

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
 Data File : BF095134.D
 Acq On : 15 May 2017 19:47
 Operator : SJ/MA
 Sample : I3144-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-002

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-BF050217.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.137	540	544	560	rBV	247561	520971	16.56%	2.239%
2	5.748	644	648	681	rBV	1270238	2264491	72.00%	9.734%
3	7.319	911	915	932	rBV	1409312	2179308	69.29%	9.368%
4	7.442	932	936	954	rVB	1791325	2547982	81.01%	10.953%
5	7.778	990	993	1004	rBV	365439	461051	14.66%	1.982%
6	8.019	1029	1034	1045	rBV	1609253	1921973	61.11%	8.262%
7	8.678	1141	1146	1163	rBV	1053504	1401758	44.57%	6.026%
8	9.795	1331	1336	1350	rBV	449745	616100	19.59%	2.648%
9	11.566	1632	1637	1662	rBV	2506152	3145099	100.00%	13.519%
10	12.260	1751	1755	1771	rBV	183508	302678	9.62%	1.301%
11	12.624	1812	1817	1828	rBV2	544666	766764	24.38%	3.296%
12	13.919	2032	2037	2050	rBV	996259	1516561	48.22%	6.519%
13	15.030	2221	2226	2242	rBV	427750	626238	19.91%	2.692%
14	15.983	2384	2388	2395	rBV4	63963	115820	3.68%	0.498%
15	17.348	2615	2620	2632	rBV	1570158	1811402	57.59%	7.786%
16	18.606	2828	2834	2835	rBV4	26408	39045	1.24%	0.168%
17	18.701	2846	2850	2864	rVB	336190	455897	14.50%	1.960%
18	20.100	3084	3088	3092	rBV	94689	108291	3.44%	0.465%
19	20.324	3124	3126	3130	rBV4	23915	32379	1.03%	0.139%
20	20.371	3130	3134	3145	rVV	308294	469147	14.92%	2.017%
21	20.453	3145	3148	3153	rVB5	24190	33344	1.06%	0.143%
22	20.730	3191	3195	3201	rVB2	27262	52158	1.66%	0.224%
23	20.836	3209	3213	3218	rVB	61704	74145	2.36%	0.319%
24	21.047	3247	3249	3255	rVB	37387	63256	2.01%	0.272%
25	21.912	3391	3396	3398	rBV6	18279	32937	1.05%	0.142%
26	22.200	3436	3445	3452	rVB6	72739	214430	6.82%	0.922%
