

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
 Data File : BF096825.D
 Acq On : 17 Jul 2017 17:55
 Operator : SJ/JU
 Sample : I4203-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DL-SB02C

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-BF071317.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	4.787	472	476	489	rVB	190767	263855	4.21%	0.786%
2	5.222	546	550	565	rBV	2144185	2281645	36.41%	6.799%
3	6.263	722	727	738	rBV	2359960	2557242	40.81%	7.621%
4	6.387	743	748	751	rBV	2658912	2439187	38.92%	7.269%
5	6.610	782	786	790	rBV	837745	669945	10.69%	1.996%
6	6.769	809	813	816	rBV	2178277	1887073	30.11%	5.624%
7	7.175	877	882	885	rBV	1714517	1539938	24.57%	4.589%
8	7.892	1000	1004	1007	rBV	1084940	893415	14.26%	2.662%
9	8.969	1182	1187	1190	rBV	2383728	2012122	32.11%	5.996%
10	9.363	1250	1254	1259	rBV	214693	202917	3.24%	0.605%
11	9.639	1296	1301	1304	rBV	724782	668938	10.67%	1.993%
12	10.422	1430	1434	1437	rBV	970411	880225	14.05%	2.623%
13	11.110	1547	1551	1554	rBV	583807	478164	7.63%	1.425%
14	11.657	1641	1644	1648	rBV	96677	79209	1.26%	0.236%
15	12.316	1753	1756	1762	rVB	91721	82123	1.31%	0.245%
16	12.539	1790	1794	1796	rBV	75319	78839	1.26%	0.235%
17	12.574	1796	1800	1812	rVV	518666	704902	11.25%	2.101%
18	12.692	1816	1820	1824	rVB	1436431	1306008	20.84%	3.892%
19	13.604	1971	1975	1981	rVB2	190273	246166	3.93%	0.734%
20	13.733	1993	1997	2000	rBV	644327	643997	10.28%	1.919%
21	14.233	2079	2082	2086	rBV2	85456	104412	1.67%	0.311%
22	14.521	2129	2131	2134	rBV3	68882	78390	1.25%	0.234%
23	14.733	2165	2167	2173	rBV2	65569	99987	1.60%	0.298%
24	15.110	2227	2231	2236	rVB	437524	500311	7.98%	1.491%
25	16.921	2534	2539	2549	rVB	78129	184768	2.95%	0.551%
26	17.104	2565	2570	2578	rVB5	104960	241791	3.86%	0.721%
27	17.309	2600	2605	2614	rVB3	276532	598426	9.55%	1.783%
28	17.404	2615	2621	2632	rVB7	204027	542672	8.66%	1.617%
