

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031418\
 Data File : BF103652.D
 Acq On : 14 Mar 2018 20:26
 Operator : SJ/JU
 Sample : J1909-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1-3-RO-COMP

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

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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	5.098	509	512	525	rBV	37074	80808	2.70%	0.311%
2	5.487	575	578	609	rBV	1138575	2690199	89.97%	10.363%
3	6.498	747	750	769	rBV	1205751	2653135	88.73%	10.220%
4	6.628	769	772	799	rVB	2042966	2990036	100.00%	11.518%
5	6.857	808	811	833	rVB	456148	788871	26.38%	3.039%
6	7.010	833	837	863	rVB	1721805	2137971	71.50%	8.236%
7	7.428	905	908	940	rBV	879591	1893253	63.32%	7.293%
8	8.139	1026	1029	1052	rBV	572746	990528	33.13%	3.816%
9	9.075	1185	1188	1195	rVB	55296	56361	1.88%	0.217%
10	9.210	1203	1211	1226	rBV	2250054	2644522	88.44%	10.187%
11	9.316	1226	1229	1238	rVV3	51083	82291	2.75%	0.317%
12	9.416	1241	1246	1255	rBV6	25925	74782	2.50%	0.288%
13	9.628	1279	1282	1289	rBV4	35313	36656	1.23%	0.141%
14	9.898	1324	1328	1343	rVB	758564	909896	30.43%	3.505%
15	10.510	1429	1432	1439	rBV	273018	223026	7.46%	0.859%
16	10.698	1460	1464	1476	rBV	760591	1232123	41.21%	4.746%
17	10.780	1476	1478	1490	rVB5	33046	64473	2.16%	0.248%
18	10.957	1505	1508	1517	rBV	144702	207437	6.94%	0.799%
19	11.022	1517	1519	1535	rVB2	48749	121684	4.07%	0.469%
20	11.398	1579	1583	1595	rBV	503911	792723	26.51%	3.054%
21	11.480	1595	1597	1603	rVV6	18104	36971	1.24%	0.142%
22	11.539	1603	1607	1613	rVV	111458	109861	3.67%	0.423%
23	11.904	1666	1669	1672	rBV	167232	181900	6.08%	0.701%
24	11.933	1672	1674	1680	rVB	490146	459175	15.36%	1.769%
25	12.451	1760	1762	1765	rVB	42471	33984	1.14%	0.131%
26	12.622	1788	1791	1797	rBV	90591	115571	3.87%	0.445%
27	12.780	1814	1818	1823	rBV	38699	46417	1.55%	0.179%