27	22.324	3462	3466	3470	rVV5	27608	41344	1.31%	0.178%
28	22.618	3510	3516	3526	rVB8	80232	244376	7.77%	1.050%
29	22.877	3547	3560	3568	rBV8	56278	231267	7.35%	0.994%
30	23.041	3581	3588	3596	rVB7	75602	192450	6.12%	0.827%
31	23.759	3699	3710	3723	rBV7	79488	389790	12.39%	1.676%
32	23.888	3725	3732	3741	rVB6	135680	391143	12.44%	1.681%

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-PS-01-002

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

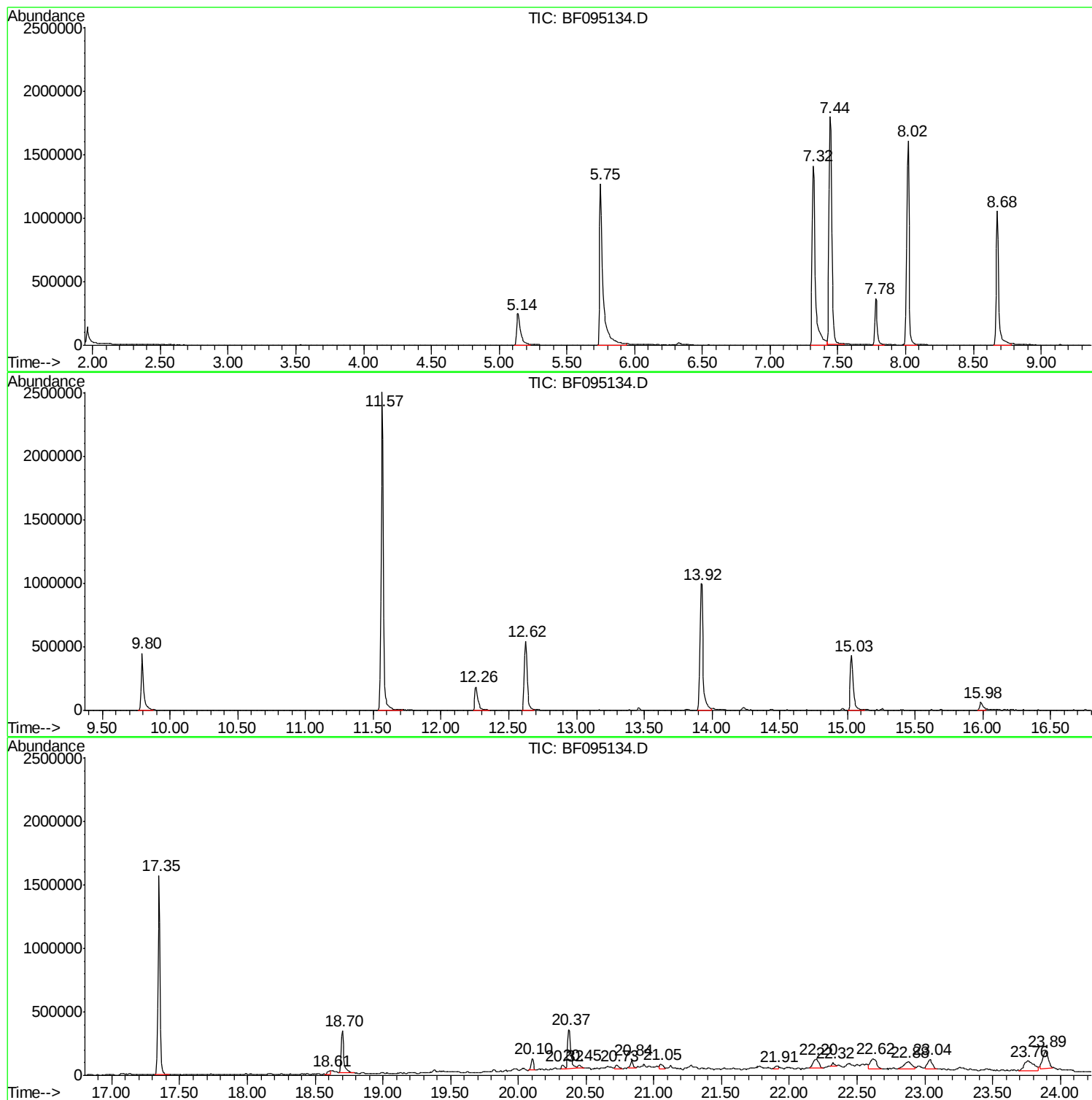
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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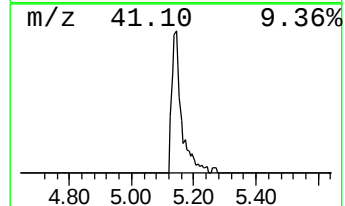
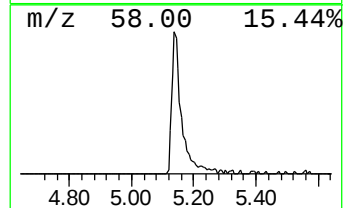
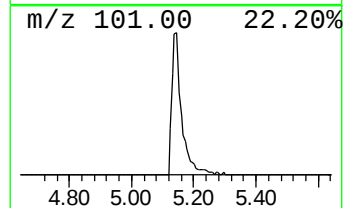
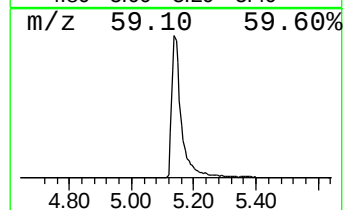
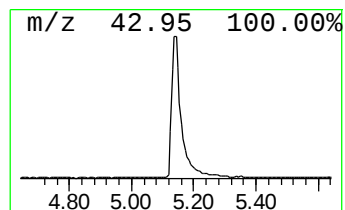
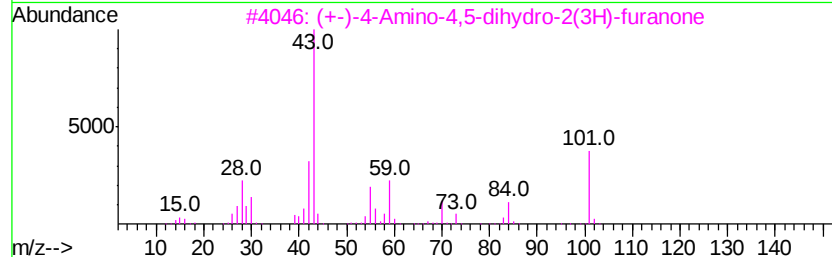
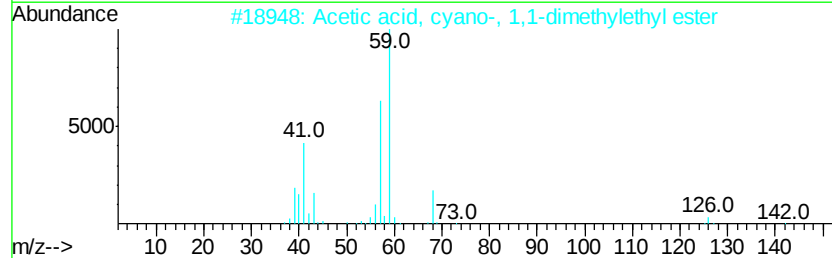
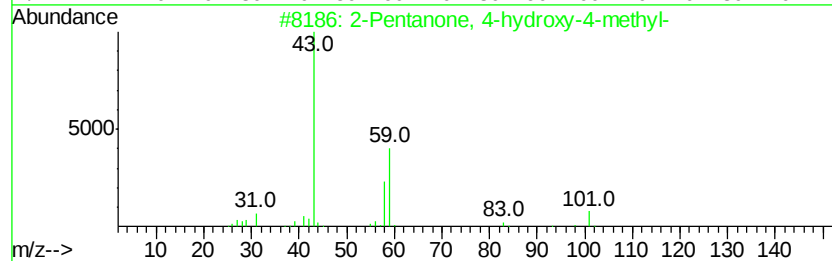
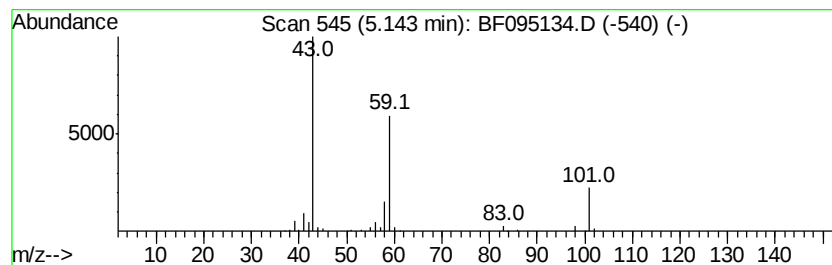
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	22.60 ng	520971	1,4-Dichlorobenzene-d4	7.78

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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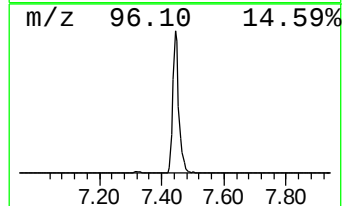
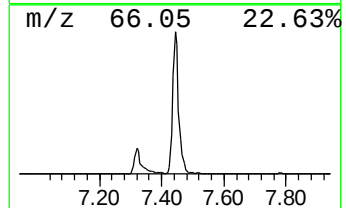
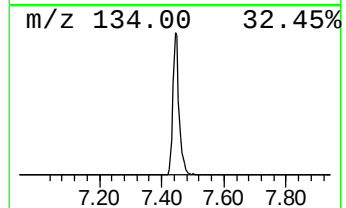
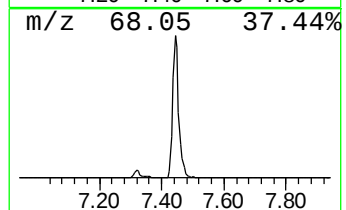
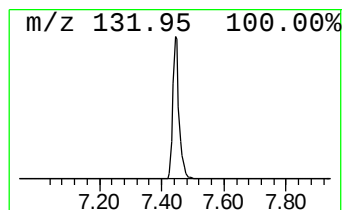
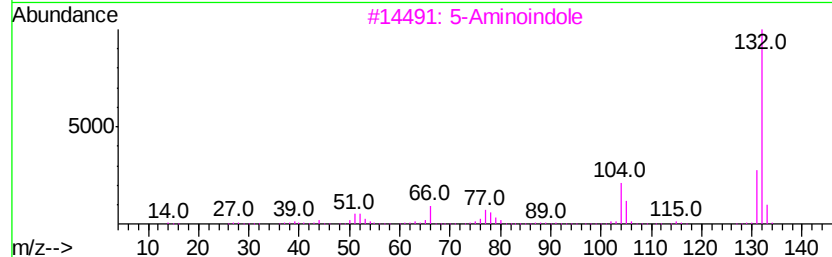
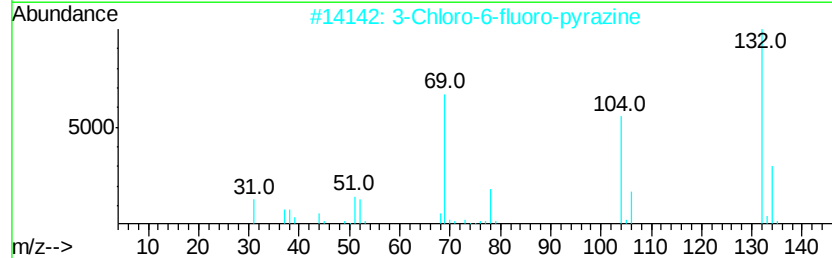
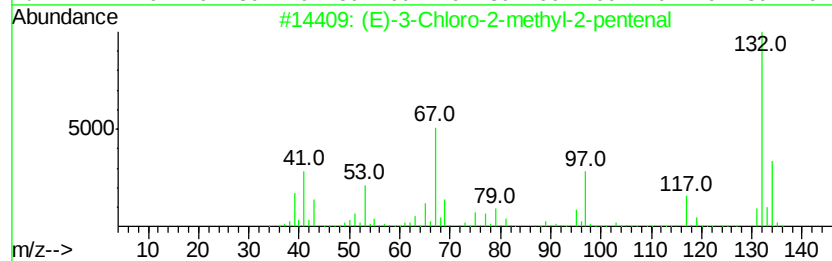
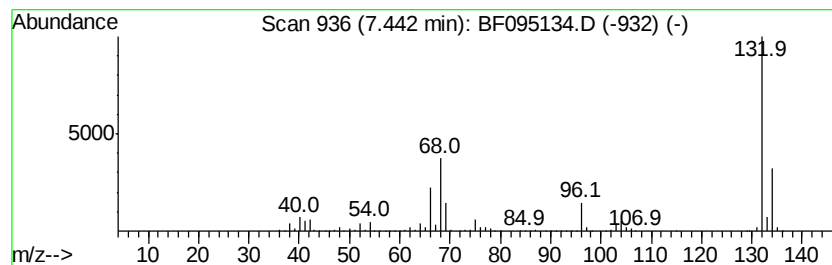
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	110.53 ng	2547980	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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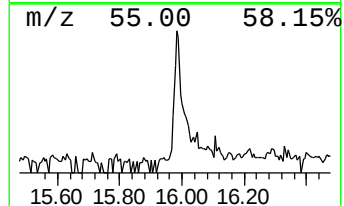
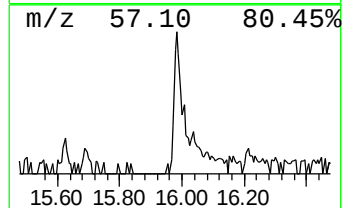
