	13.825	1025	1027	1030	rVV	888798	1107389	20.21%	2.247%
34	14.019	1042	1044	1051	rBV3	28732	55102	1.01%	0.112%

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S4-B014(25-27)

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-BF020116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.339	1065	1072	1077	rBV2	75476	259866	4.74%	0.527%
36	14.614	1092	1096	1098	rBV2	36233	59130	1.08%	0.120%
37	14.911	1120	1122	1124	rBV	50842	65287	1.19%	0.132%
38	14.957	1124	1126	1132	rVB6	34396	96547	1.76%	0.196%
39	15.208	1145	1148	1150	rBV	837722	1001750	18.28%	2.032%
40	15.699	1187	1191	1200	rBV2	73261	286263	5.22%	0.581%
41	16.065	1219	1223	1229	rBV5	27499	91063	1.66%	0.185%
42	17.048	1303	1309	1313	rBV5	67428	180043	3.29%	0.365%
43	17.174	1318	1320	1326	rVB3	23527	57566	1.05%	0.117%
44	17.471	1341	1346	1350	rVB	198142	413631	7.55%	0.839%

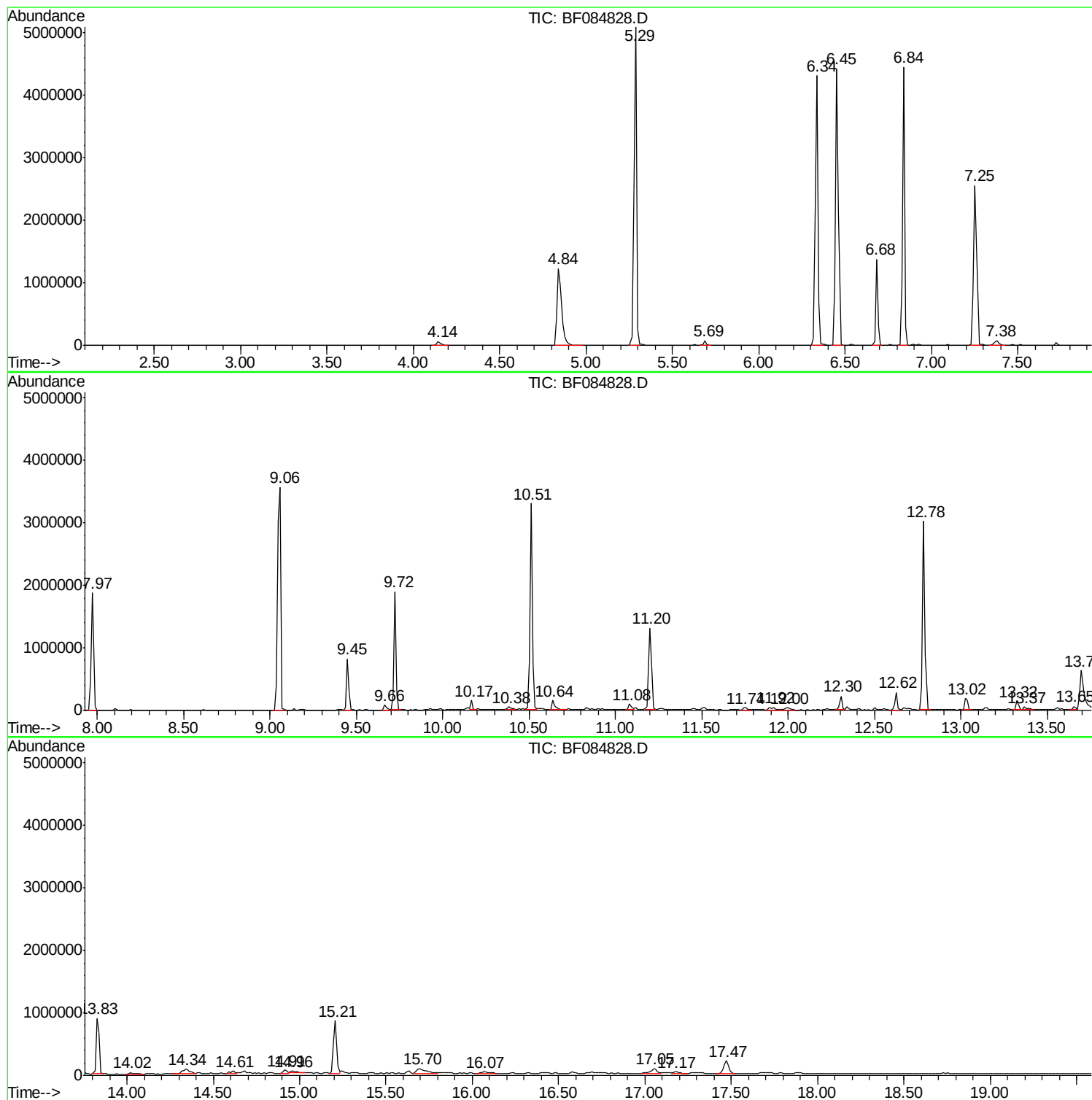
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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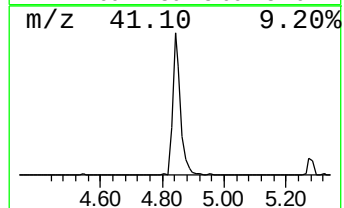
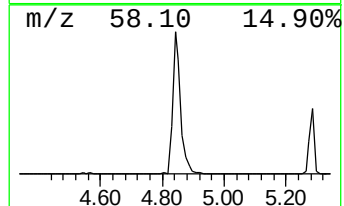
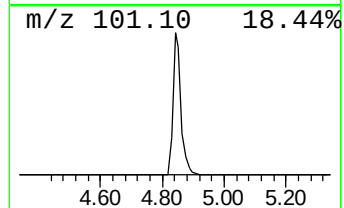
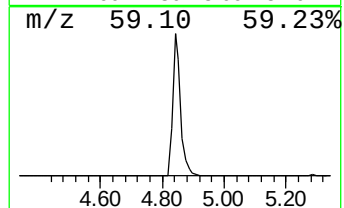
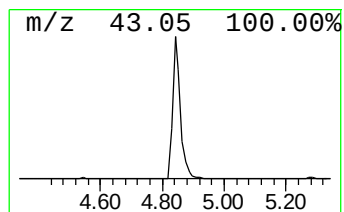
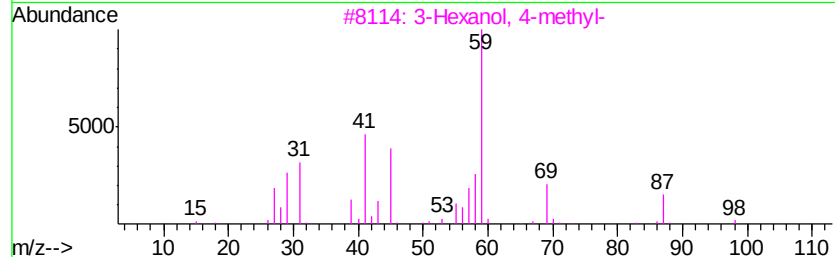
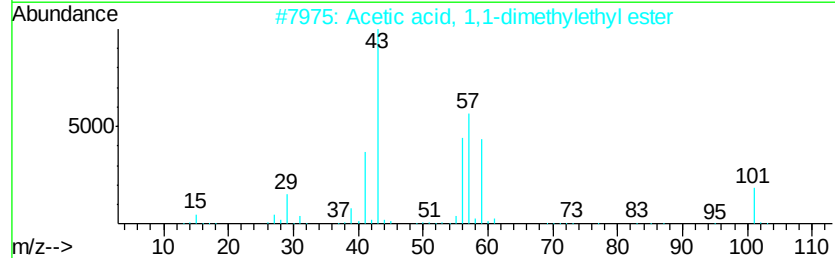
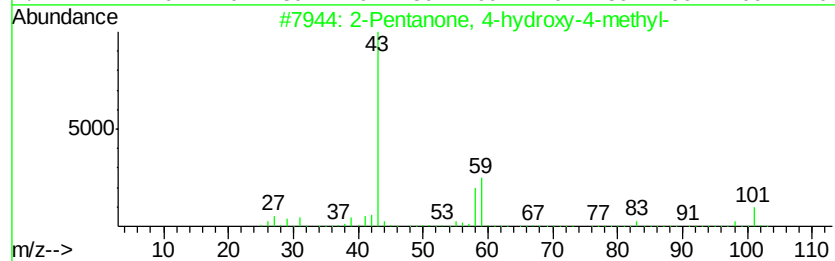
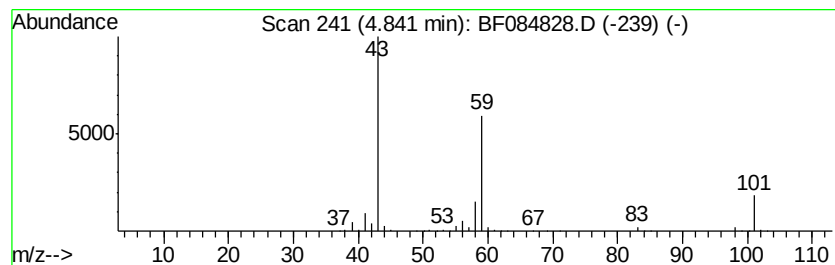