29	17.633	2649	2660	2677	rBV4	1123461	4498920	71.79%	13.407%
30	17.851	2689	2697	2706	rVB5	178772	524147	8.36%	1.562%
31	18.239	2748	2763	2773	rBV5	1615949	6266643	100.00%	18.675%

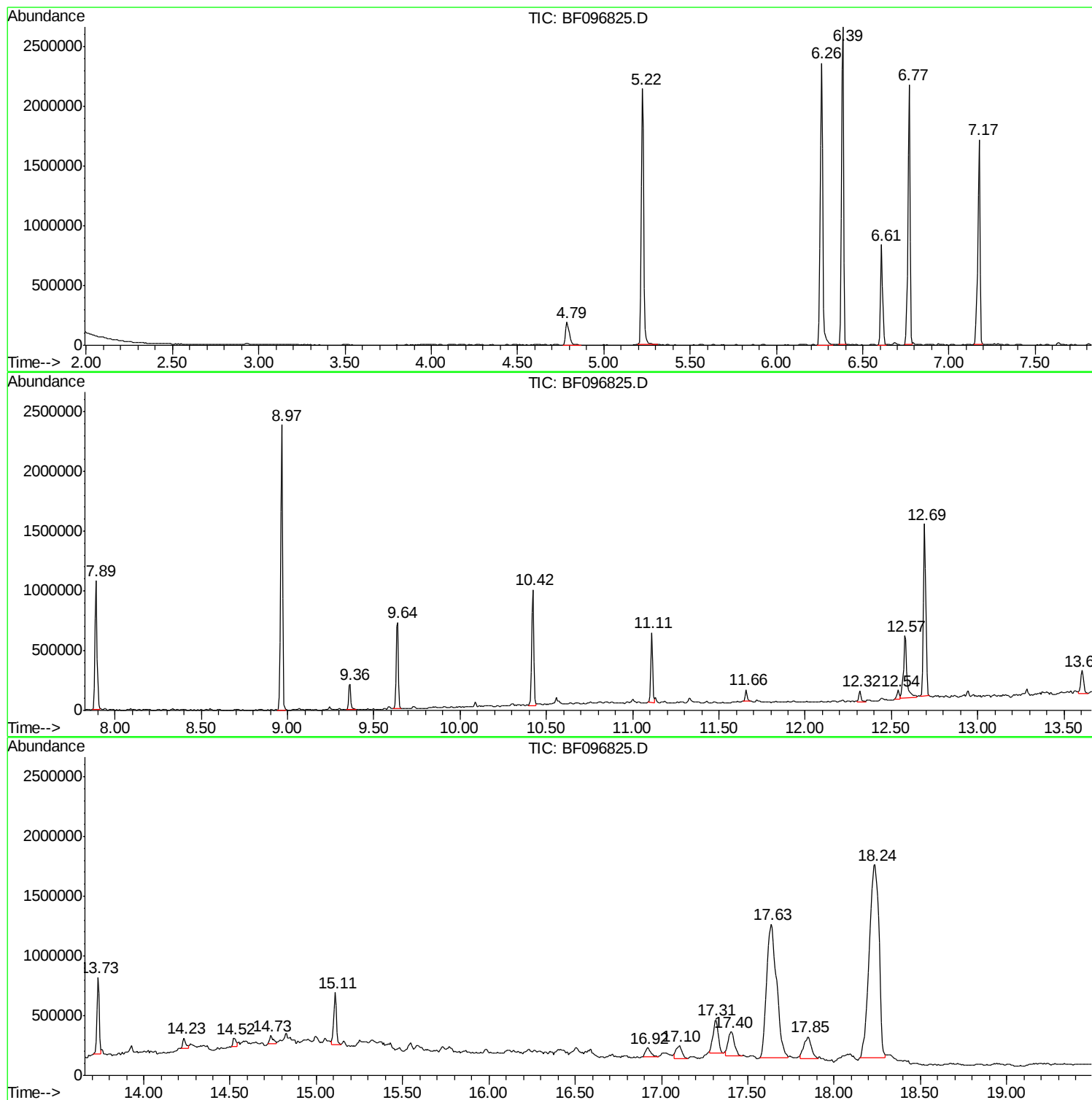
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ClientSampleId :
DL-SB02C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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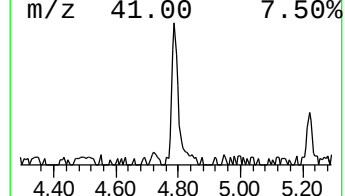
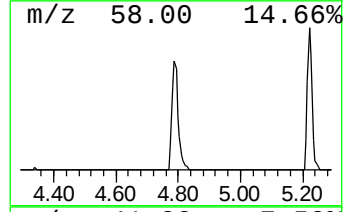
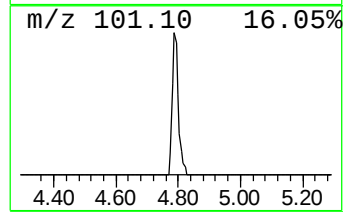
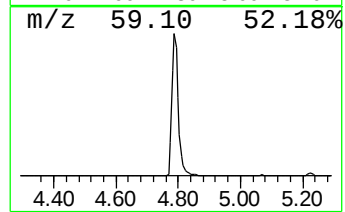
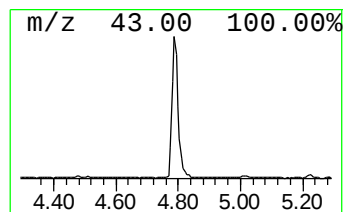
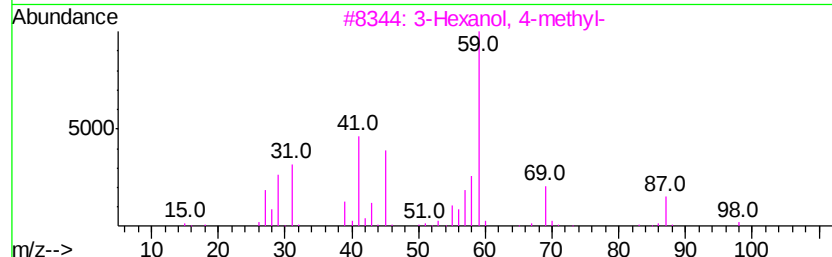
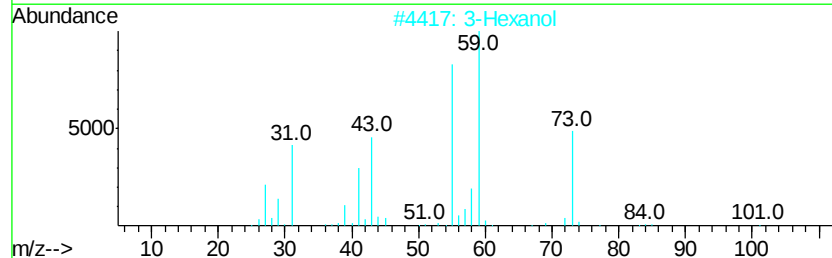
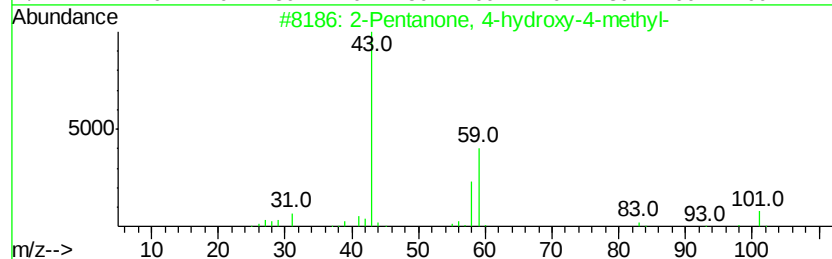
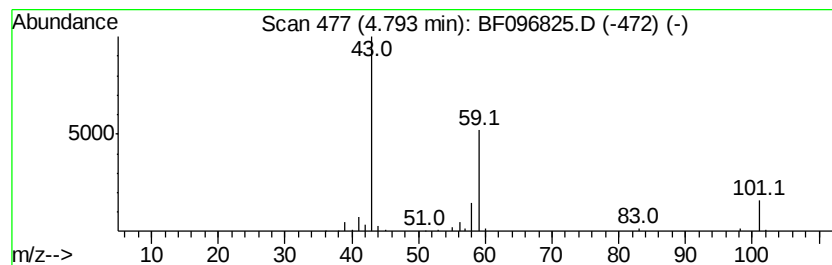
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	7.88 ng	263855	1,4-Dichlorobenzene-d4	6.61

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol	102	C6H14O	000623-37-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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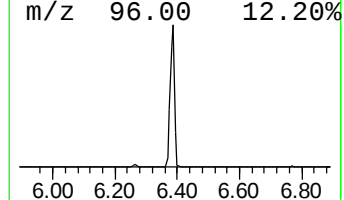
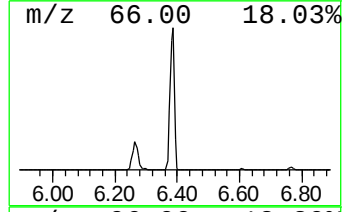
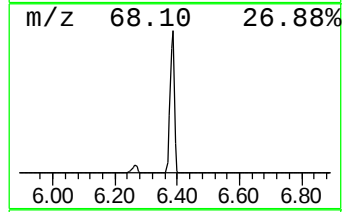
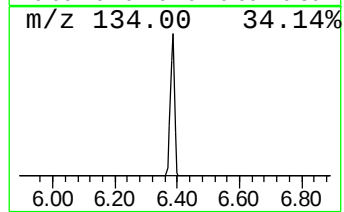
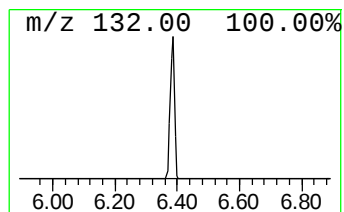
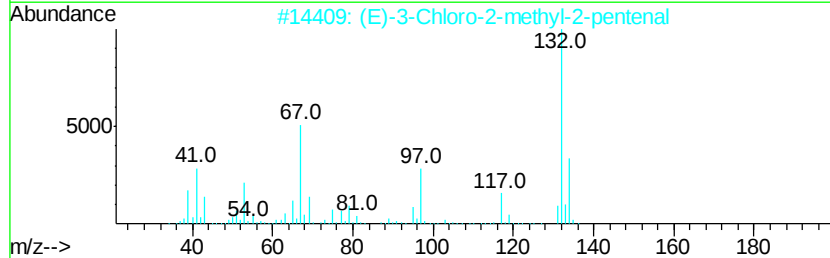
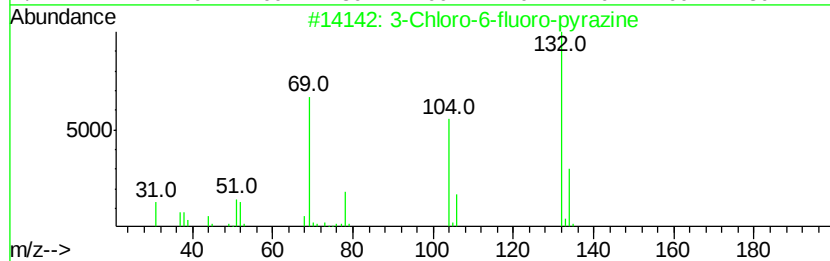
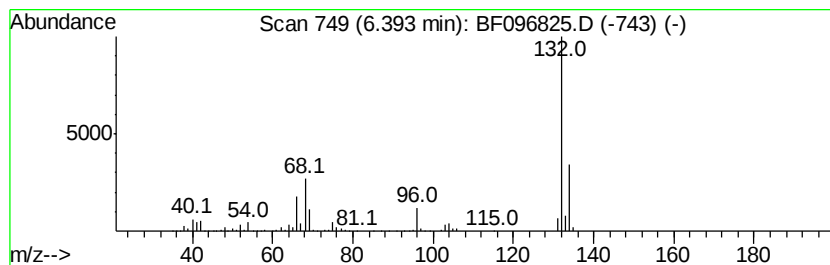
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.39 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	72.82 ng	2439190	1,4-Dichlorobenzene-d4	6.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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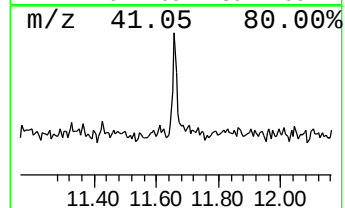
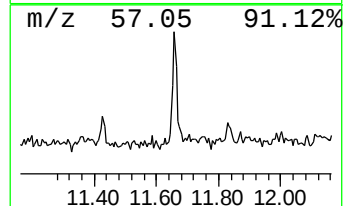
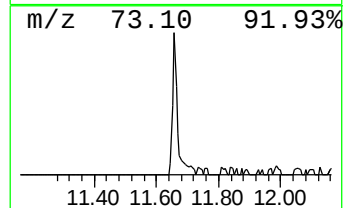
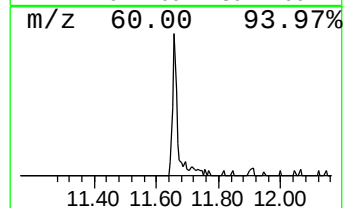
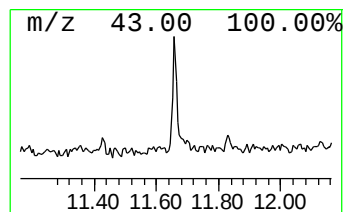