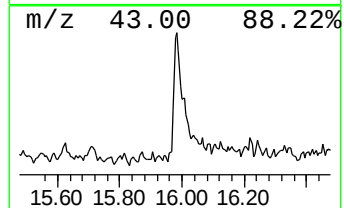
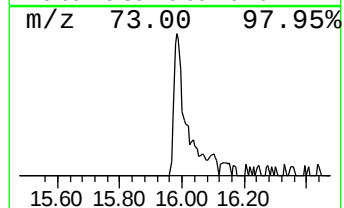
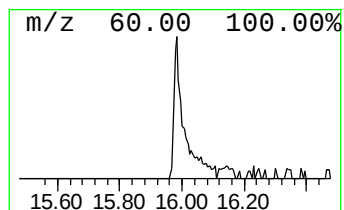
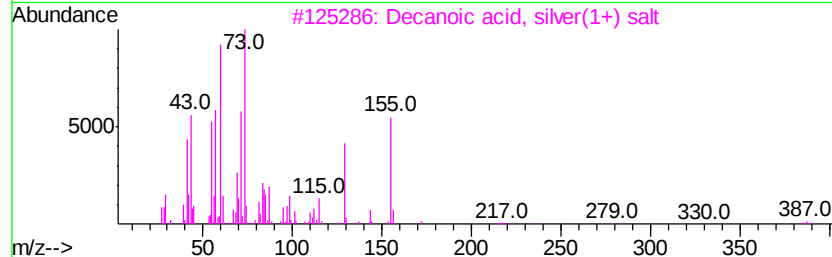
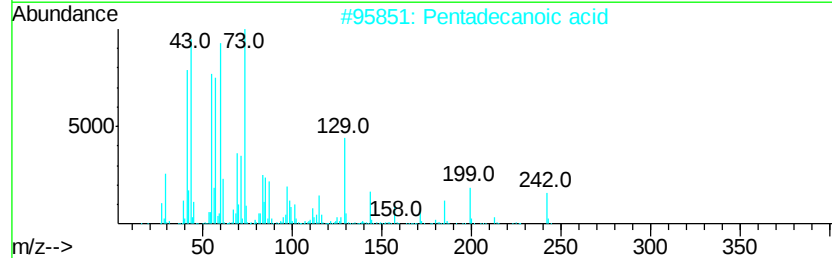
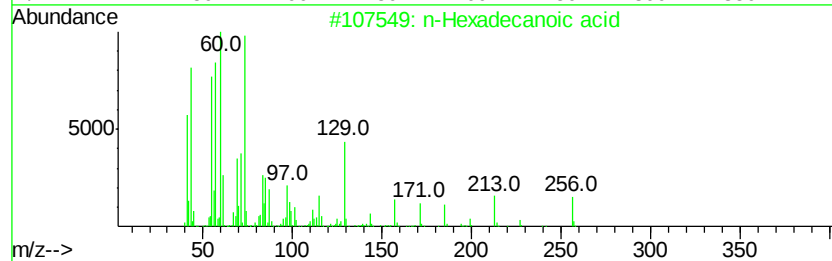
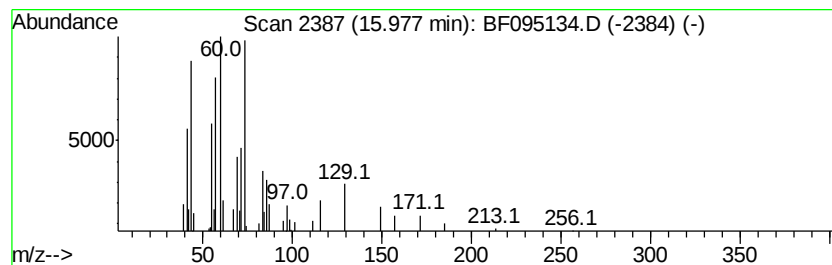
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	3.70 ng	115820	Phenanthrene-d10	15.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	53



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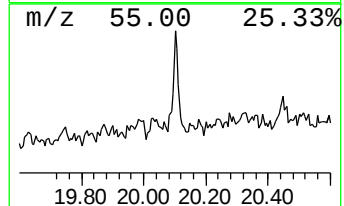
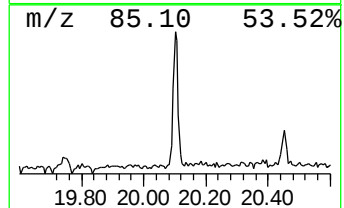
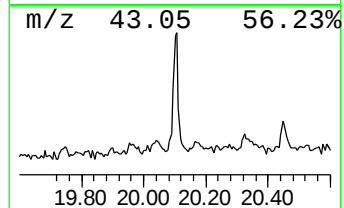
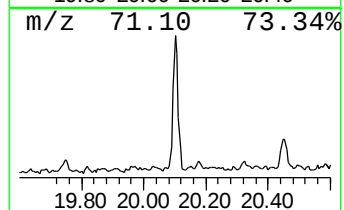
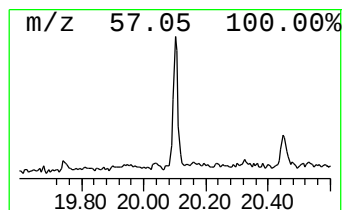
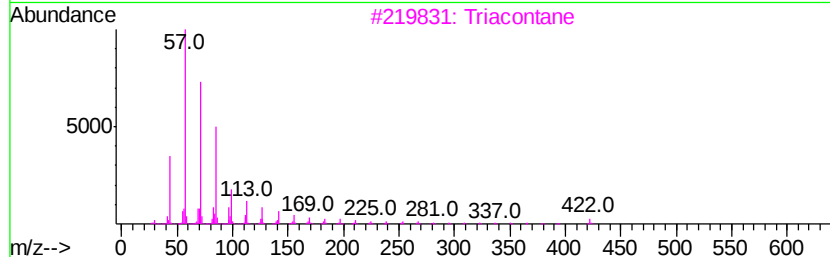
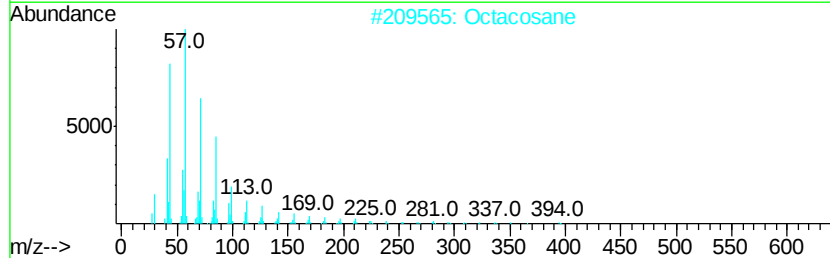
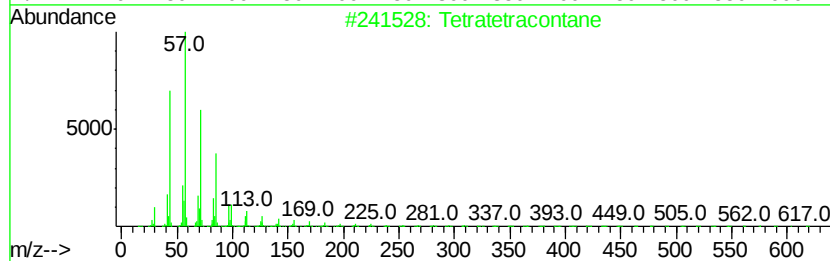
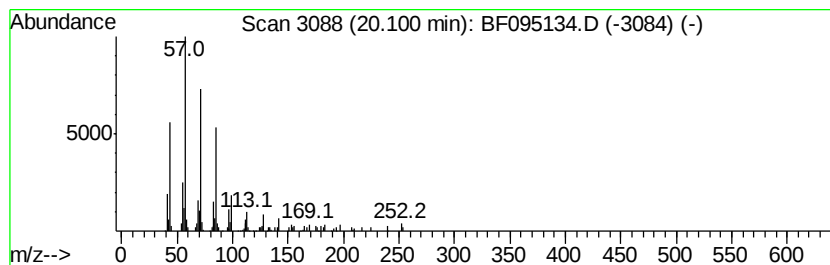
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.10	4.62 ng	108291	Perylene-d12	20.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Triacosane	422	C30H62	000638-68-6	91
4		Hexacosane	366	C26H54	000630-01-3	90
5		Heneicosane	296	C21H44	000629-94-7	90



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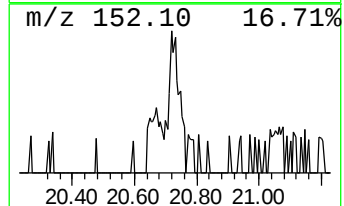
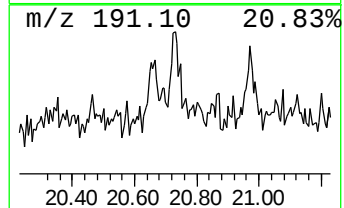
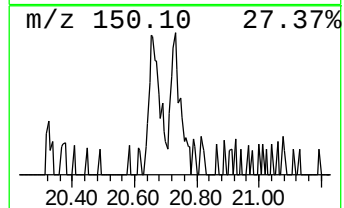
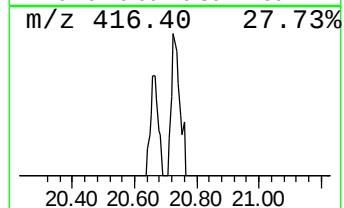
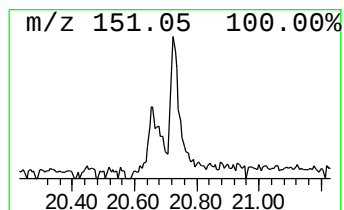
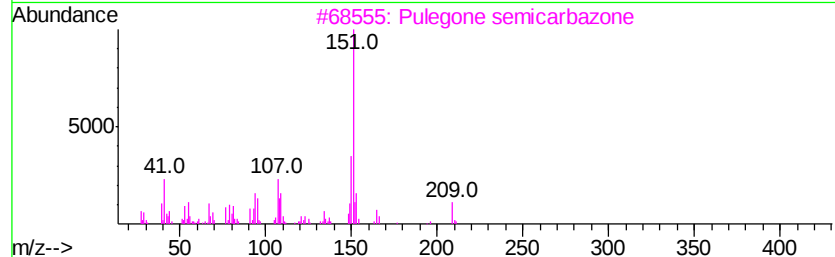
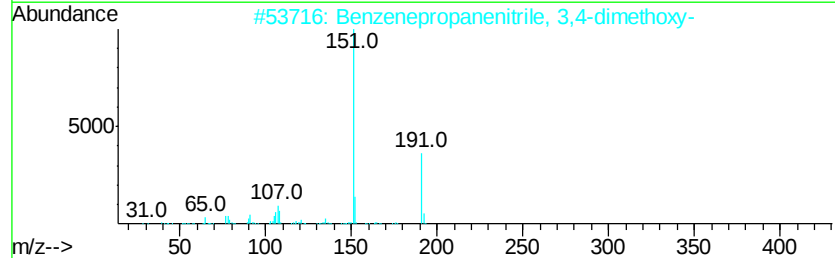
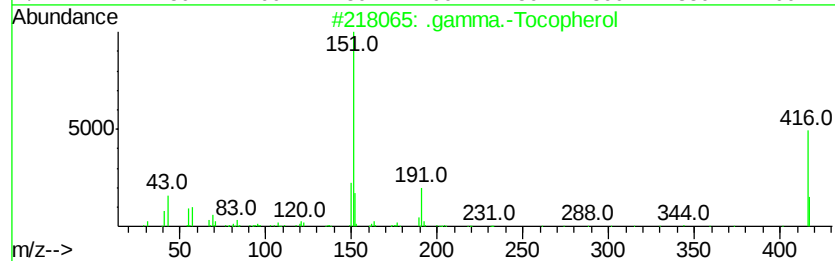
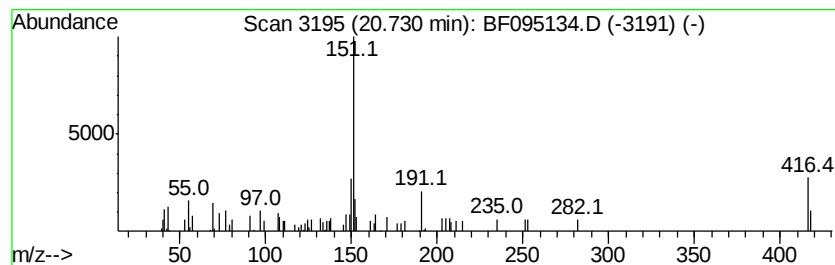
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 .gamma.-Tocopherol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.73	2.22 ng	52158	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	80