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.84	36.42 ng	2173900	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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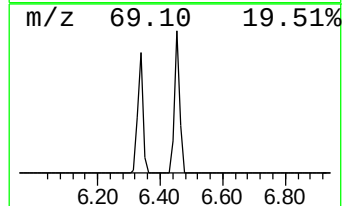
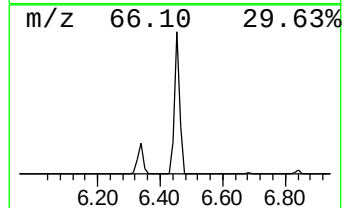
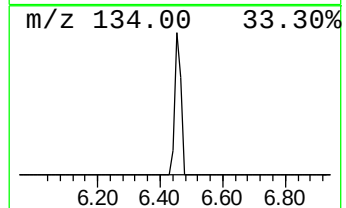
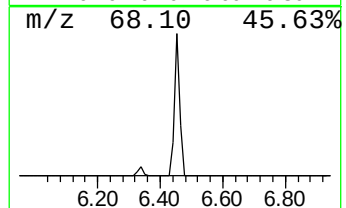
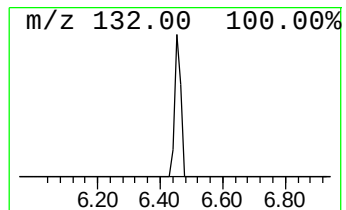
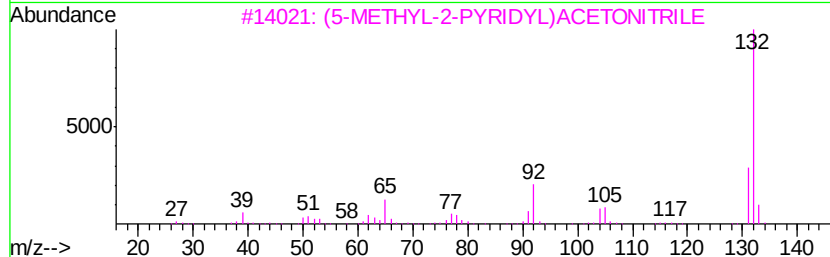
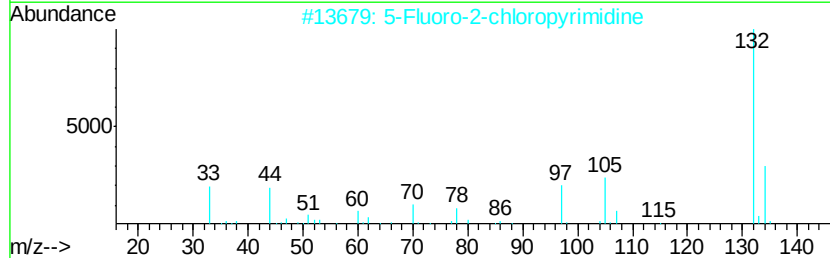
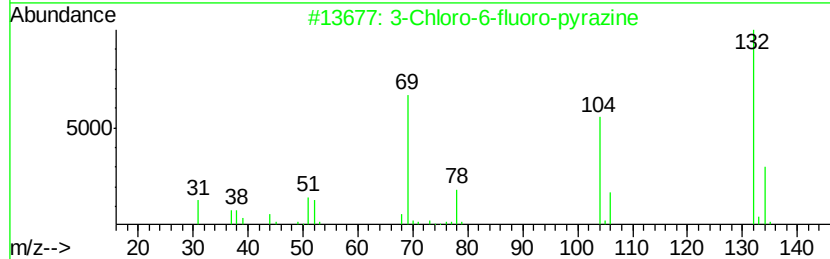
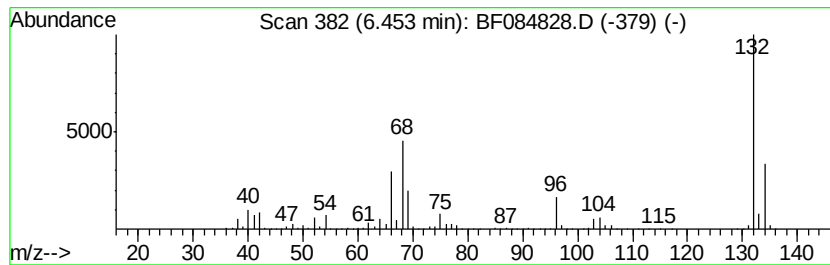
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Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	85.88 ng	5126400	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Xenon	132	Xe	007440-63-3	9



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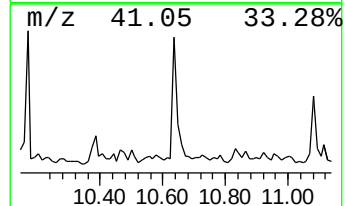
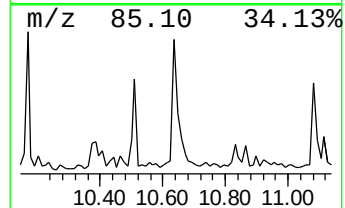
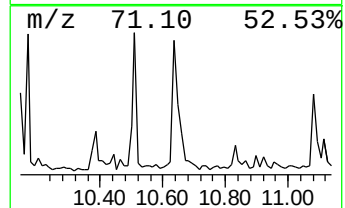
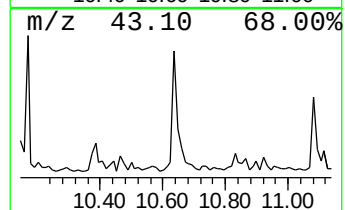
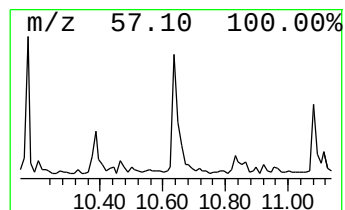
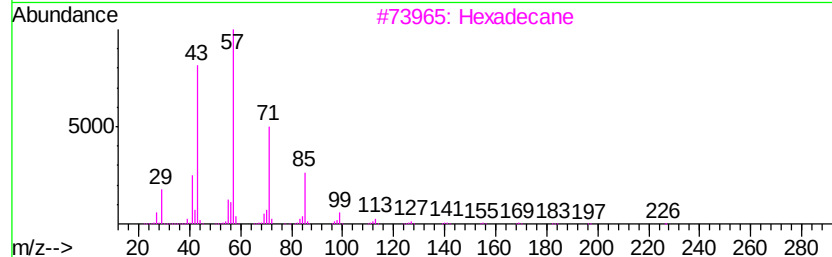
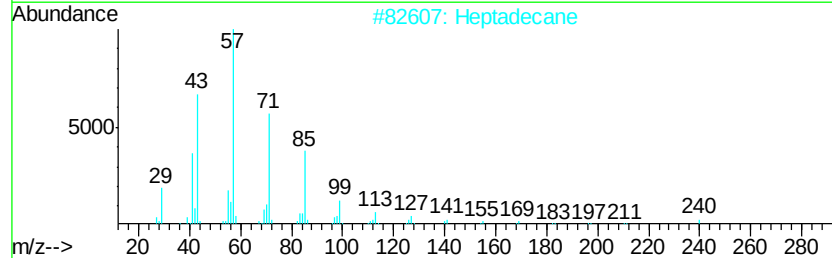
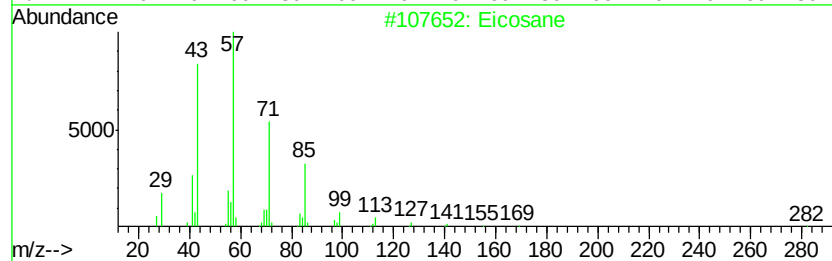
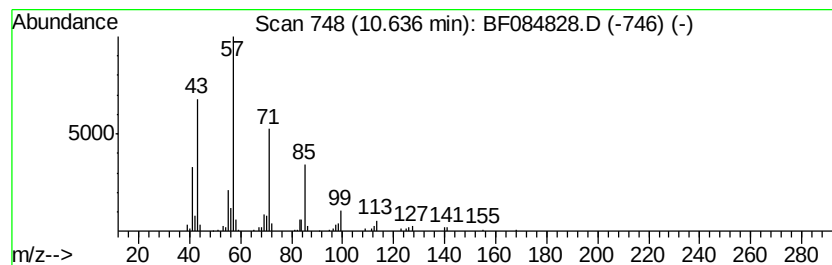
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.64	2.52 ng	176650	Phenanthrene-d10		11.20	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heptadecane		240	C17H36	000629-78-7	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Tetradecane		198	C14H30	000629-59-4	87
5	Tridecane		184	C13H28	000629-50-5	86