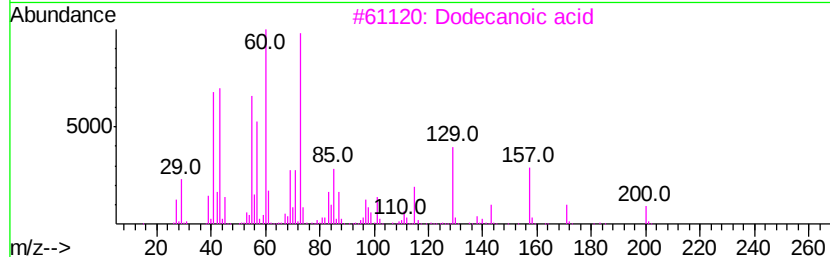
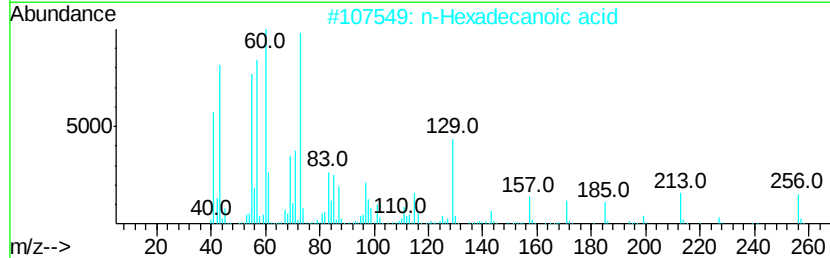
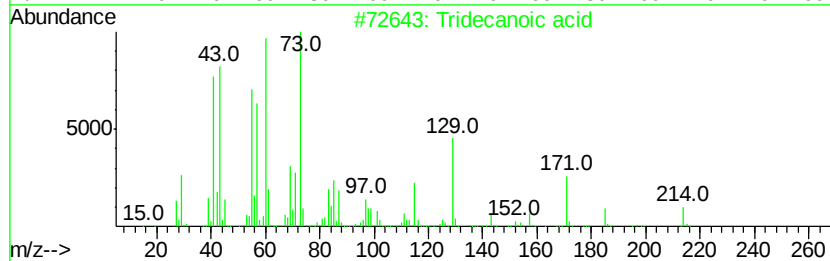
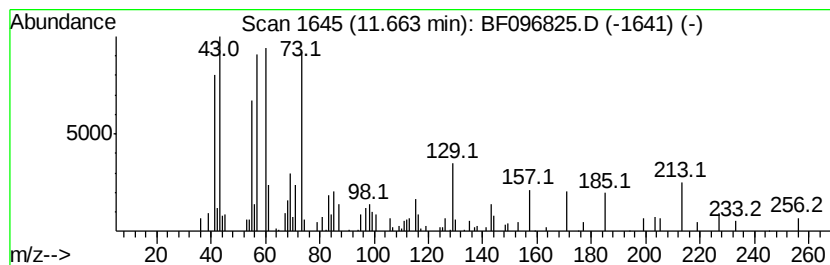
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Tridecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	3.31 ng	79209	Phenanthrene-d10	11.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	94
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Dodecanoic acid	200	C12H24O2	000143-07-7	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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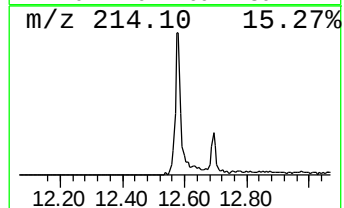
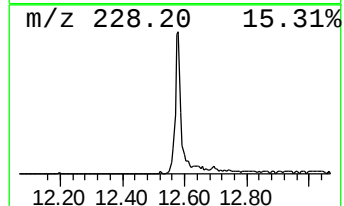
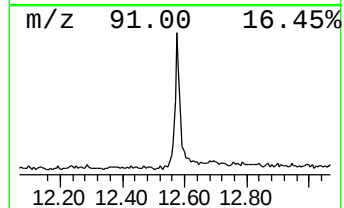
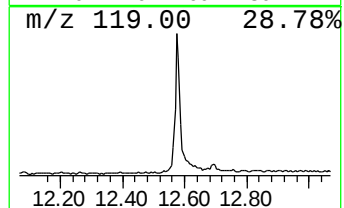
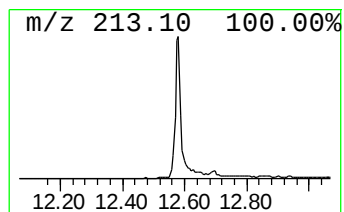
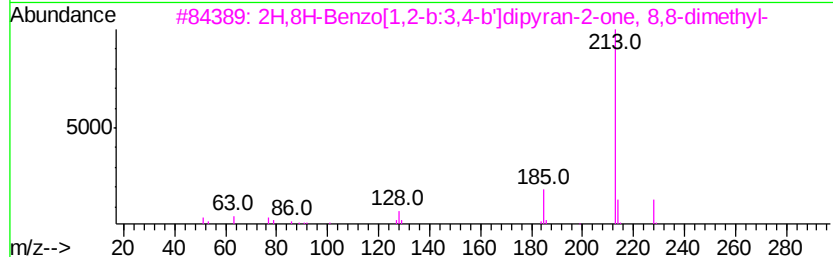
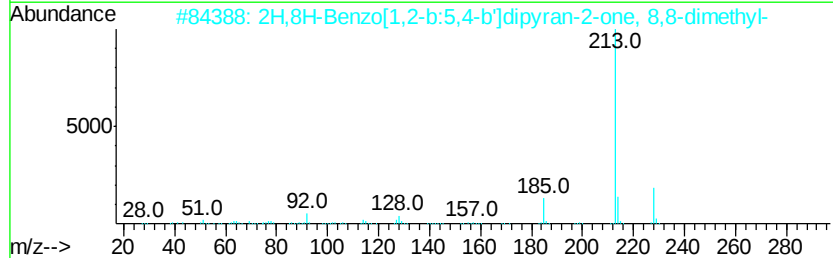
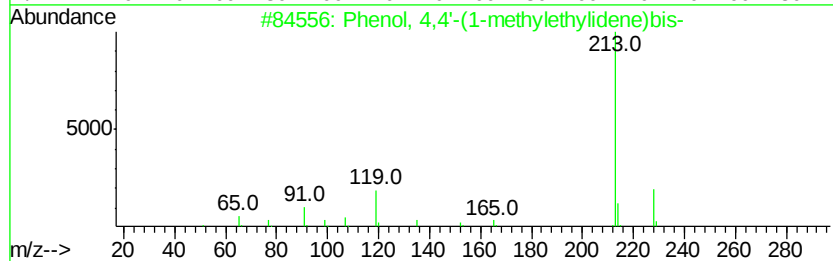
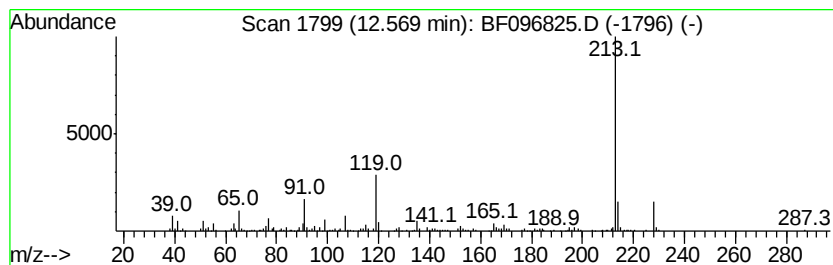
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	21.89 ng	704902	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96	
2	2H,8H-Benzo[1,2-b:5,4-b']dipyr...	228	C14H12O3	000553-19-5	58	
3	2H,8H-Benzo[1,2-b:3,4-b']dipyr...	228	C14H12O3	000523-59-1	58	
4	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	47	
5	1,4-Naphthalenedione, 2-(1-buten...	228	C14H12O3	029366-43-6	47	



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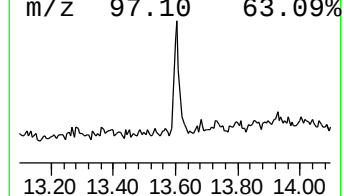
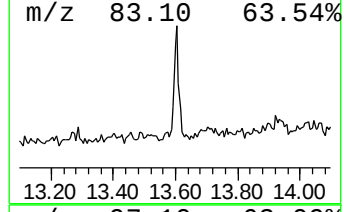
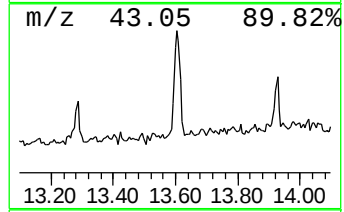
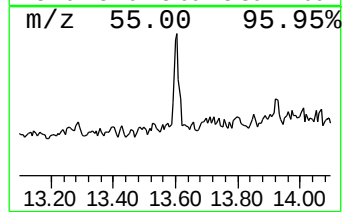
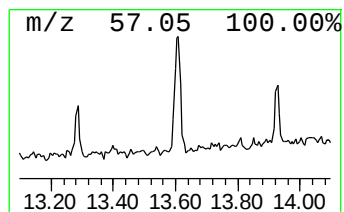
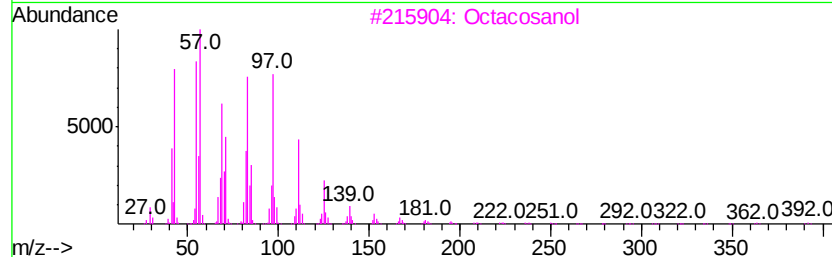
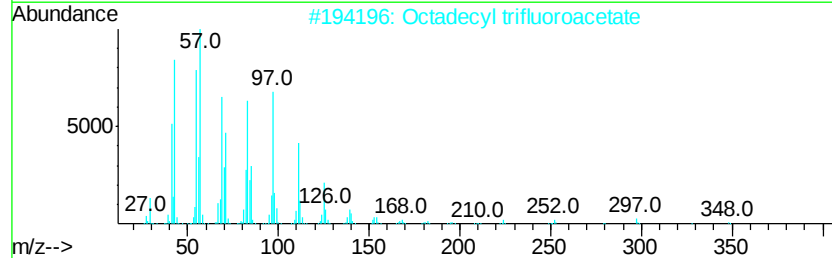
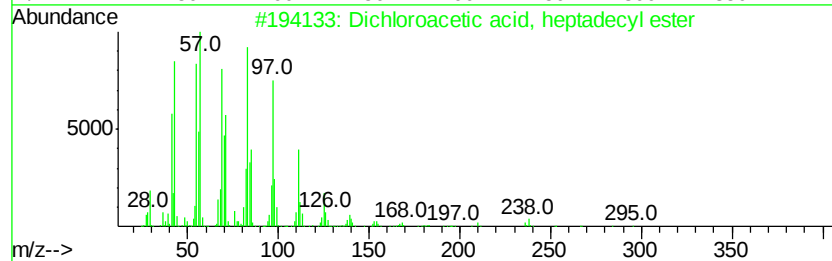
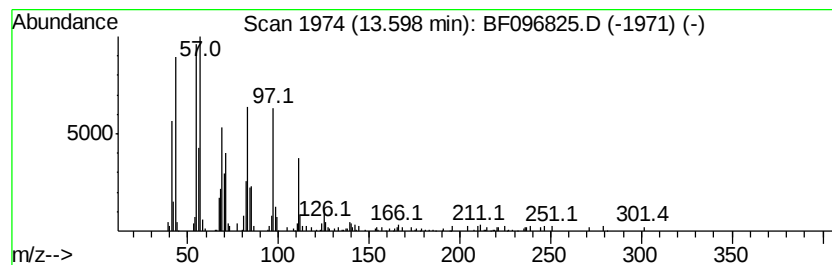
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	7.64 ng	246166	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3		Octacosanol	410	C28H58O	000557-61-9	87