2		Benzenepropanenitrile, 3,4-dimet...	191	C11H13N02	049621-56-9	47
3		Pulegone semicarbazone	209	C11H19N3O	023733-71-3	47
4		2'-Hydroxy-6'-methoxyacetophenon...	208	C11H12O4	1000352-92-5	46
5		4-Amino-2,1,3-benzothiadiazole	151	C6H5N3S	000767-64-6	38



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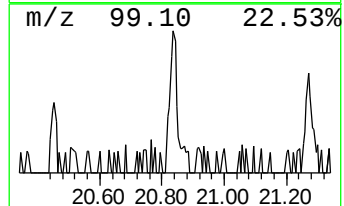
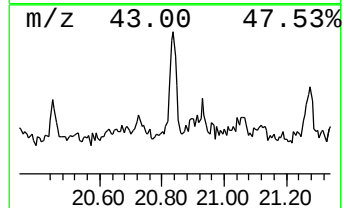
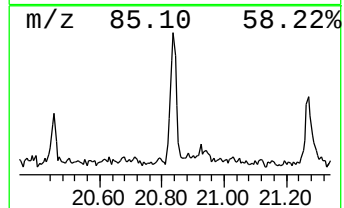
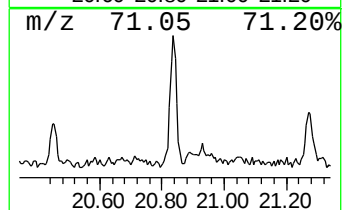
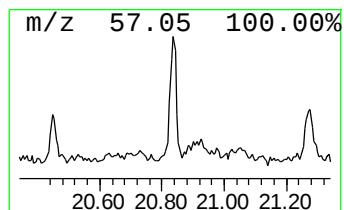
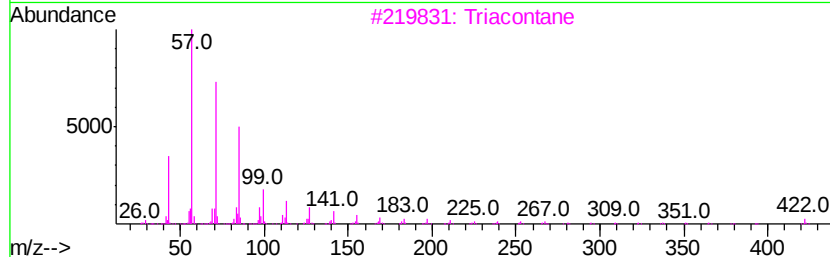
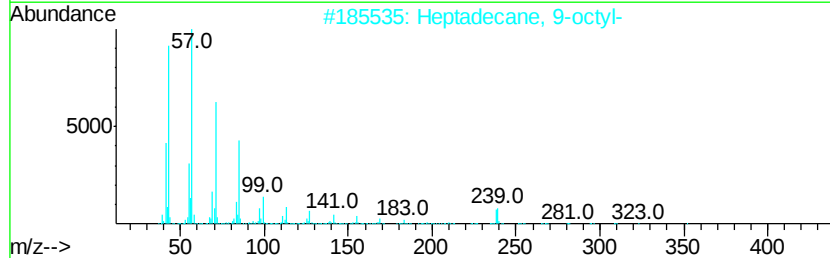
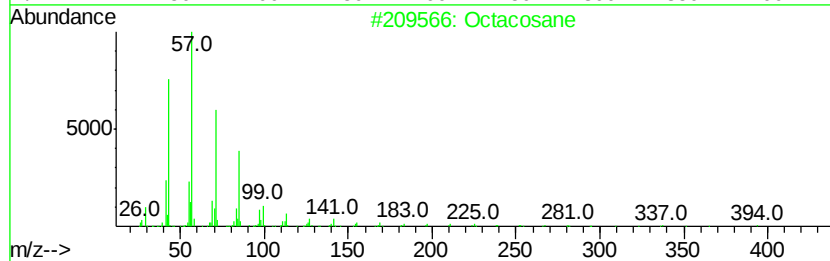
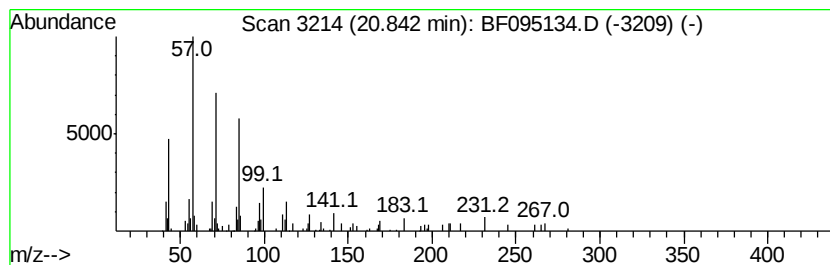
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	3.16 ng	74145	Perylene-d12	20.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	Triacontane		422	C30H62	000638-68-6	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Pentacosane		352	C25H52	000629-99-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095134.D
Acq On : 15 May 2017 19:47
Operator : SJ/MA
Sample : I3144-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-PS-01-002

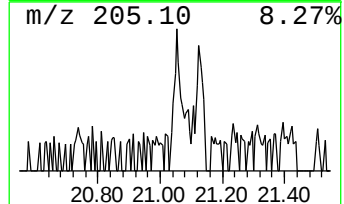
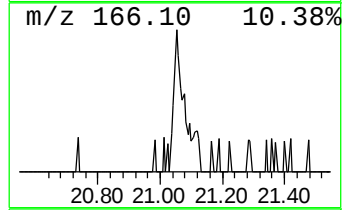
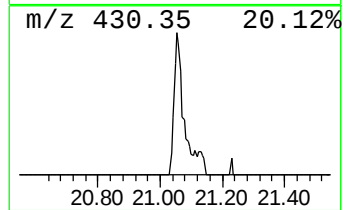
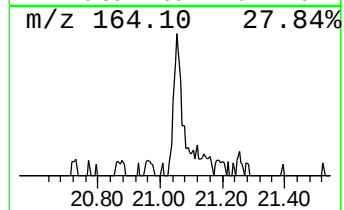
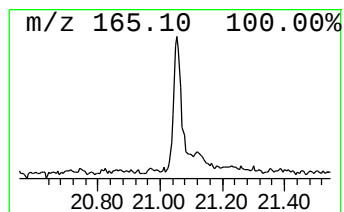
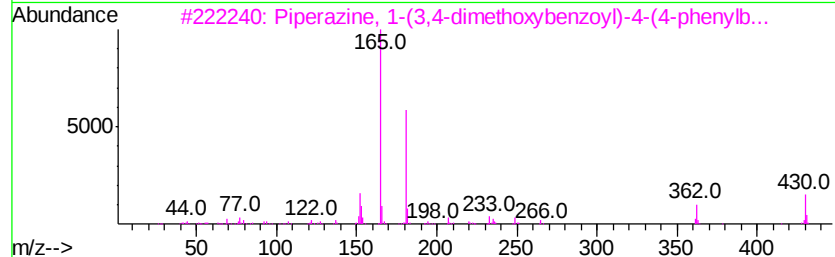
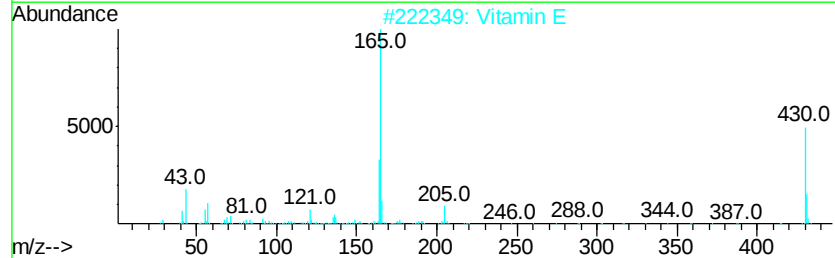
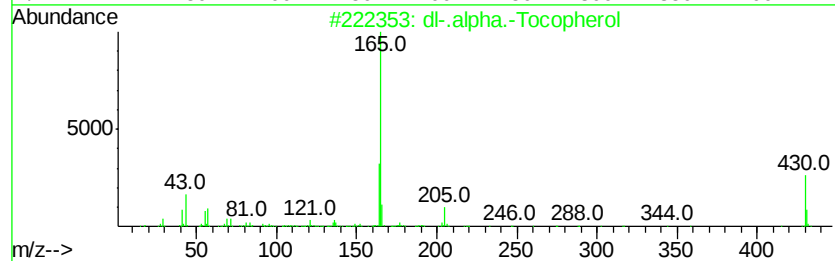
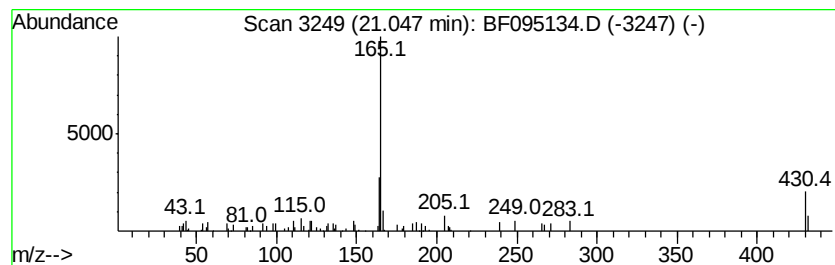
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 dl-.alpha.-Tocopherol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.05	2.70 ng	63256	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	dl-.alpha.-Tocopherol	430	C29H50O2	010191-41-0	87
2		Vitamin E	430	C29H50O2	000059-02-9	80