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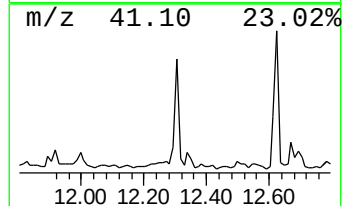
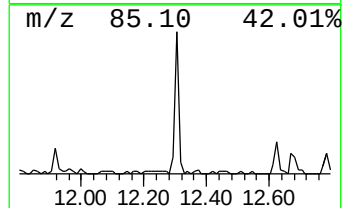
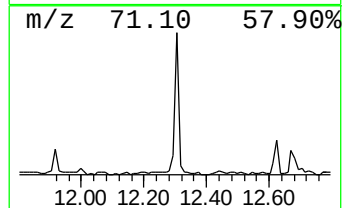
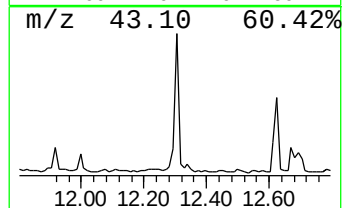
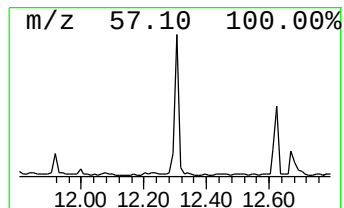
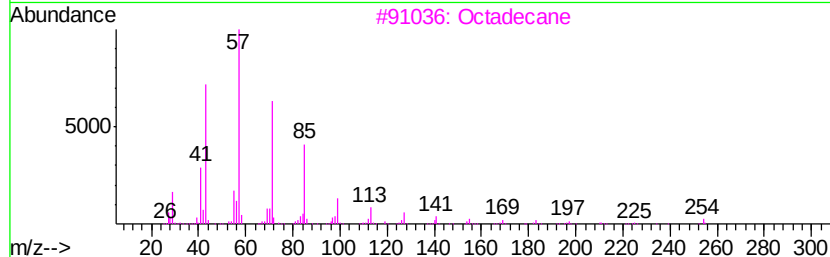
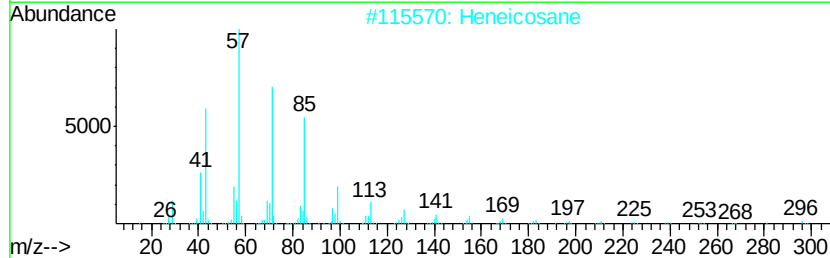
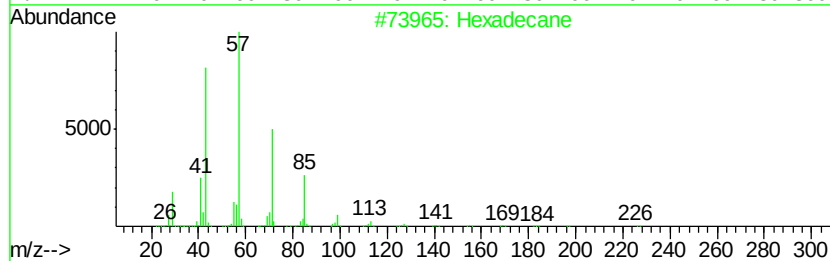
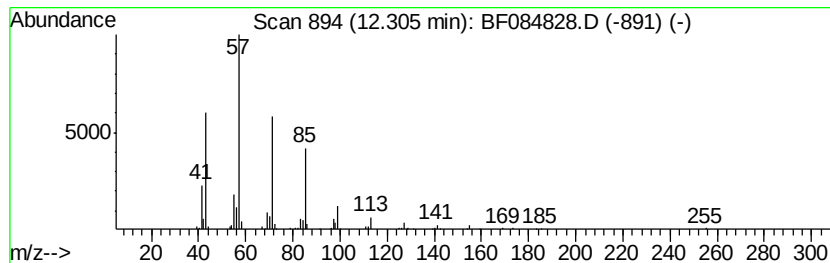
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.59 ng	181561	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Heneicosane		296	C21H44	000629-94-7	90
3	Octadecane		254	C18H38	000593-45-3	86
4	Eicosane		282	C20H42	000112-95-8	83
5	Heptacosane		380	C27H56	000593-49-7	83



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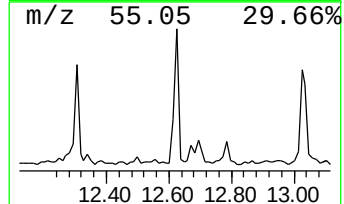
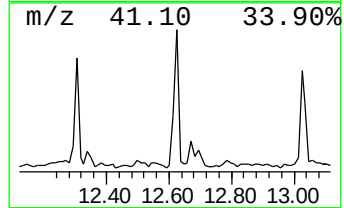
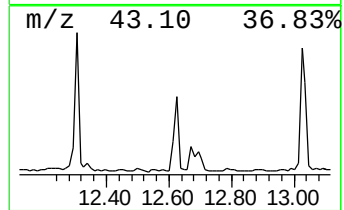
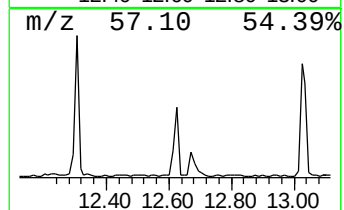
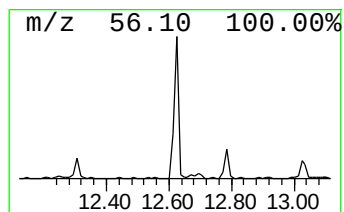
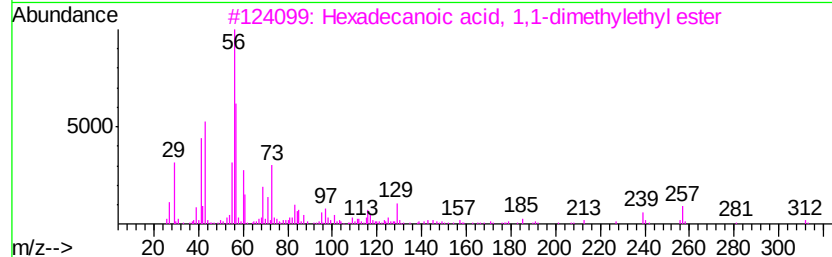
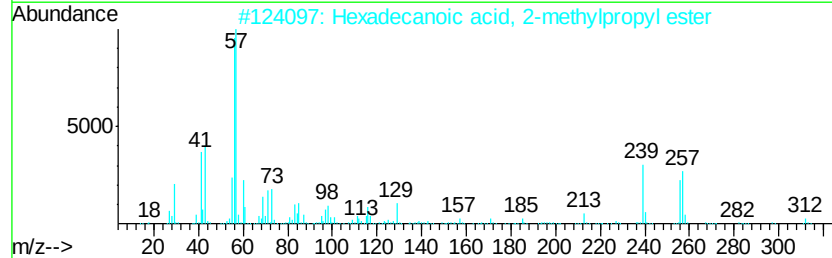
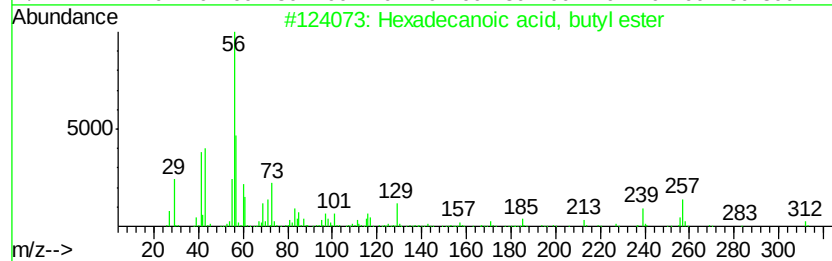
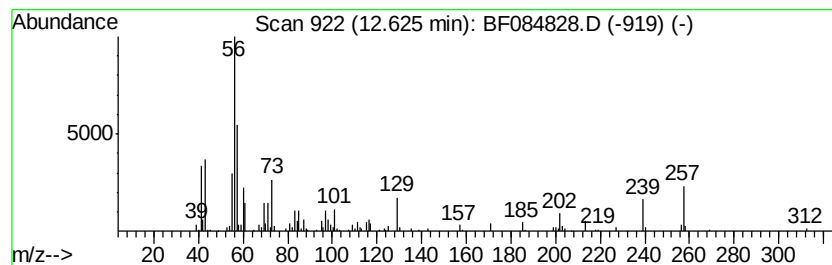
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.62	4.85 ng	268679	Chrysene-d12	13.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 2-methylpropyl ester	312	C20H40O2	000110-34-9	64
3	Hexadecanoic acid, 1,1-dimethylethyl ester	312	C20H40O2	031158-91-5	50
4	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