28	12.827	1823	1826	1828	rBV	82144	79931	2.67%	0.308%
29	12.851	1828	1830	1836	rVB	103519	108882	3.64%	0.419%
30	12.974	1847	1851	1863	rBV	1454207	1559535	52.16%	6.008%
31	13.069	1865	1867	1873	rVB3	28865	41471	1.39%	0.160%
32	13.180	1881	1886	1890	rVB	107896	120481	4.03%	0.464%
33	13.527	1941	1945	1948	rBV	86741	84766	2.83%	0.327%
34	13.821	1991	1995	1998	rBV2	66502	101976	3.41%	0.393%

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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-BF022218.M
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35	13.857	1998	2001	2007	rVV2	221419	280146	9.37%	1.079%
36	13.992	2021	2024	2029	rVB	126884	112808	3.77%	0.435%
37	14.057	2030	2035	2044	rBV	553673	822645	27.51%	3.169%
38	14.174	2052	2055	2057	rVB2	34938	33913	1.13%	0.131%
39	15.127	2214	2217	2221	rBV	105068	146658	4.90%	0.565%
40	15.510	2279	2282	2287	rVB	68415	96994	3.24%	0.374%
41	15.568	2287	2292	2304	rBV	330993	596945	19.96%	2.300%
42	15.951	2353	2357	2362	rVB2	79646	117684	3.94%	0.453%

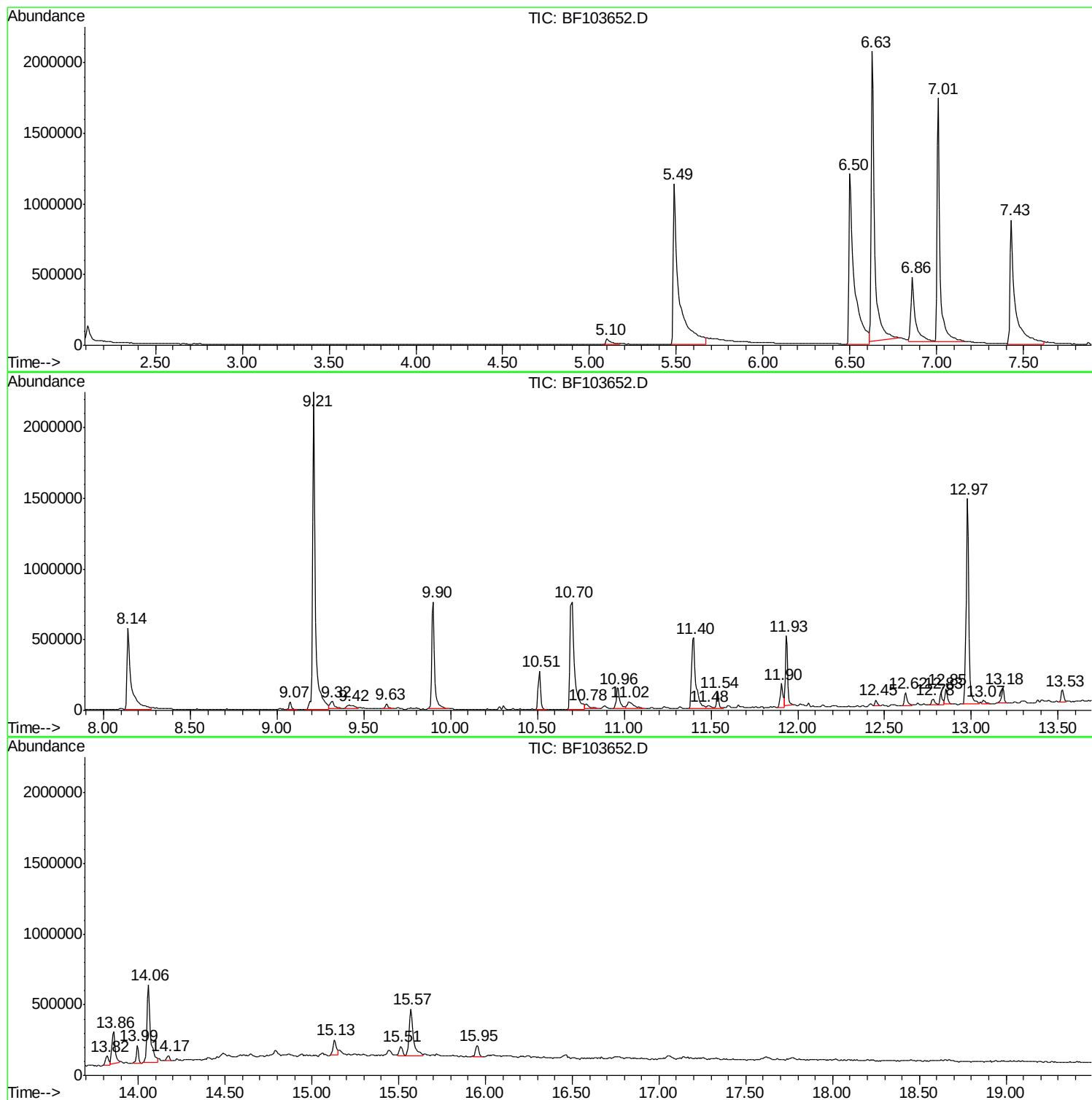
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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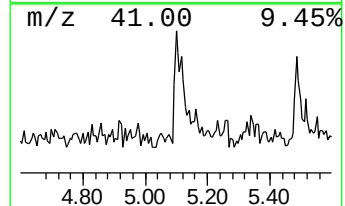
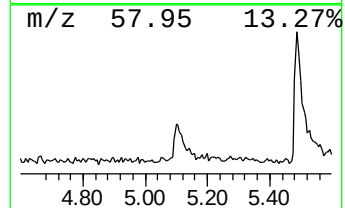
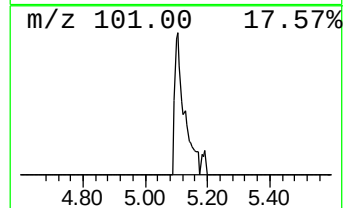
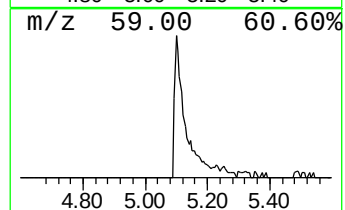
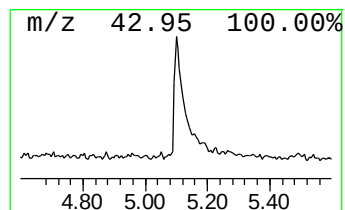
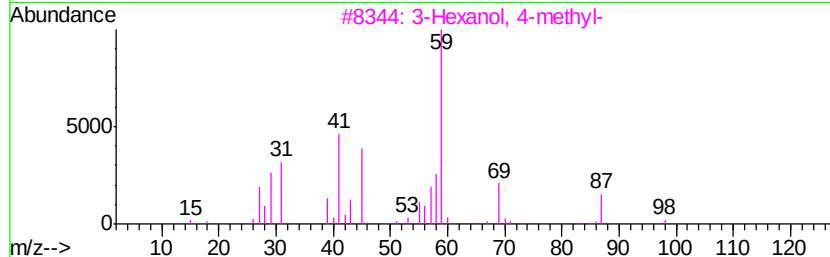
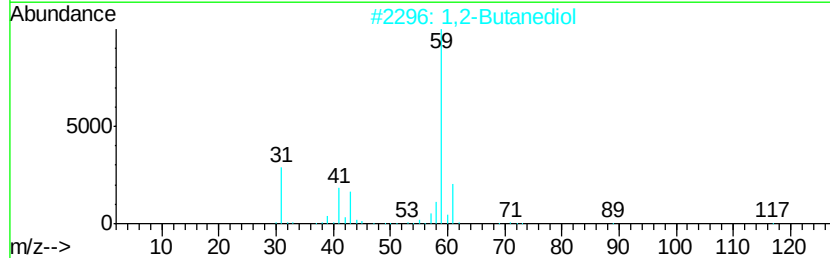
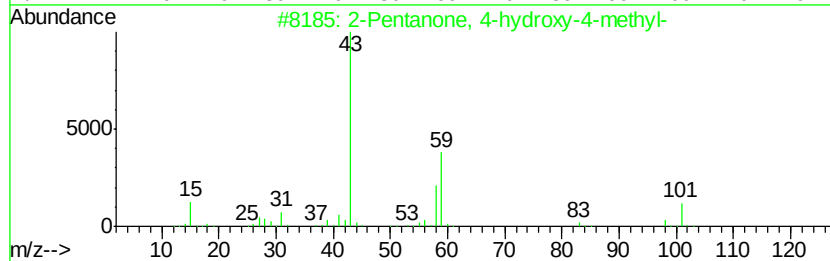
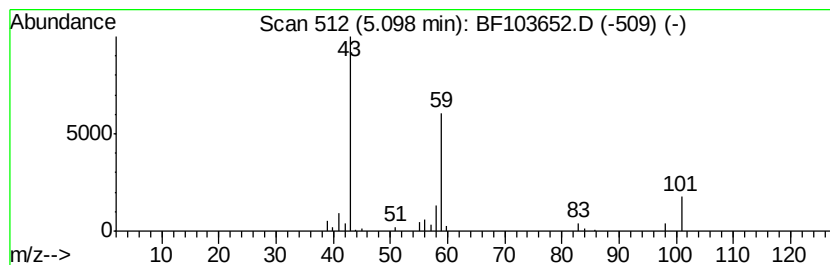
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.05 ng	80808	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			1,2-Butanediol	90	C4H10O2	000584-03-2	37
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
4			3-Hexanol	102	C6H14O	000623-37-0	25
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25



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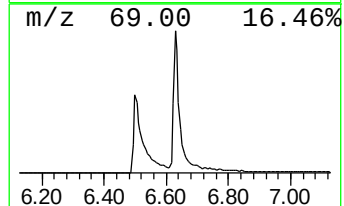