3		Piperazine, 1-(3,4-dimethoxybenz...	430	C26H26N2O4	333756-87-9	64
4		Furo[3,4-c]pyridine-3,4(1H,5H)-d...	165	C8H7NO3	007472-18-6	50
5		3,6-Dimethyl-5-oxo-1,2,3,5-tetra...	165	C8H11N3O	058910-42-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
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Misc :
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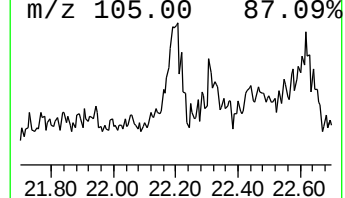
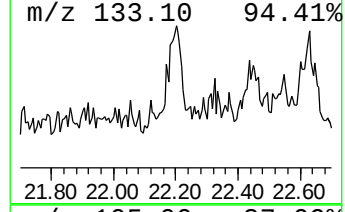
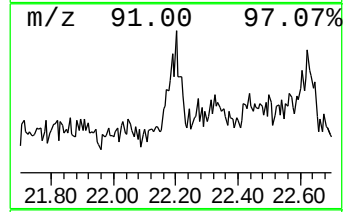
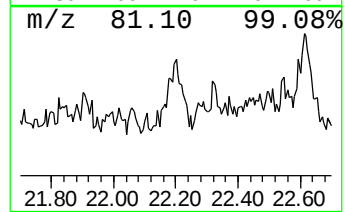
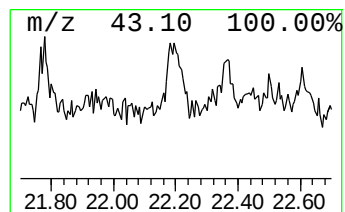
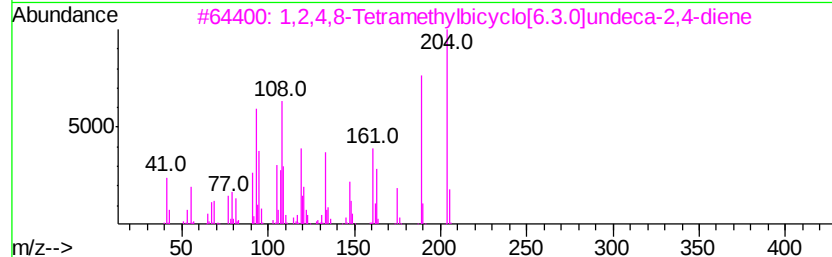
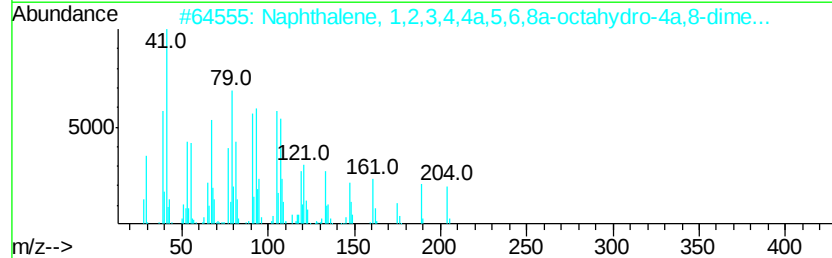
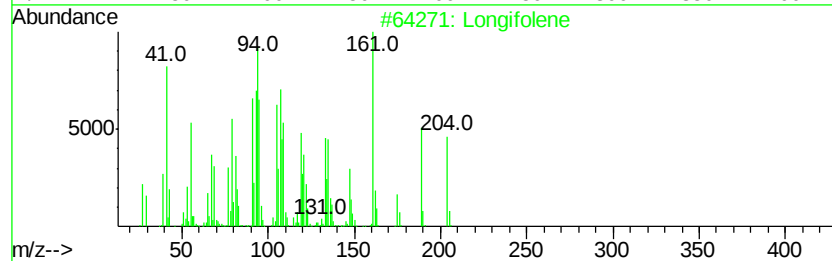
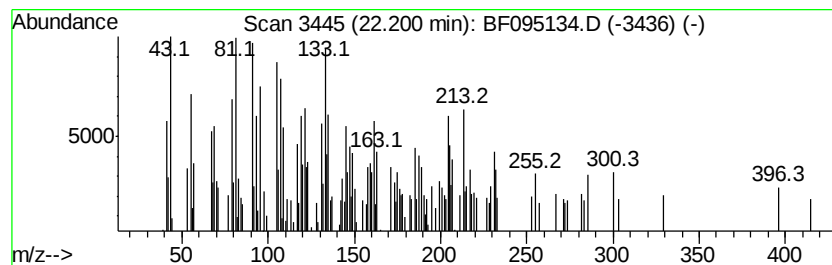
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Longifolene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.20	9.14 ng	214430	Perylene-d12	20.37
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Longifolene	204 C15H24	000475-20-7	55
2	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204 C15H24	000473-13-2	48
3	1,2,4,8-Tetramethylbicyclo[6.3.0]...	204 C15H24	137235-51-9	44
4	Aciphyllene	204 C15H24	087745-31-1	42
5	Methanol, 6,8,9-trimethyl-4-(2-p...	300 C20H28O2	1000277-01-1	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
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Acq On : 15 May 2017 19:47
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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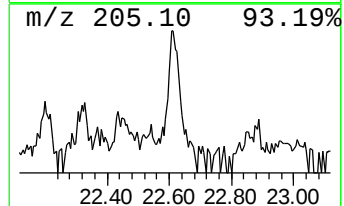
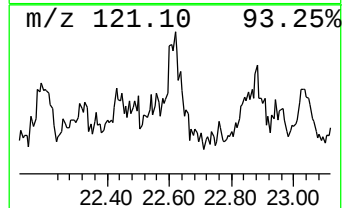
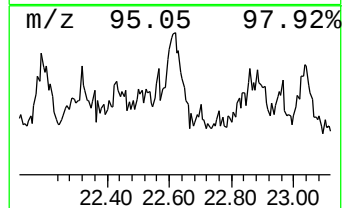
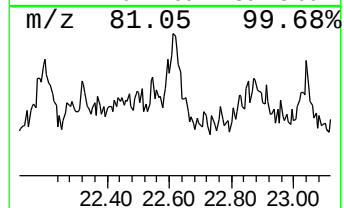
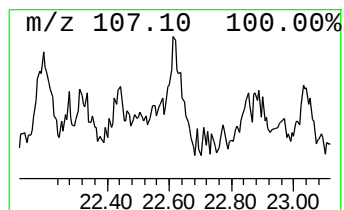
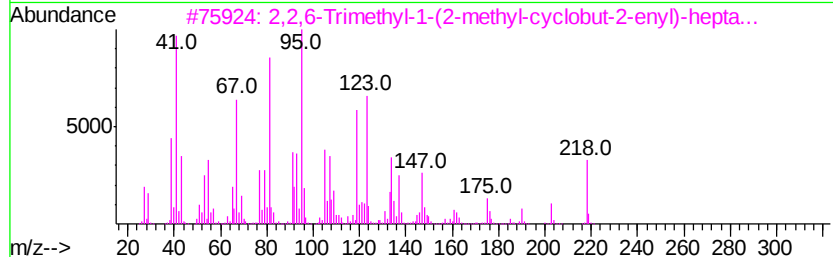
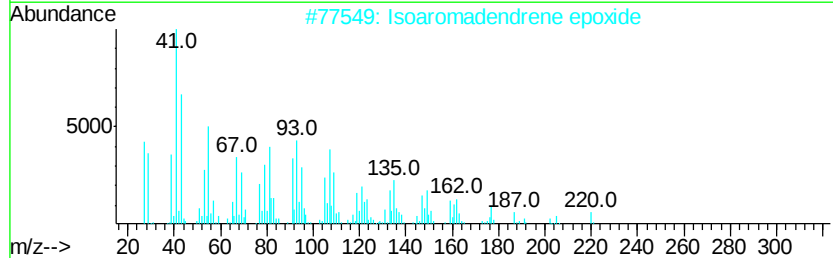
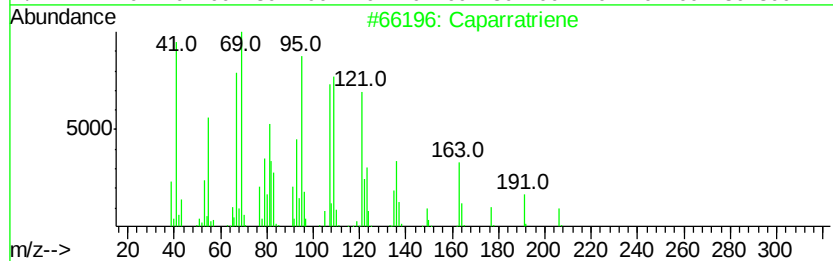