Data File : BF084828.D
Acq On : 4 Feb 2016 11:37
Operator : SJ/IZ
Sample : H1322-12
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S4-B014(25-27)

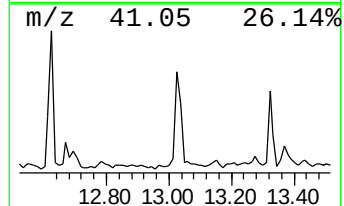
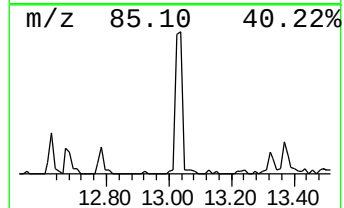
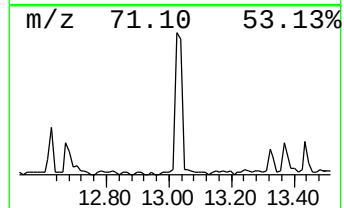
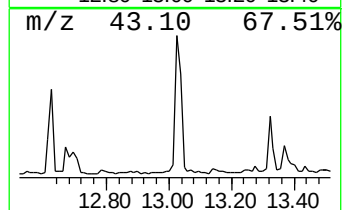
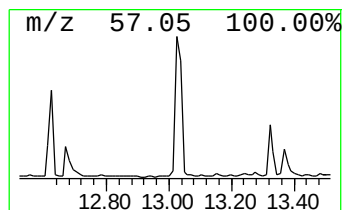
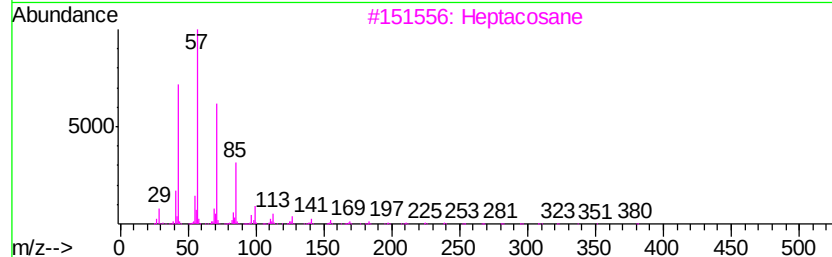
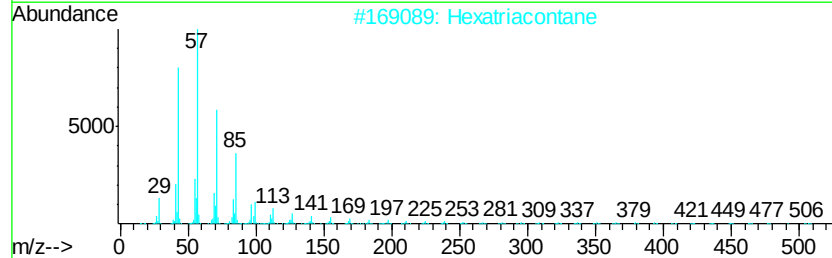
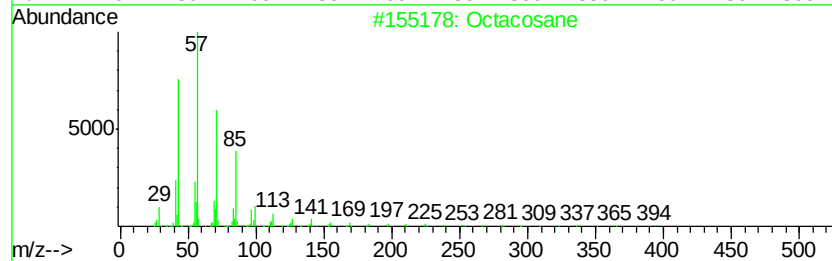
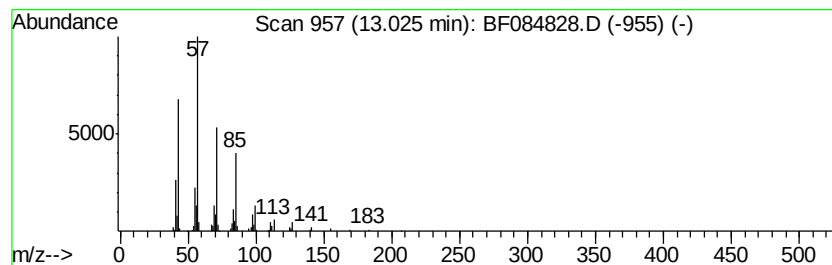
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.02	4.47 ng	247434	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexatriacontane	507	C36H74	000630-06-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Tetratetracontane	619	C44H90	007098-22-8	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
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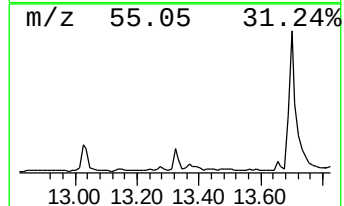
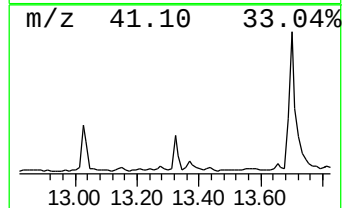
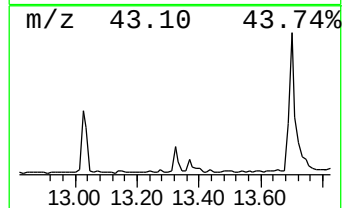
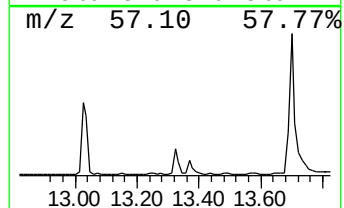
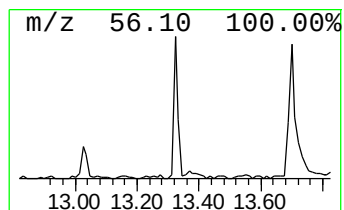
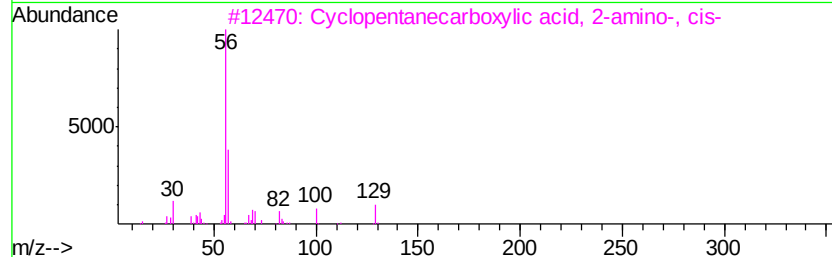
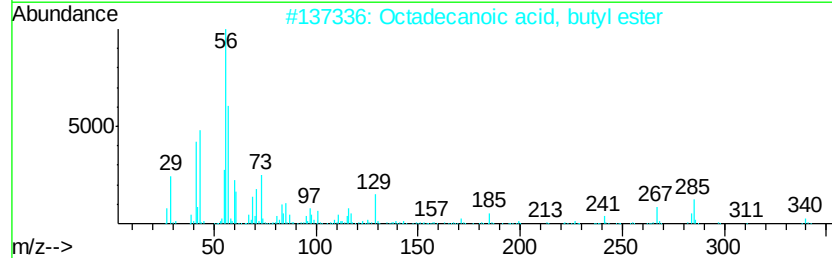
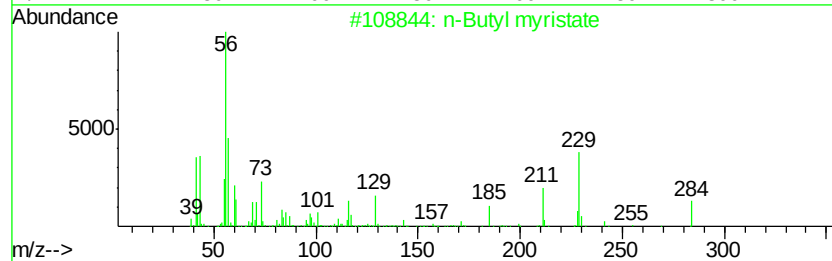
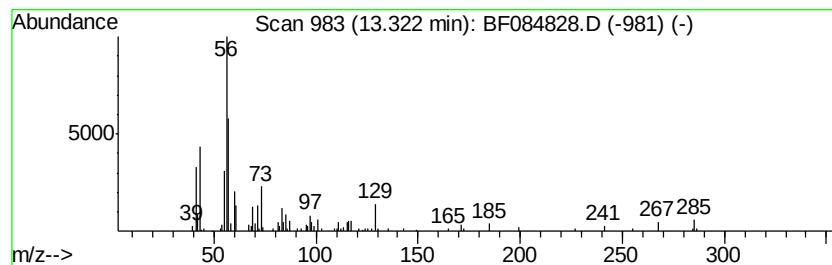
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Butyl myristate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	2.80 ng	155231	Chrysene-d12	13.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Butyl myristate	284 C18H36O2	000110-36-1	86