4		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83
5		Hexadecane, 1-(ethenyloxy)-	268	C18H36O	000822-28-6	76



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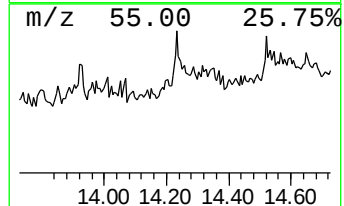
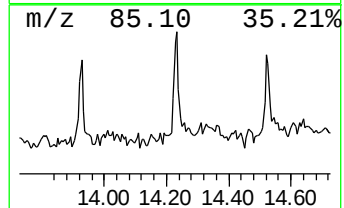
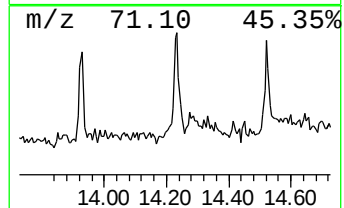
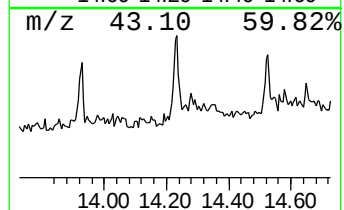
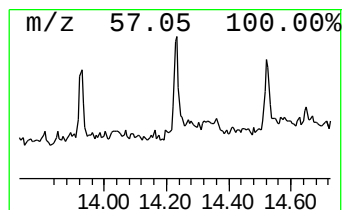
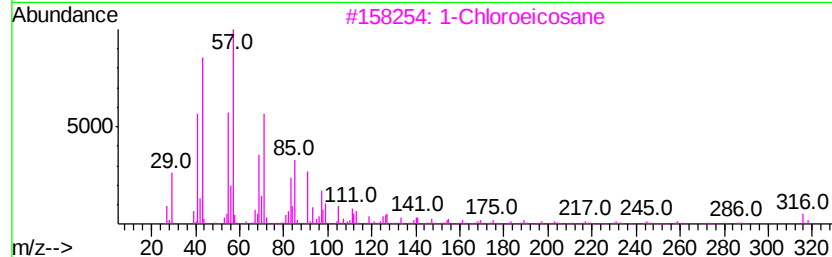
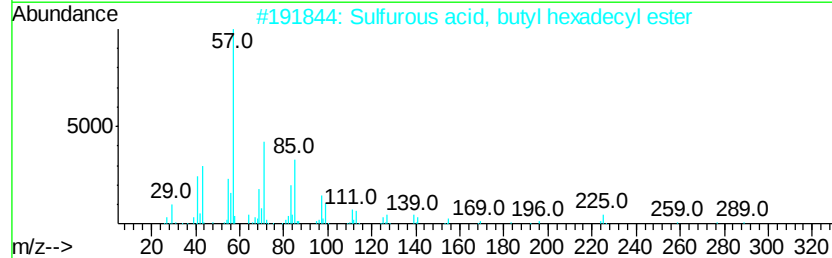
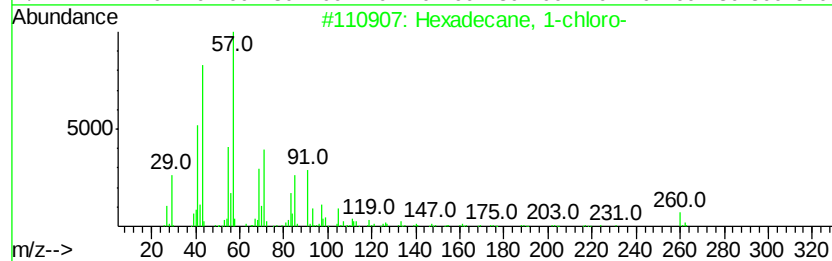
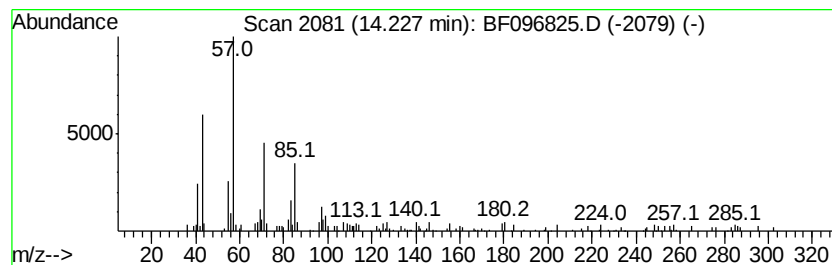
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ClientSampleId :
DL-SB02C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane, 1-chloro- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	3.24 ng	104412	Chrysene-d12	13.73
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane, 1-chloro-	260 C16H33Cl	004860-03-1	91
2	Sulfurous acid, butyl hexadecyl ...	362 C20H42O3S	1000309-18-3	90
3	1-Chloroeicosane	316 C20H41Cl	042217-02-7	86
4	Pentadecane	212 C15H32	000629-62-9	78
5	Sulfurous acid, octadecyl 2-prop...	376 C21H44O3S	1000309-12-7	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071717\
Data File : BF096825.D
Acq On : 17 Jul 2017 17:55
Operator : SJ/JU
Sample : I4203-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

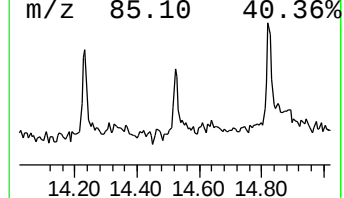
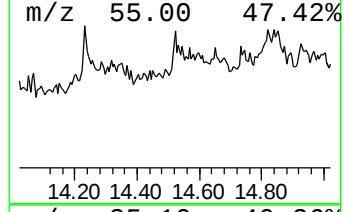
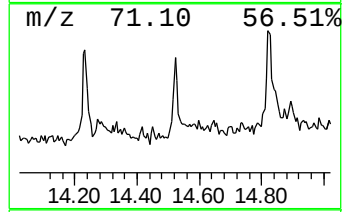
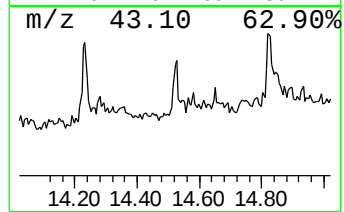
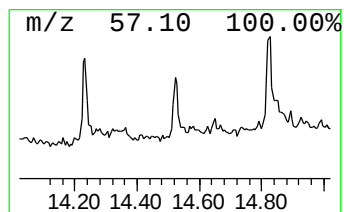
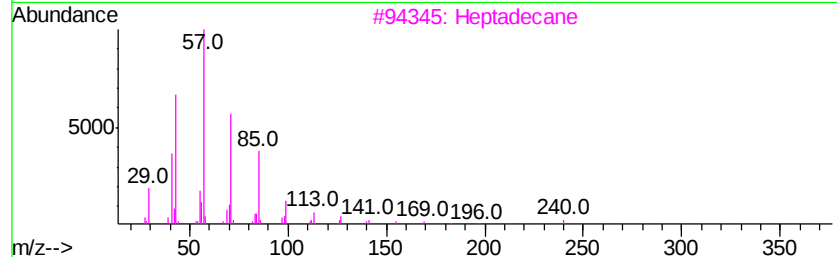
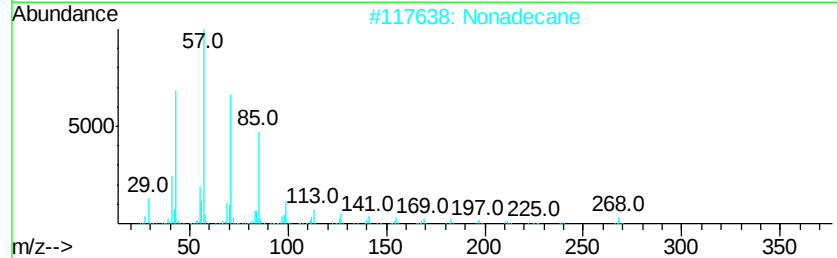
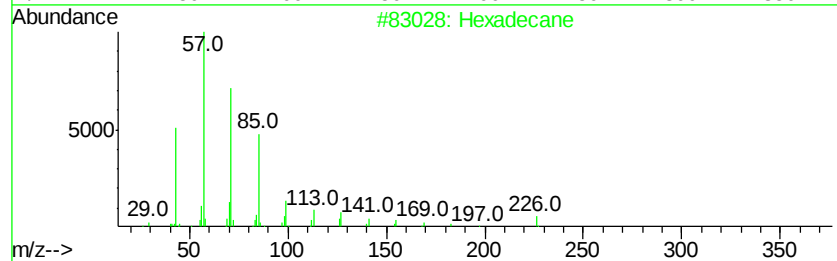
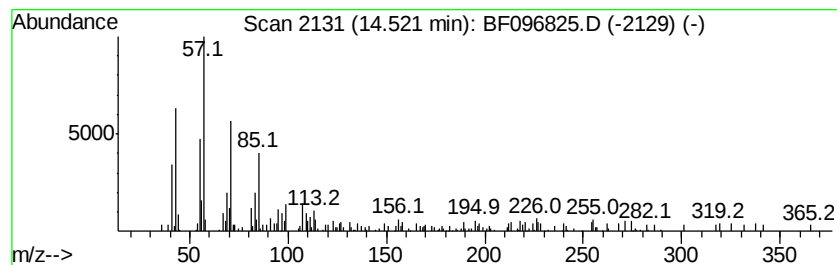
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.52	3.13 ng	78390	Perylene-d12		15.11
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Nonadecane	268	C19H40	000629-92-5	95