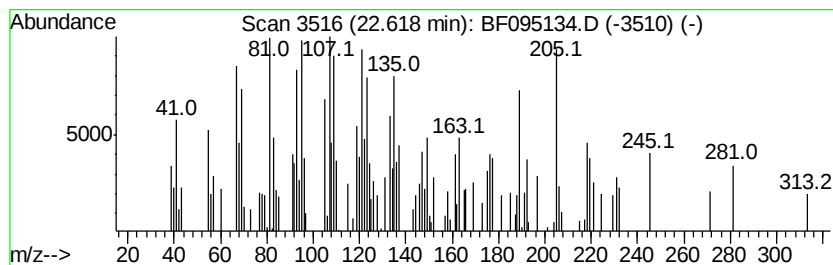
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown22.62 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.62	10.42 ng	244376	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Caparratriene	206	C15H26	1000374-08-7	43
2		Isoaromadendrene epoxide	220	C15H24O	1000159-36-6	38
3		2,2,6-Trimethyl-1-(2-methyl-cyclobut-2-enyl)-hepta...	218	C15H22O	1000188-72-8	35
4		2-Butenal, 2-methyl-4-(2,6,6-trimethyl-3-cyclohexyl)-	206	C14H22O	003155-71-3	30
5		Cyclohexane, 1,1,2-trimethyl-3,5-dimethyl-	206	C15H26	062337-96-6	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
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Acq On : 15 May 2017 19:47
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Misc :
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ClientSampleId :
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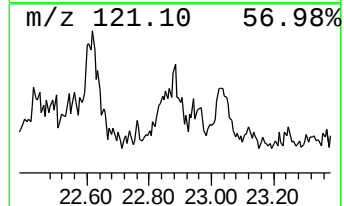
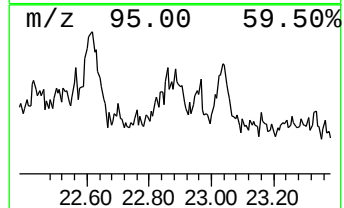
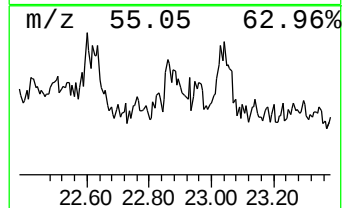
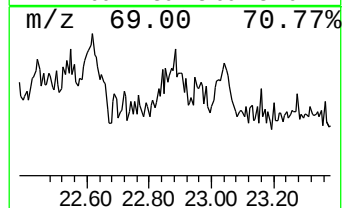
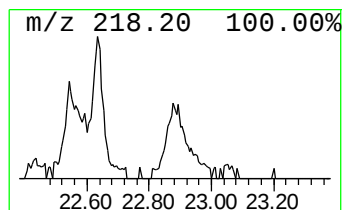
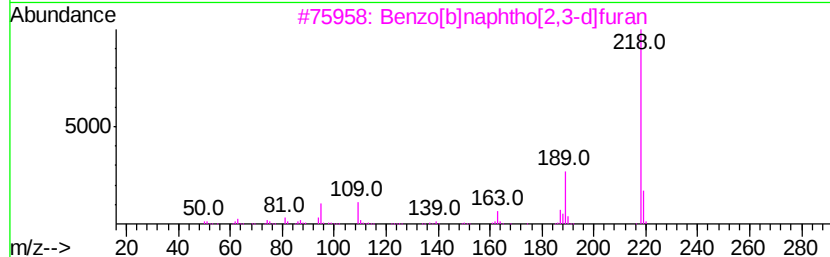
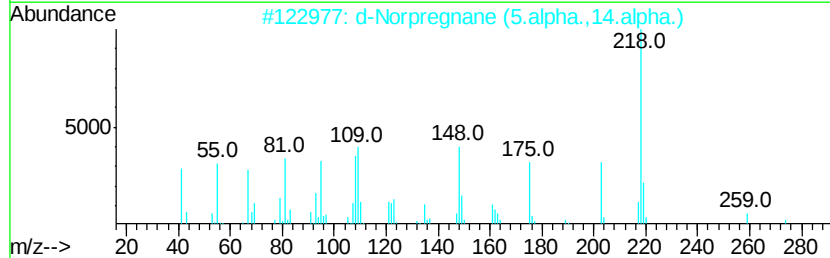
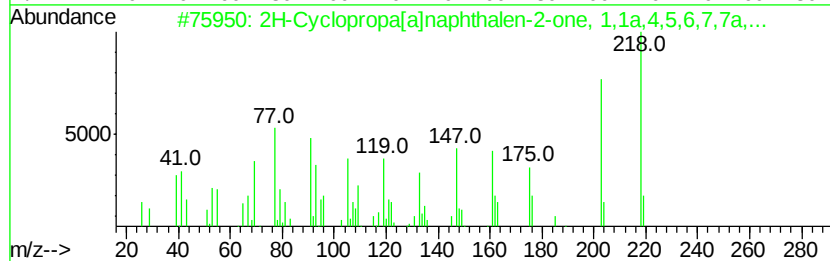
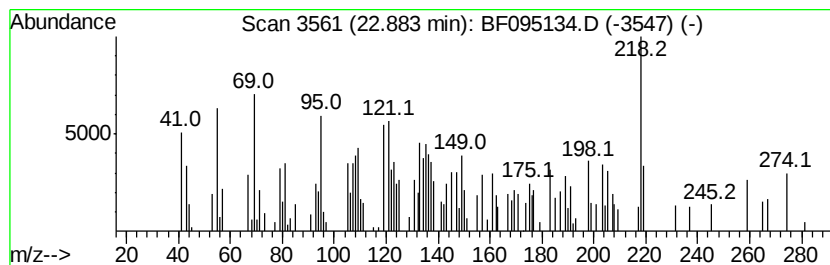
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown22.88 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.88	9.86 ng	231267	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	38
2		d-Norpregnane (5.alpha.,14.alpha.)	274	C20H34	1000281-13-7	35
3		Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	30
4		Pyrido[1,2-a]perimidine	218	C15H10N2	000200-42-0	27
5		Disulfide, diphenyl	218	C12H10S2	000882-33-7	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095134.D