2	Octadecanoic acid, butyl ester	340 C22H44O2	000123-95-5	58
3	Cyclopentanecarboxylic acid, 2-amino, cis-	129 C6H11NO2	037910-65-9	43
4	Oxirane, 2,3-bis(1-methylethyl)-	128 C8H16O	054644-32-5	38
5	Decane, 2,2,3-trimethyl-	184 C13H28	062338-09-4	37



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
Data File : BF084828.D
Acq On : 4 Feb 2016 11:37
Operator : SJ/IZ
Sample : H1322-12
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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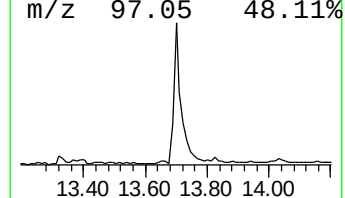
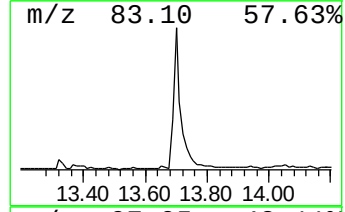
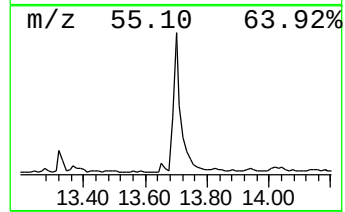
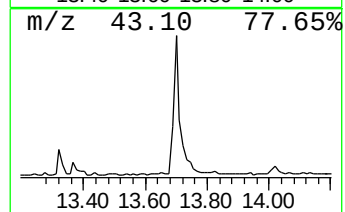
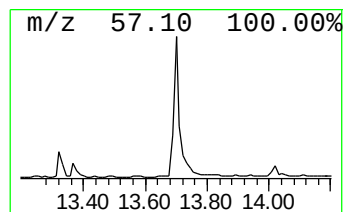
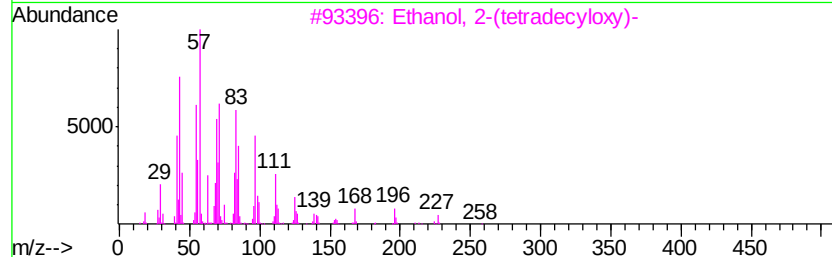
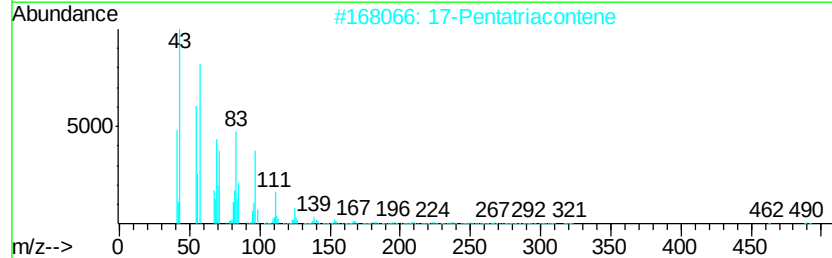
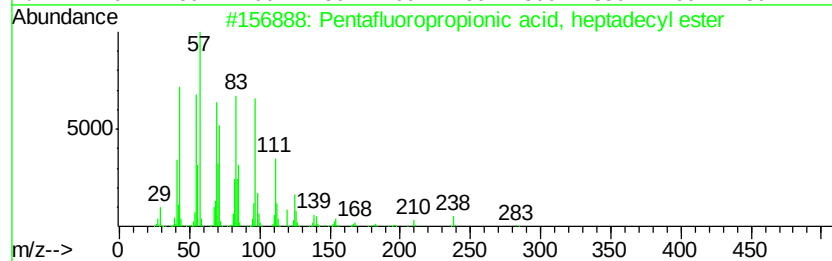
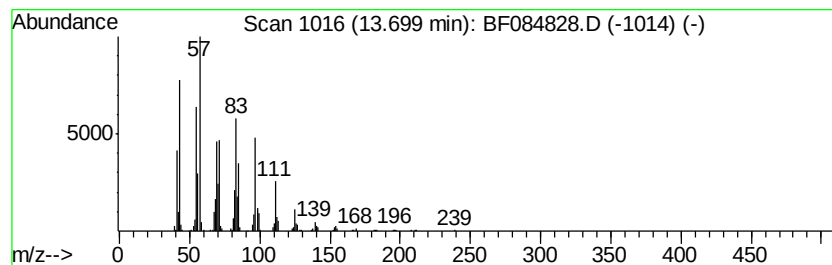
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	17.61 ng	974967	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
Data File : BF084828.D
Acq On : 4 Feb 2016 11:37
Operator : SJ/IZ
Sample : H1322-12
Misc :
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Instrument :
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ClientSampled :
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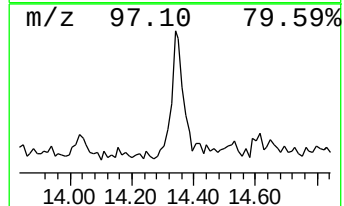
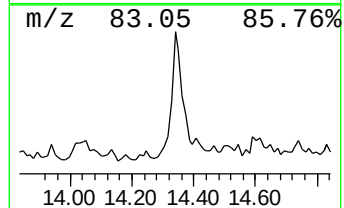