3	Heptadecane	240	C17H36	000629-78-7	93
4	Pentadecane	212	C15H32	000629-62-9	93
5	Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096825.D
Acq On : 17 Jul 2017 17:55
Operator : SJ/JU
Sample : I4203-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

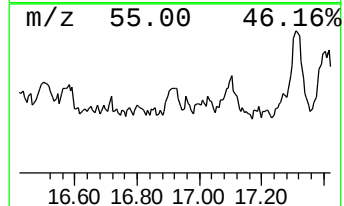
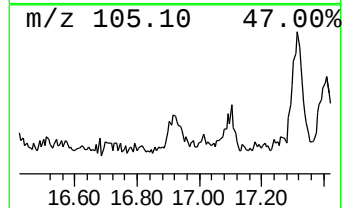
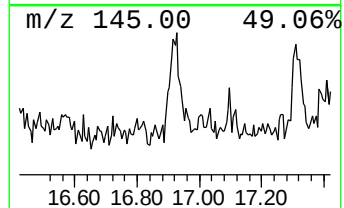
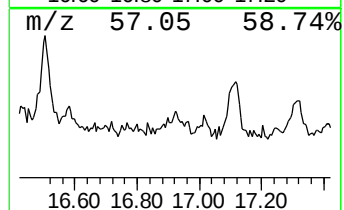
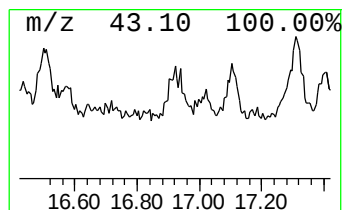
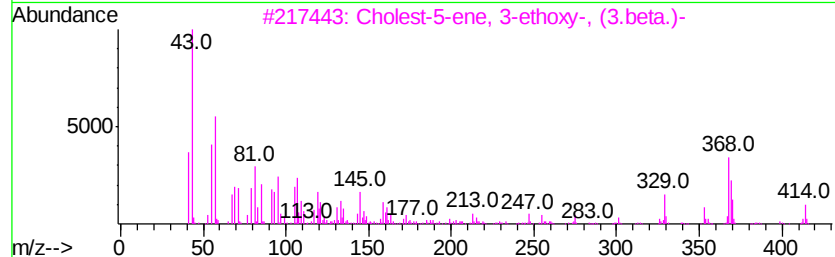
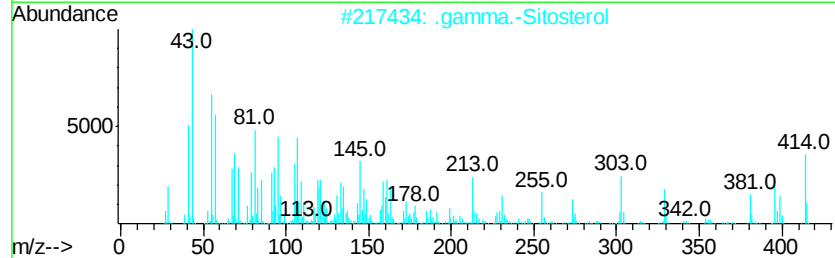
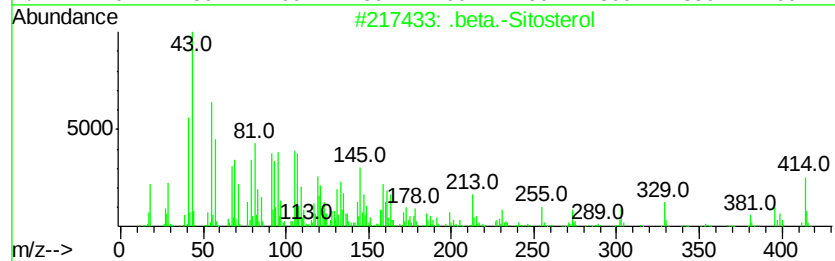
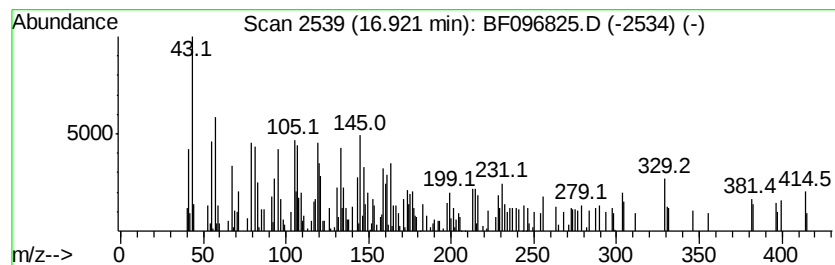
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .beta.-Sitosterol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.92	7.39 ng	184768	Perylene-d12	15.11
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 91
2		.gamma.-Sitosterol	414 C29H50O	000083-47-6 91
3		Cholest-5-ene, 3-ethoxy-, (3.beta...	414 C29H50O	000986-19-6 64
4		17-(1,5-Dimethylhexyl)-10,13-dim...	414 C29H50O	1000210-86-9 35
5		5-Pregnen-3.beta.-ol-20-one, met...	330 C22H34O2	1000364-94-5 25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071717\
Data File : BF096825.D
Acq On : 17 Jul 2017 17:55
Operator : SJ/JU
Sample : I4203-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DL-SB02C

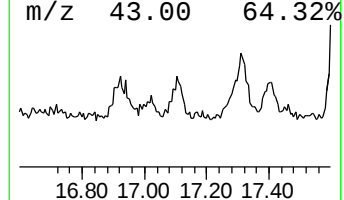
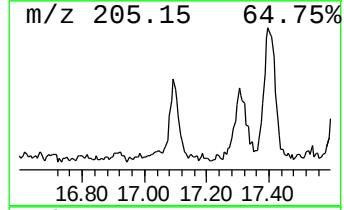
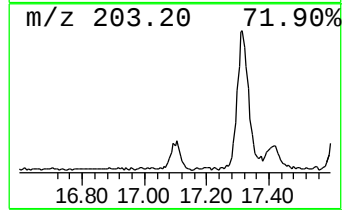
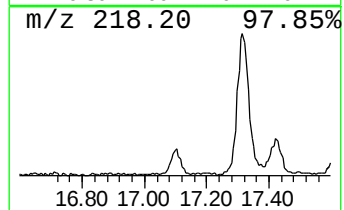
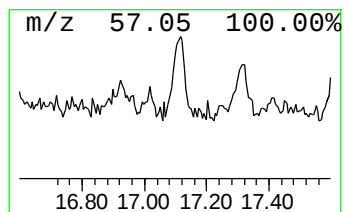
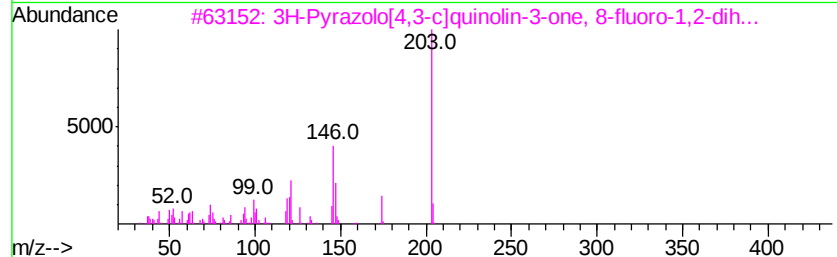
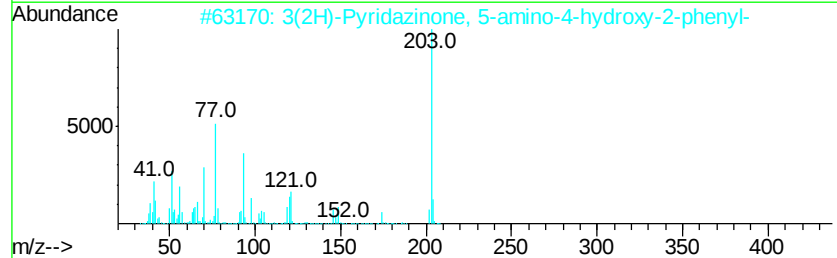
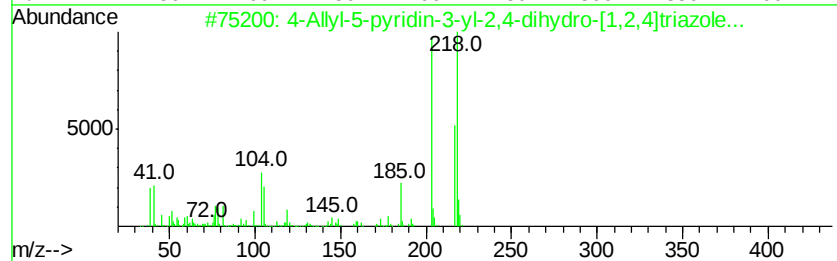
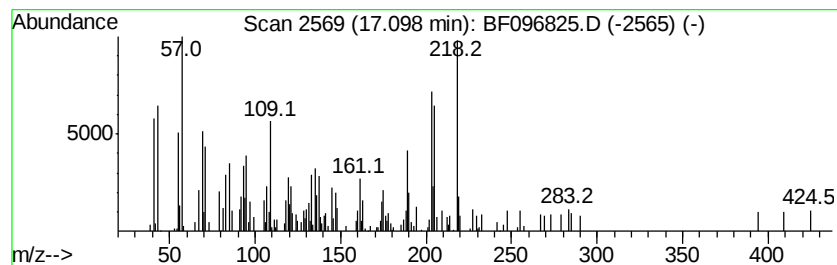
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.10 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.10	9.67 ng	241791	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Allyl-5-pyridin-3-yl-2,4-dihyd...	218	C10H10N4S	1000300-40-5	38