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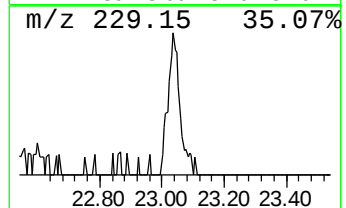
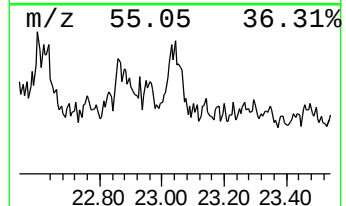
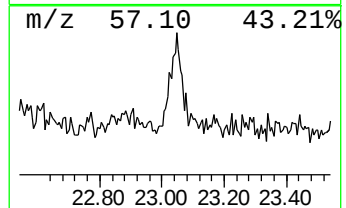
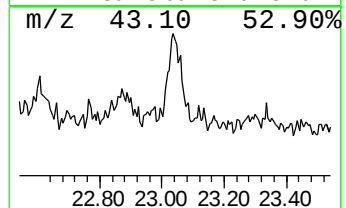
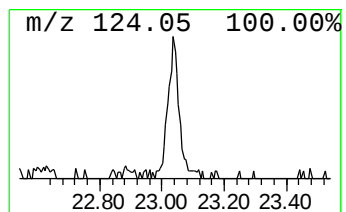
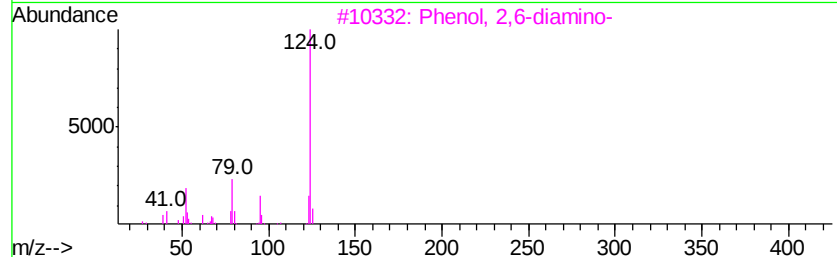
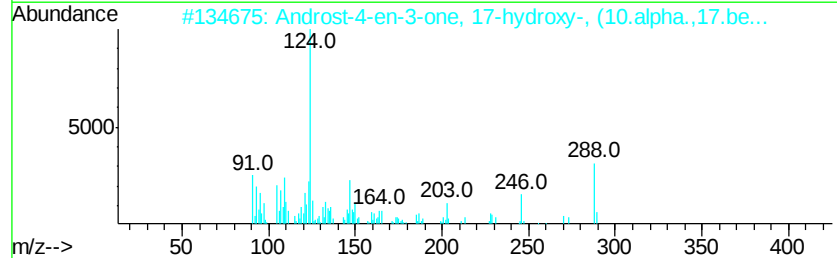
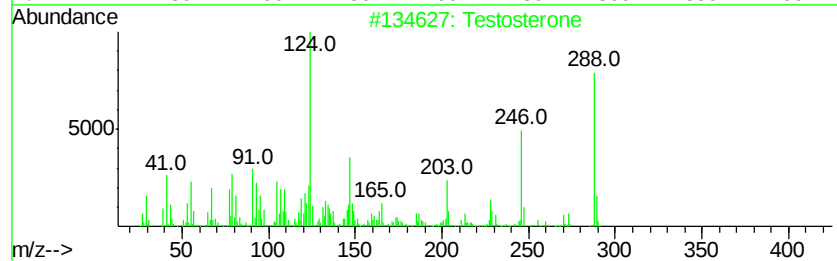
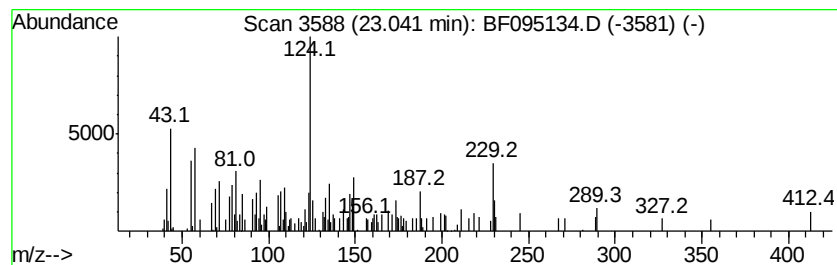
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown23.04 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.04	8.20 ng	192450	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Testosterone	288	C19H28O2	000058-22-0	41
2		Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	38
3		Phenol, 2,6-diamino-	124	C6H8N2O	022440-82-0	35
4		2,6,8-Trimethylbicyclo[4.2.0]oct...	182	C11H18O2	1000187-22-4	35
5		Benzenemethanol, 3-hydroxy-	124	C7H8O2	000620-24-6	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
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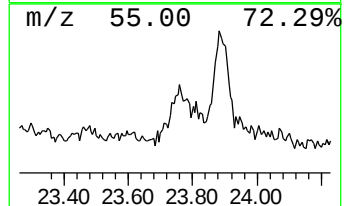
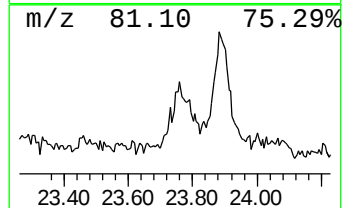
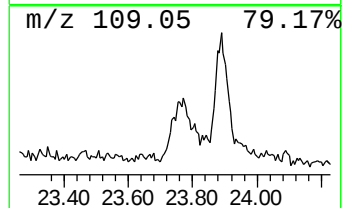
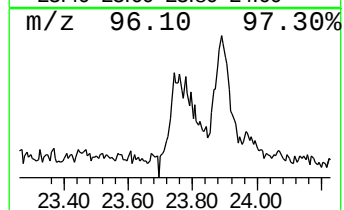
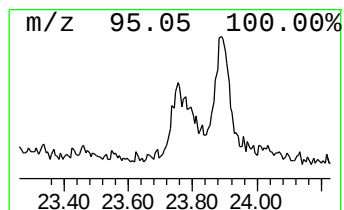
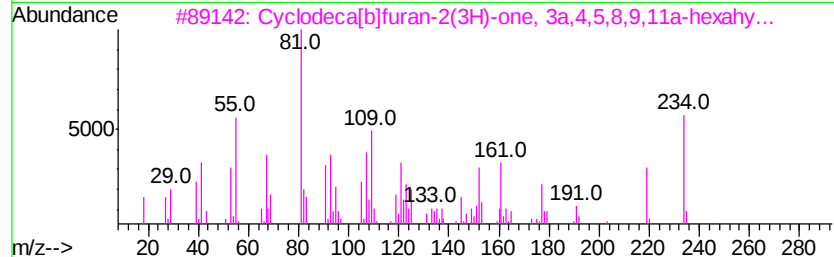
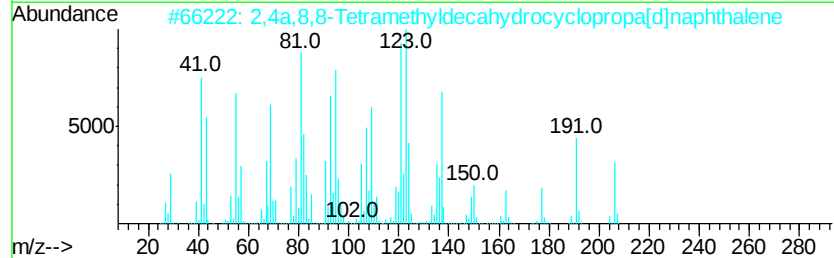
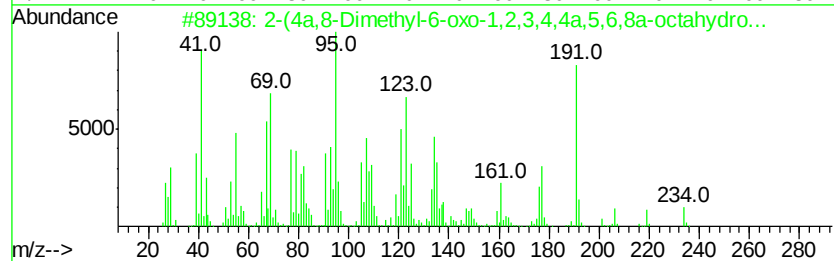
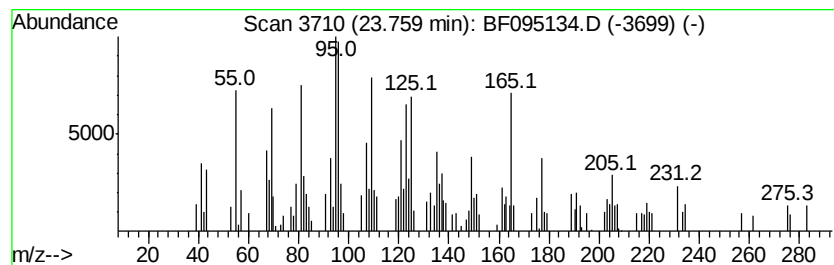
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 2-(4a,8-Dimethyl-6-oxo-1,2,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.76	16.62 ng	389790	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	60
2		2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	42
3		Cyclodeca[b]furan-2(3H)-one, 3a,...	234	C15H22O2	002225-79-8	41
4		4-[3-(4-Fluorobenzoyloxy)propyl]-...	234	C13H15FN2O	1000311-87-2	38
5		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095134.D