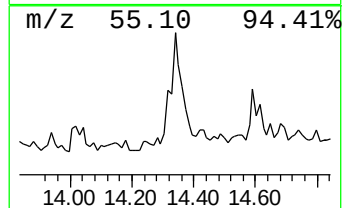
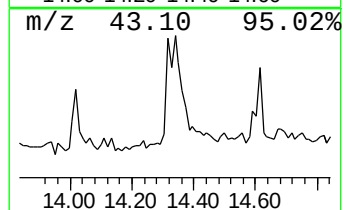
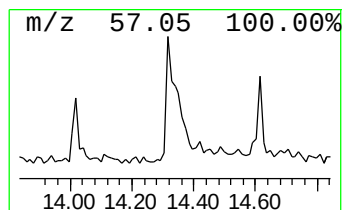
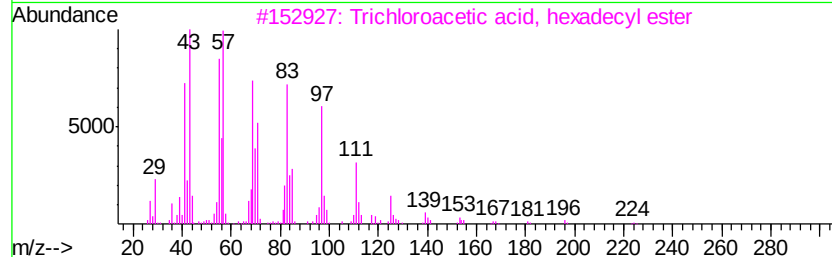
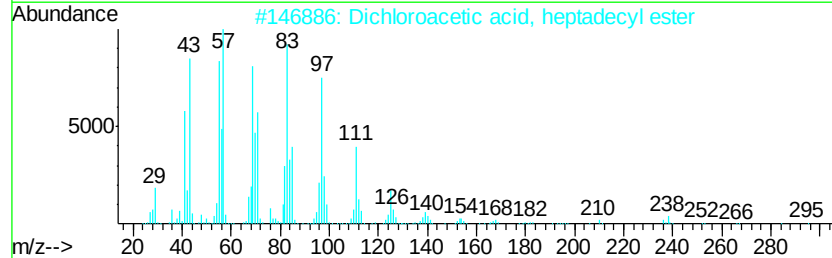
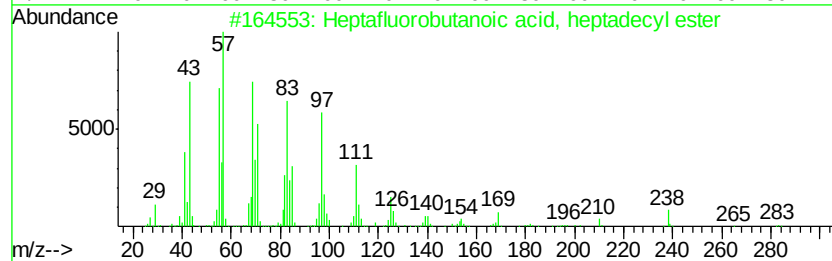
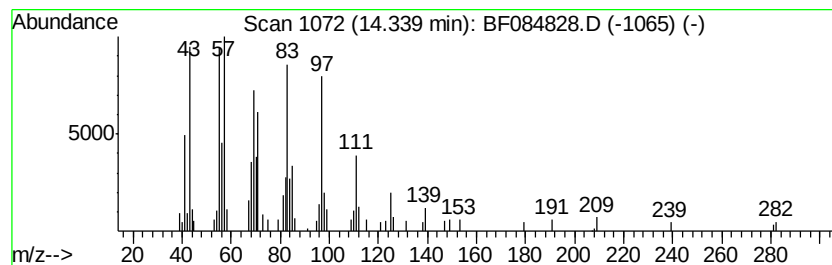
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptafluorobutanoic acid, h... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	4.69 ng	259866	Chrysene-d12	13.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
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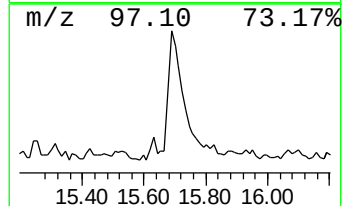
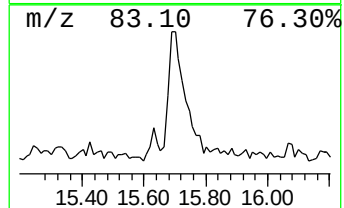
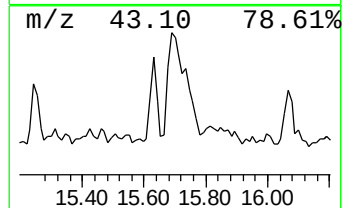
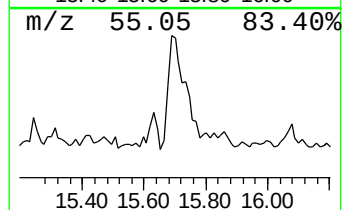
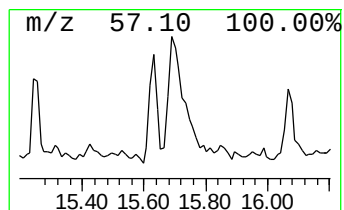
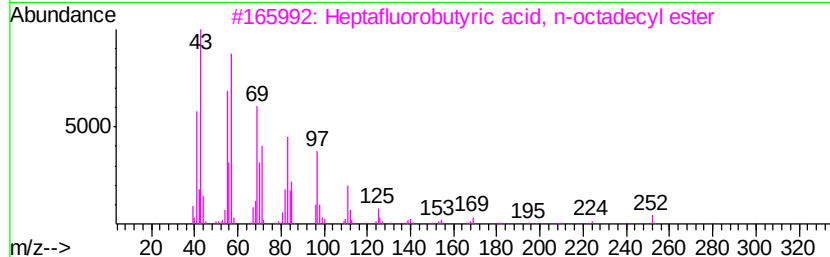
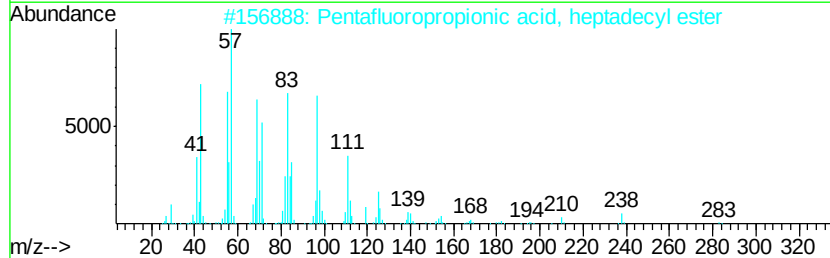
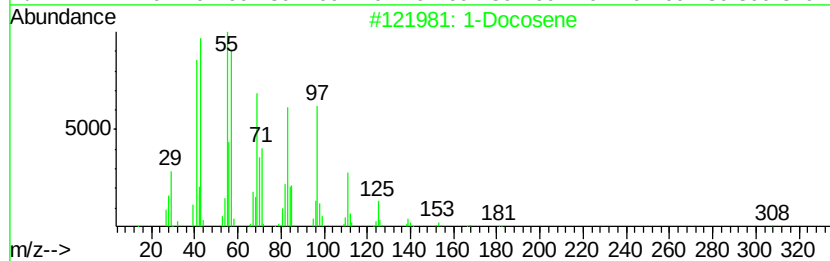
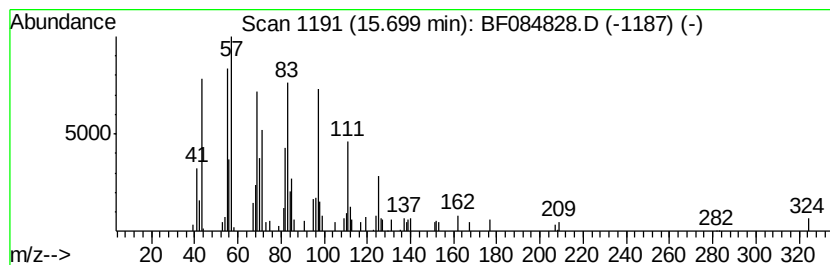
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	5.72 ng	286263	Perylene-d12	15.21
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 90
2	Pentafluoropropionic acid, hepta...		402 C20H35F5O2	1000283-04-2 87
3	Heptafluorobutyric acid, n-octad...		466 C22H37F7O2	000400-57-7 83
4	Bromoacetic acid, octadecyl ester		390 C20H39BrO2	018992-03-5 74
5	Acetic acid, octadecyl ester		312 C20H40O2	000822-23-1 74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020316\
Data File : BF084828.D