2		3(2H)-Pyridazinone, 5-amino-4-hy...	203	C10H9N3O2	1000338-12-1	25
3		3H-Pyrazolo[4,3-c]quinolin-3-one...	203	C10H6FN3O	1000362-68-8	25
4		2,4-Dichlorophenyl isothiocyanate	203	C7H3Cl2NS	006590-96-1	25
5		5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096825.D
Acq On : 17 Jul 2017 17:55
Operator : SJ/JU
Sample : I4203-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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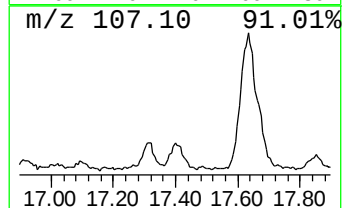
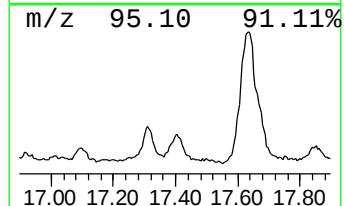
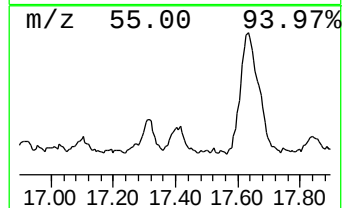
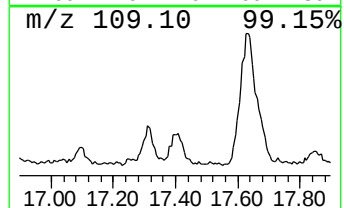
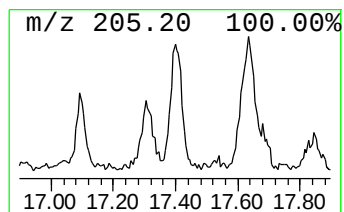
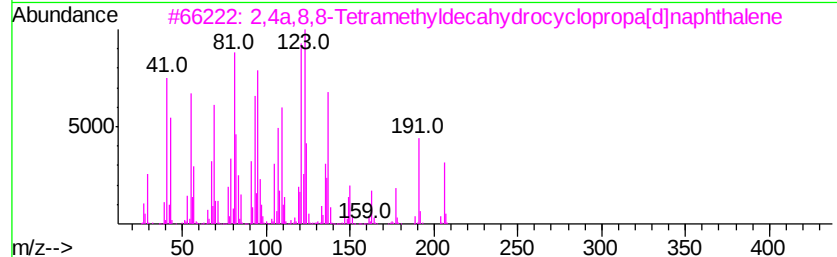
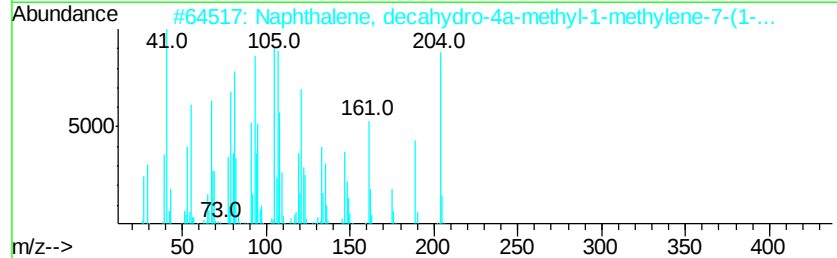
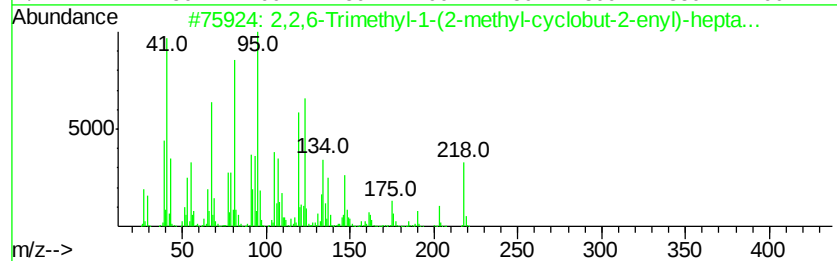
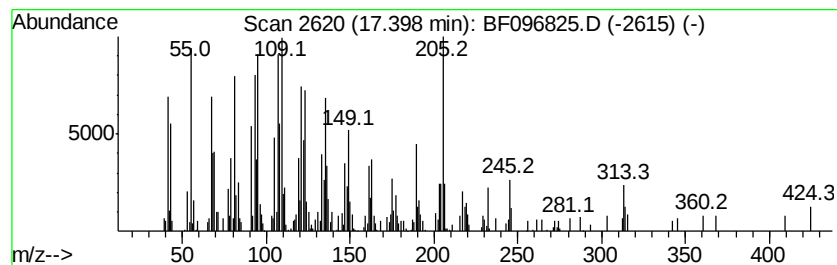
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,2,6-Trimethyl-1-(2-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.40	21.69 ng	542672	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	90
2		Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	62
3		2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	43
4		Dimethylbis(4,8,8-trimethyldec...	500	C32H56O2Si	1000364-69-0	43
5		1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071717\
Data File : BF096825.D
Acq On : 17 Jul 2017 17:55
Operator : SJ/JU
Sample : I4203-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

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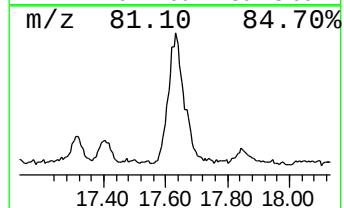
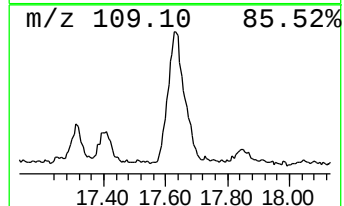
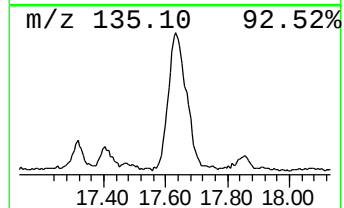
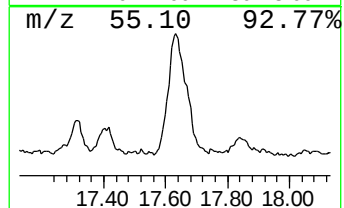
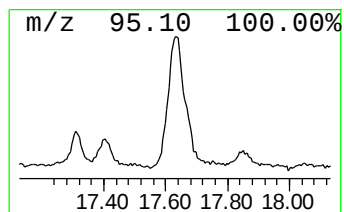
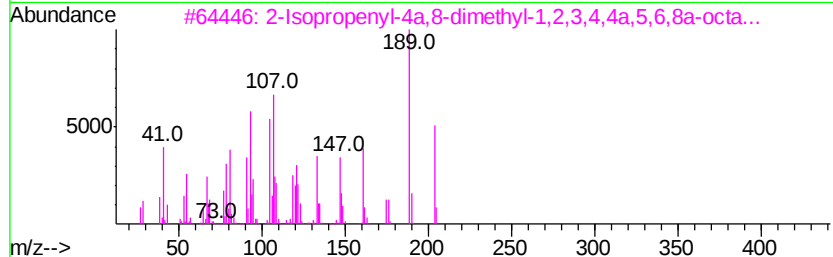
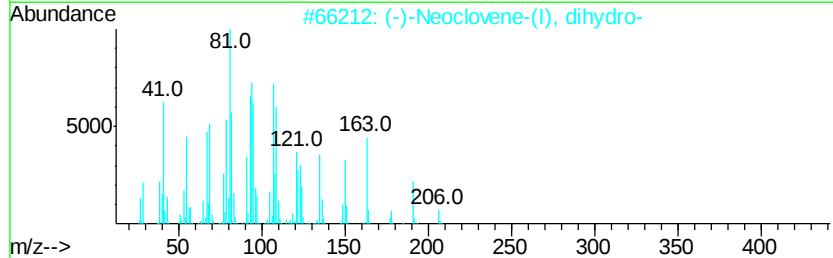
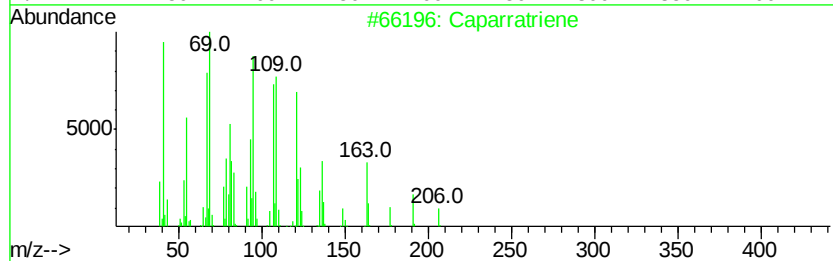