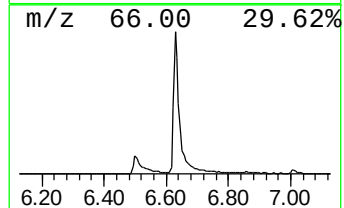
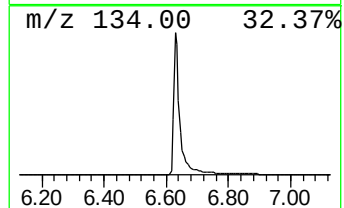
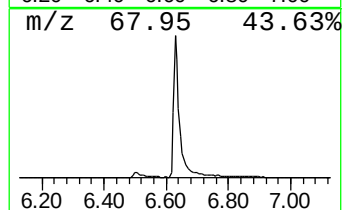
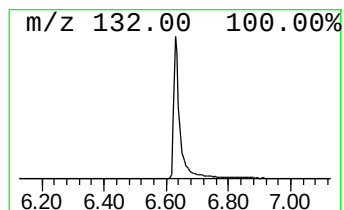
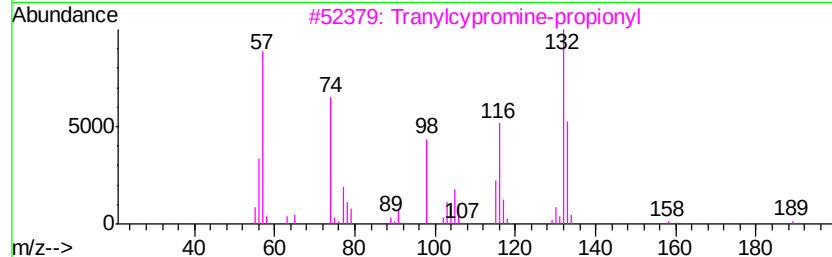
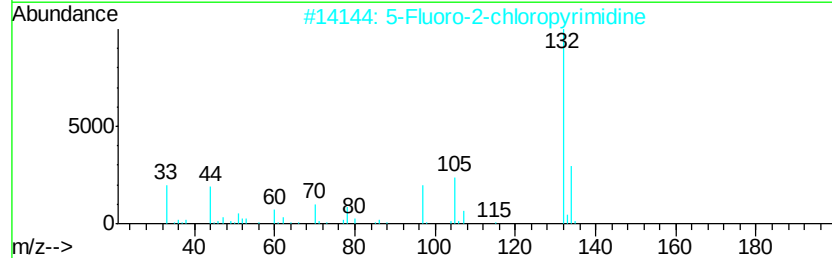
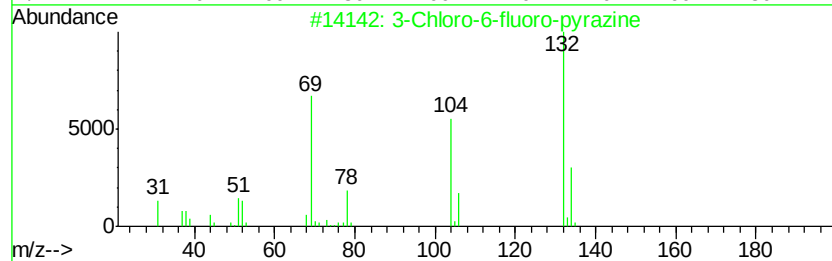
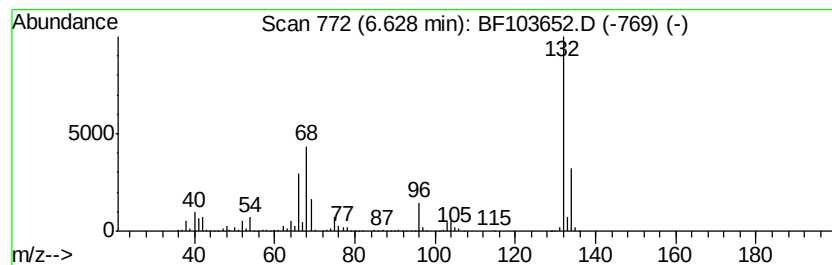
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	75.81 ng	2990040	1,4-Dichlorobenzene-d4	6.86

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	16
3		Tranvlcypromine-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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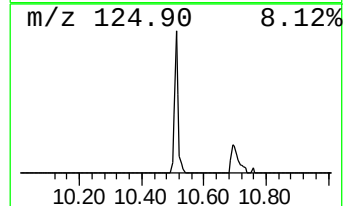
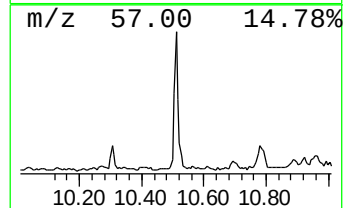
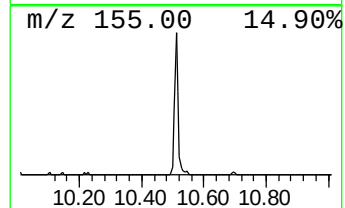
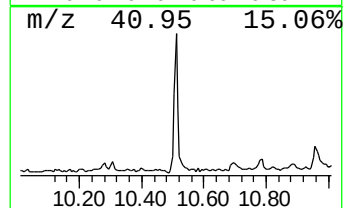
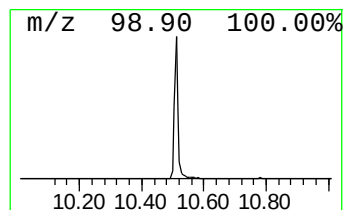
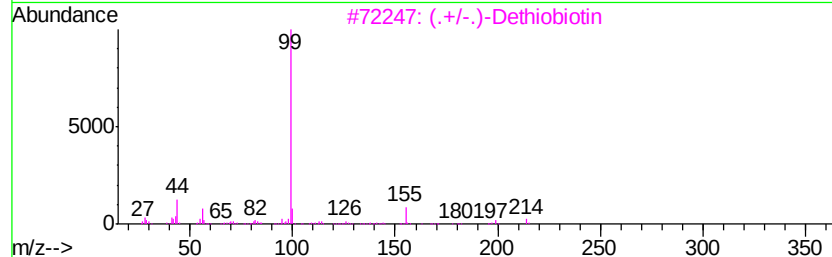
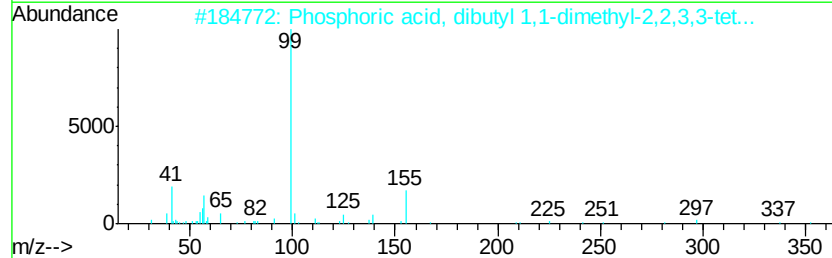