Acq On : 4 Feb 2016 11:37
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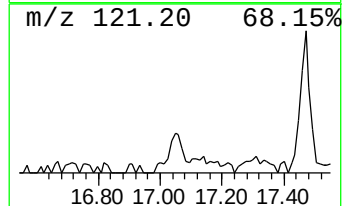
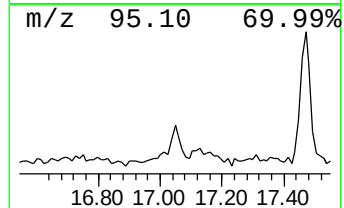
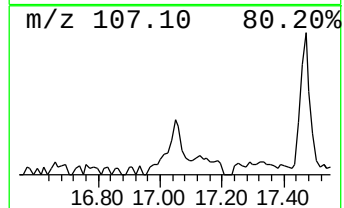
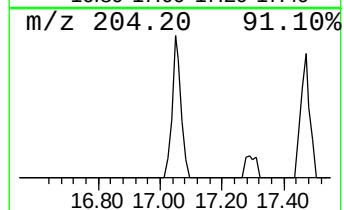
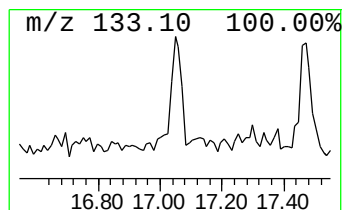
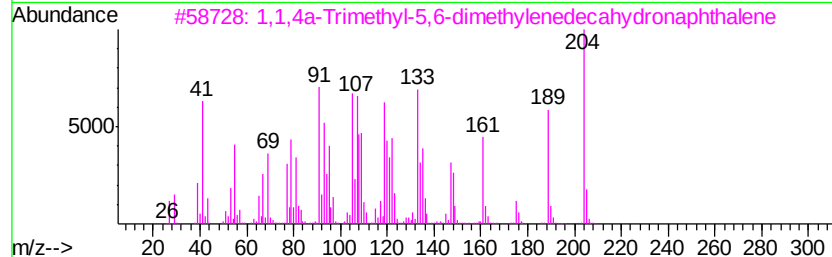
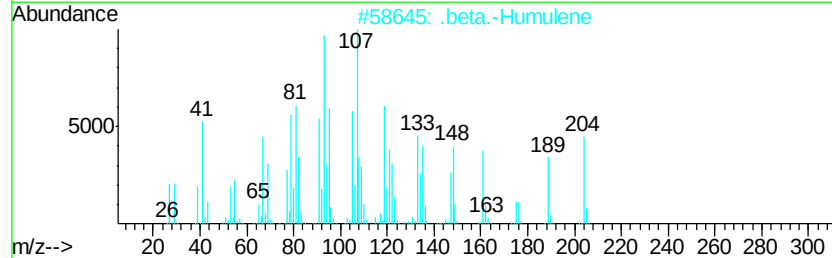
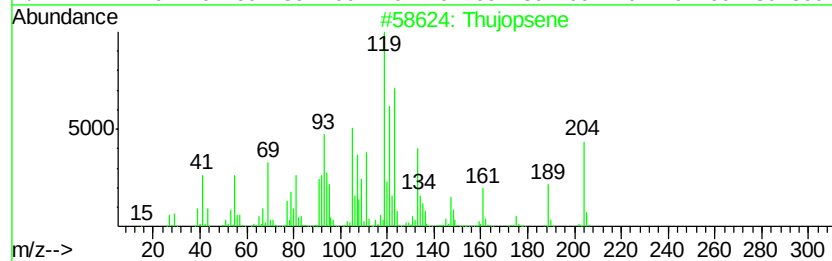
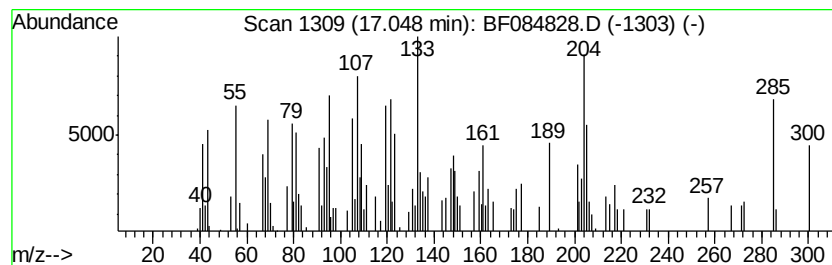
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Thujopsene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.05	3.59 ng	180043	Perylene-d12	15.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thujopsene	204	C15H24	000470-40-6	78
2			.beta.-Humulene	204	C15H24	000116-04-1	55
3			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	49
4			Azulene, 1,2,3,4,5,6,7,8-octahyd...	204	C15H24	003691-12-1	46
5			Himachala-2,4-diene	204	C15H24	060909-27-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
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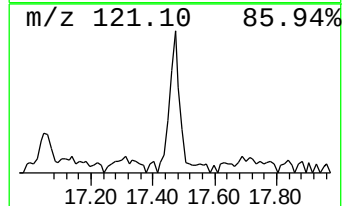
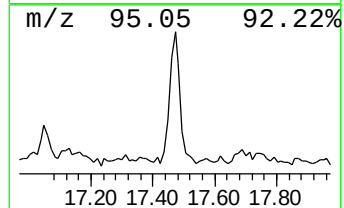
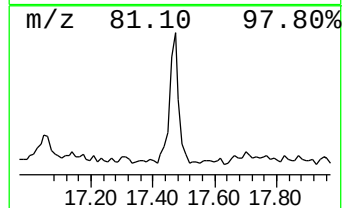
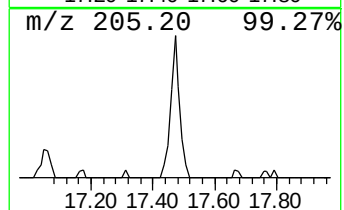
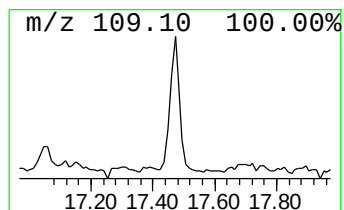
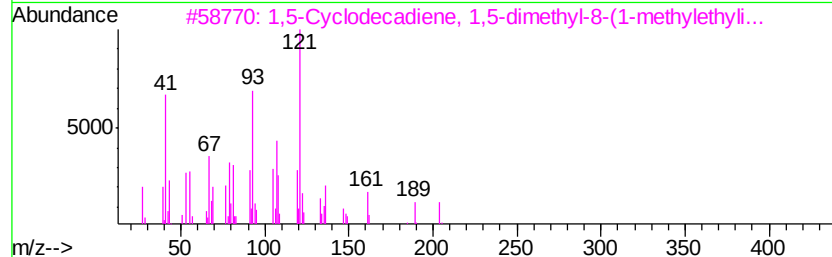
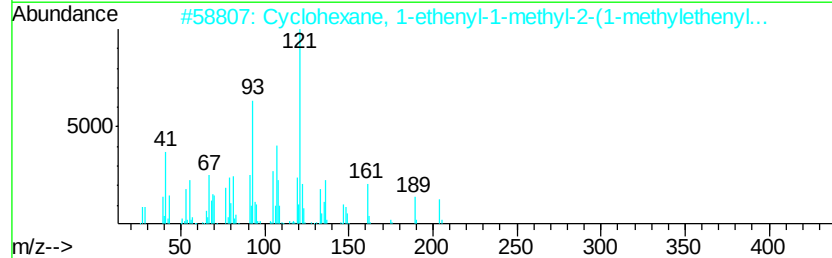
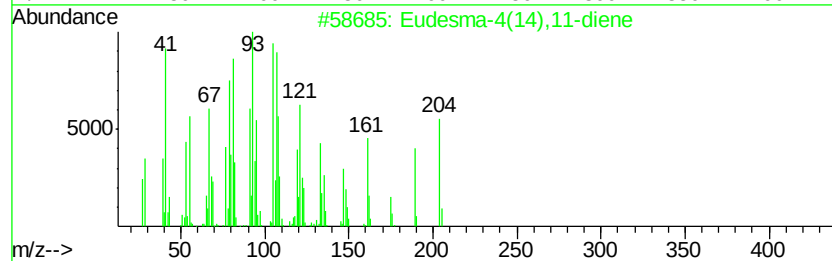
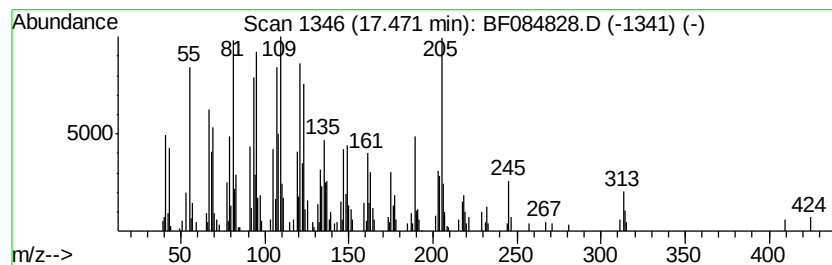