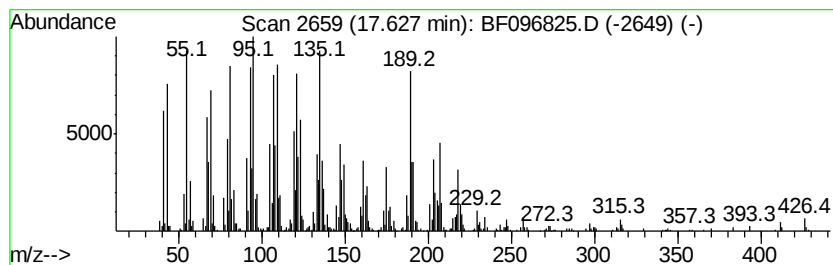
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Caparratriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.63	179.85 ng	4498920	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Caparratriene	206	C15H26	1000374-08-7	50
2		(-)-Neoclovene-(I), dihydro-	206	C15H26	1000152-82-1	50
3		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	47
4		.gamma.-Elemene	204	C15H24	029873-99-2	46
5		9,19-Cycloergost-24(28)-en-3-ol,...	468	C32H52O2	010376-42-8	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096825.D
Acq On : 17 Jul 2017 17:55
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ALS Vial : 17 Sample Multiplier: 1

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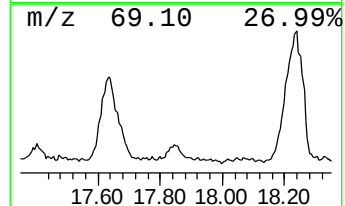
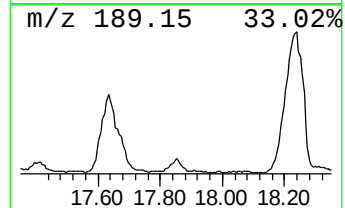
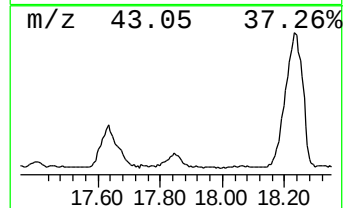
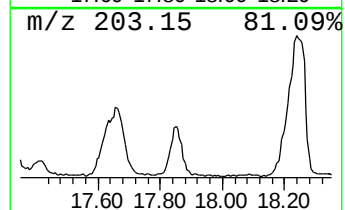
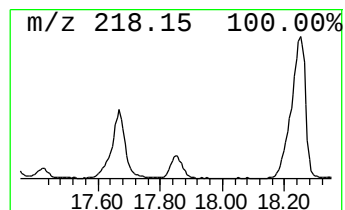
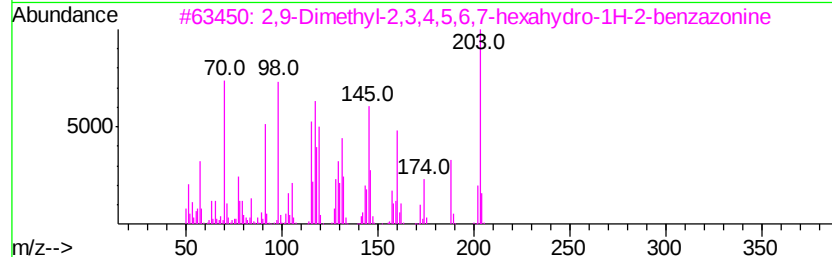
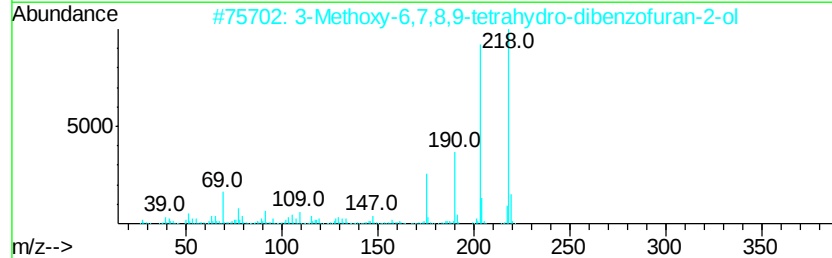
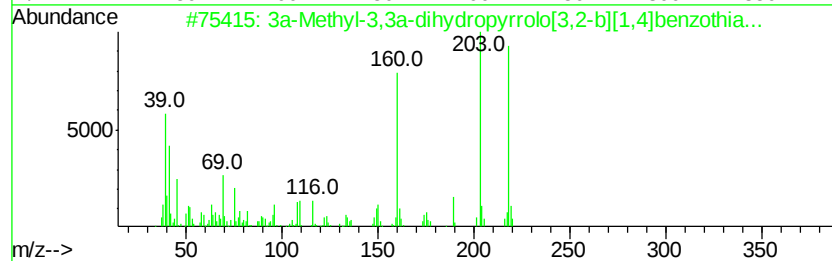
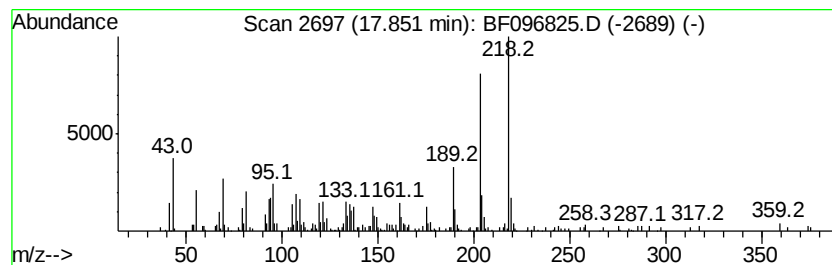
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 3a-Methyl-3,3a-dihydropyrro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	20.95 ng	524147	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3a-Methyl-3,3a-dihydropyrrolo[3,...	218	C11H10N2OS	017163-68-7	64
2		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	62
3		2,9-Dimethyl-2,3,4,5,6,7-hexahyd...	203	C14H21N	077581-11-4	60
4		8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	53
5		2H-1-Benzopyran-2-one, 6-acetyl-...	260	C14H12O5	129812-31-3	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071717\
Data File : BF096825.D
Acq On : 17 Jul 2017 17:55
Operator : SJ/JU
Sample : I4203-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DL-SB02C

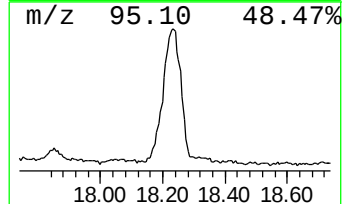