Acq On : 15 May 2017 19:47
Operator : SJ/MA
Sample : I3144-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-002

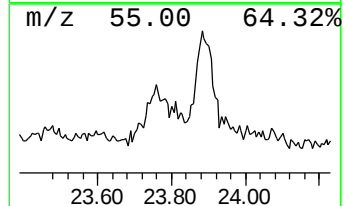
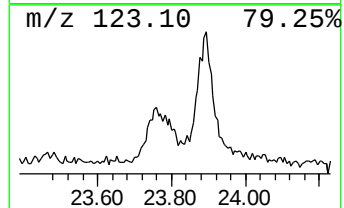
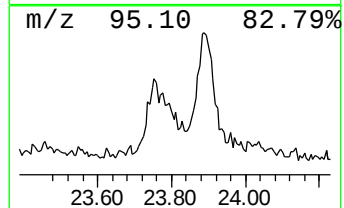
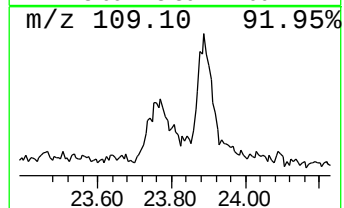
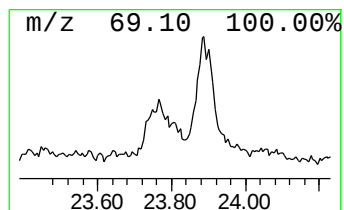
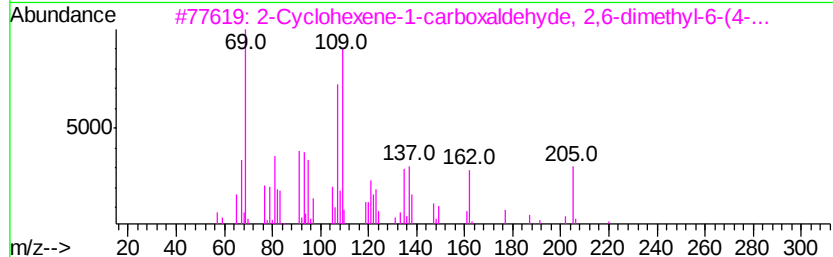
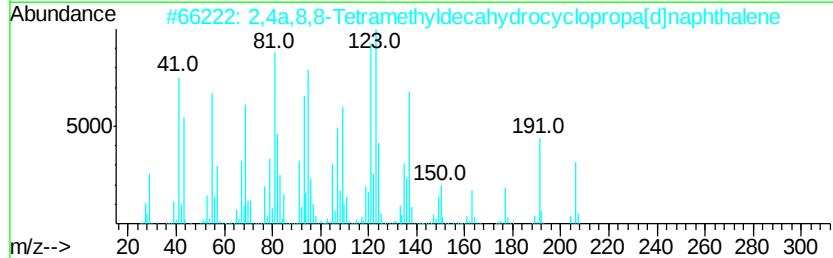
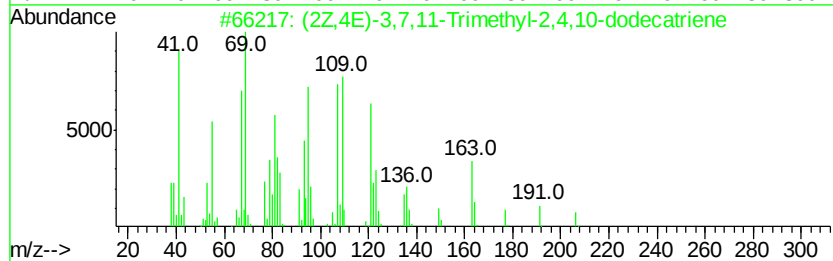
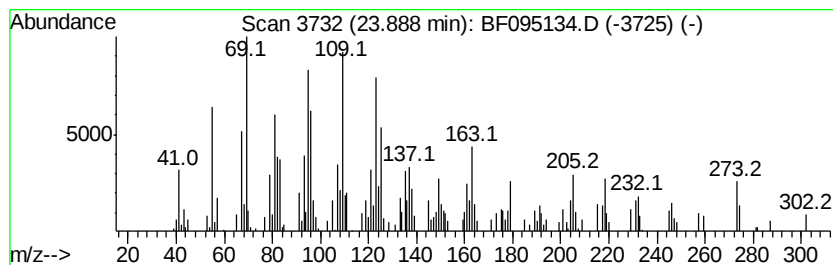
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 (2Z,4E)-3,7,11-Trimethyl-2,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.89	16.67 ng	391143	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	58
2		2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	46
3		2-Cyclohexene-1-carboxaldehyd...	220	C15H24O	056772-07-7	42
4		Sesquirosefuran	218	C15H22O	039007-93-7	38
5		(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095134.D
Acq On : 15 May 2017 19:47
Operator : SJ/MA
Sample : I3144-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	22.6	ng	520971	1	7.78	461051	20.0
unknown7.44	7.44	110.5	ng	2547980	1	7.78	461051	20.0
n-Hexadecanoic acid	15.98	3.7	ng	115820	4	15.03	626238	20.0
Tetratetracontane	20.10	4.6	ng	108291	6	20.37	469147	20.0
.gamma.-Tocopherol	20.73	2.2	ng	52158	6	20.37	469147	20.0
Octacosane	20.84	3.2	ng	74145	6	20.37	469147	20.0
dl-.alpha.-Tocoph...	21.05	2.7	ng	63256	6	20.37	469147	20.0
Longifolene	22.20	9.1	ng	214430	6	20.37	469147	20.0
unknown22.62	22.62	10.4	ng	244376	6	20.37	469147	20.0
unknown22.88	22.88	9.9	ng	231267	6	20.37	469147	20.0
unknown23.04	23.04	8.2	ng	192450	6	20.37	469147	20.0
2-(4a,8-Dimethyl-...	23.76	16.6	ng	389790	6	20.37	469147	20.0
(2Z,4E)-3,7,11-Tr...	23.89	16.7	ng	391143	6	20.37	469147	20.0