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown17.47 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	8.26 ng	413631	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eudesma-4(14),11-diene	204	C15H24	1000152-04-3	43
2		Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	003242-08-8	42
3		1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	015423-57-1	41
4		1-Naphthalenepropanol, .alpha.-e...	306	C20H34O2	004549-12-6	38
5		6-(3-Isopropenylcycloprop-1-enyl...	204	C14H20O	1000195-43-0	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020316\
 Data File : BF084828.D
 Acq On : 4 Feb 2016 11:37
 Operator : SJ/IZ
 Sample : H1322-12
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B014(25-27)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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...	4.84	36.4	ng	2173900	1	6.68	1193780	20.0
unknown6.45	6.45	85.9	ng	5126400	1	6.68	1193780	20.0
Eicosane	10.64	2.5	ng	176650	4	11.20	1400040	20.0
Hexadecane	12.30	2.6	ng	181561	4	11.20	1400040	20.0
Hexadecanoic acid...	12.62	4.8	ng	268679	5	13.82	1107390	20.0
Octacosane	13.02	4.5	ng	247434	5	13.82	1107390	20.0
n-Butyl myristate	13.32	2.8	ng	155231	5	13.82	1107390	20.0
Pentafluoropropio...	13.70	17.6	ng	974967	5	13.82	1107390	20.0
Heptafluorobutano...	14.34	4.7	ng	259866	5	13.82	1107390	20.0
1-Docosene	15.70	5.7	ng	286263	6	15.21	1001750	20.0
Thujopsene	17.05	3.6	ng	180043	6	15.21	1001750	20.0
unknown17.47	17.47	8.3	ng	413631	6	15.21	1001750	20.0