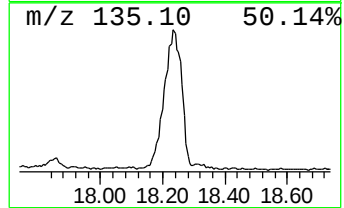
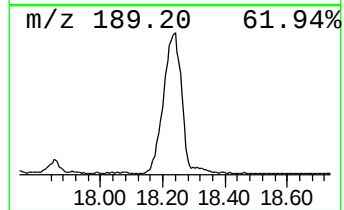
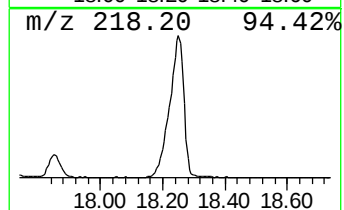
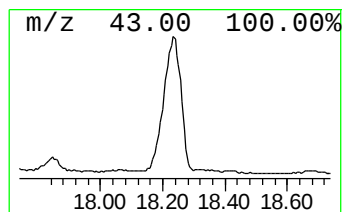
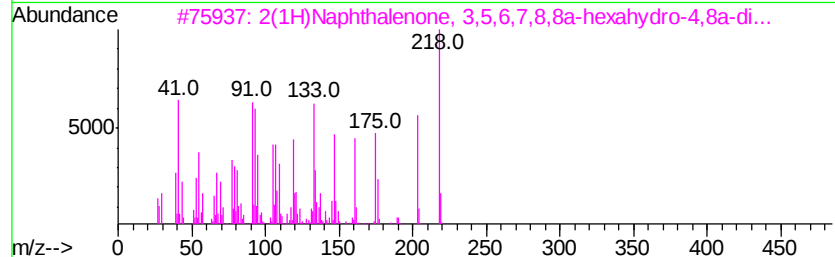
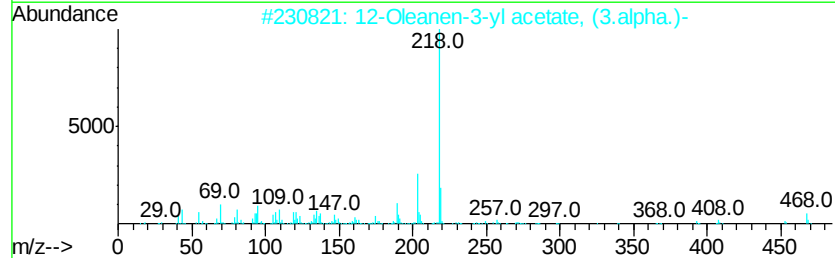
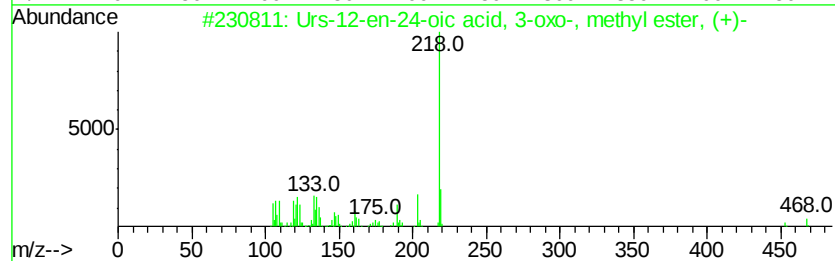
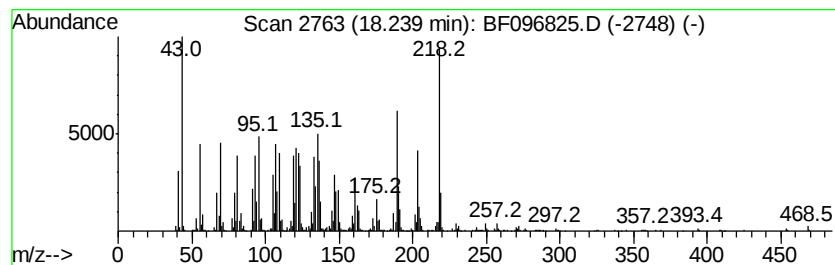
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Urs-12-en-24-oic acid, 3-ox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.24	250.51 ng	6266640	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Urs-12-en-24-oic acid, 3-oxo-, m...	468	C31H48O3	020475-86-9	90
2		12-Oleanen-3-yl acetate, (3.alpha...	468	C32H52O2	033055-28-6	89
3		2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	83
4		.alpha.-Amyrin, trimethylsilyl e...	498	C33H58OSi	1000374-76-6	64
5		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071717\
 Data File : BF096825.D
 Acq On : 17 Jul 2017 17:55
 Operator : SJ/JU
 Sample : I4203-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DL-SB02C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	4.79	7.9	ng	263855	1	6.61	669945	20.0
unknown6.39	6.39	72.8	ng	2439190	1	6.61	669945	20.0
Tridecanoic acid	11.66	3.3	ng	79209	4	11.11	478164	20.0
Phenol, 4,4'-(1-m...	12.57	21.9	ng	704902	5	13.73	643997	20.0
Dichloroacetic ac...	13.60	7.6	ng	246166	5	13.73	643997	20.0
Hexadecane, 1-chl...	14.23	3.2	ng	104412	5	13.73	643997	20.0
Hexadecane	14.52	3.1	ng	78390	6	15.11	500311	20.0
.beta.-Sitosterol	16.92	7.4	ng	184768	6	15.11	500311	20.0
unknown17.10	17.10	9.7	ng	241791	6	15.11	500311	20.0
.beta.-Amyrin	17.31	23.9	ng	598426	6	15.11	500311	20.0
2,2,6-Trimethyl-1...	17.40	21.7	ng	542672	6	15.11	500311	20.0
Caparratriene	17.63	179.8	ng	4498920	6	15.11	500311	20.0
3a-Methyl-3,3a-di...	17.85	20.9	ng	524147	6	15.11	500311	20.0
Urs-12-en-24-oic ...	18.24	250.5	ng	6266640	6	15.11	500311	20.0