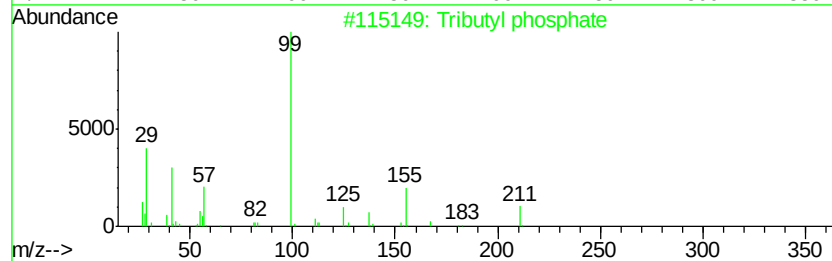
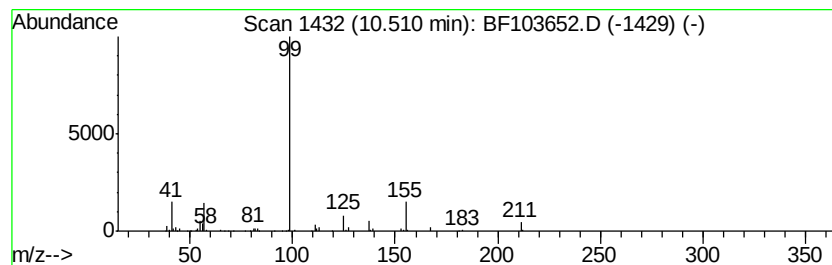
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tributyl phosphate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.51	4.90 ng	223026	Acenaphthene-d10		9.90
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	86
2	Phosphoric acid, dibutyl 1,1-dim...	352	C13H25F4O4P	1000298-93-9	72
3	(.+/-)-Dethiobiotin	214	C10H18N2O3	000636-20-4	36
4	2H-Pyran-2-one, 6-hexyltetrahydro-	184	C11H20O2	000710-04-3	10
5	1,3,2-Dioxaborolane, 4,4'-(1,4-b...	254	C12H24B2O4	074793-62-7	9



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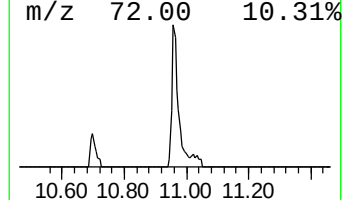
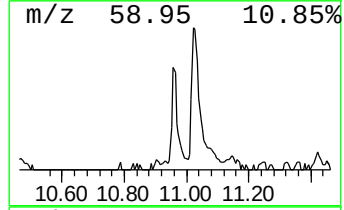
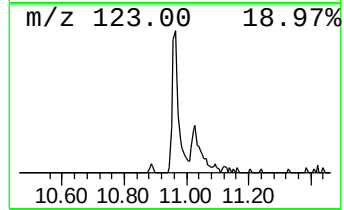
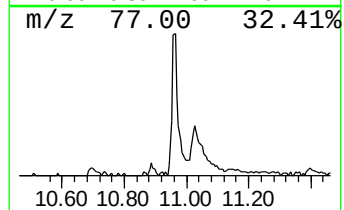
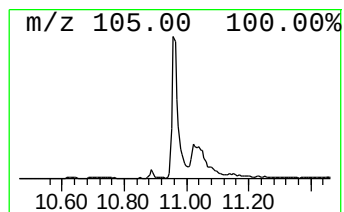
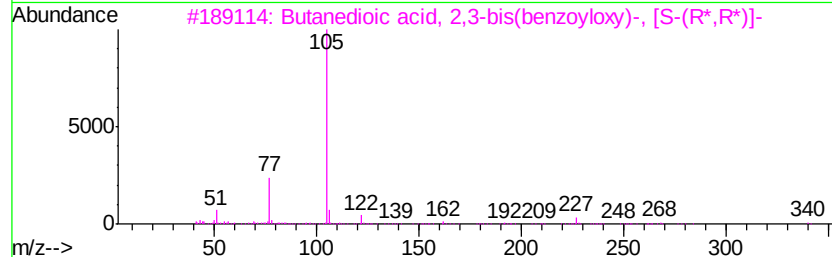
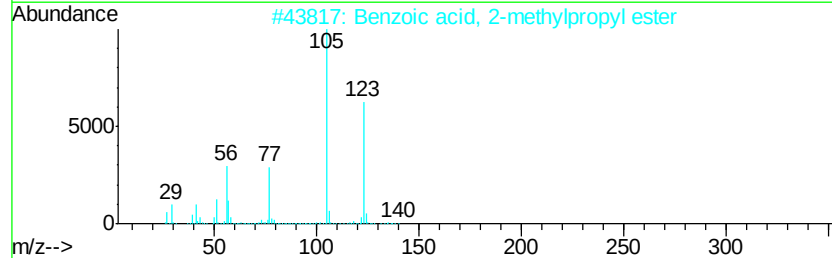
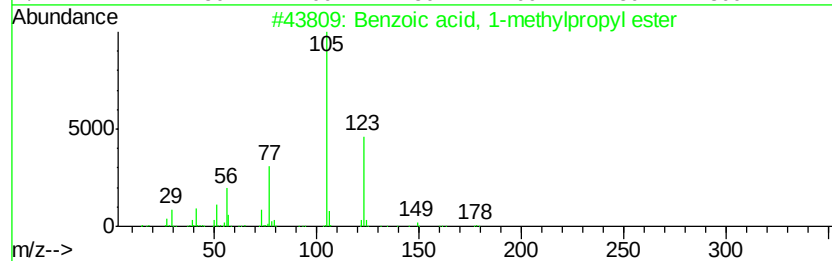
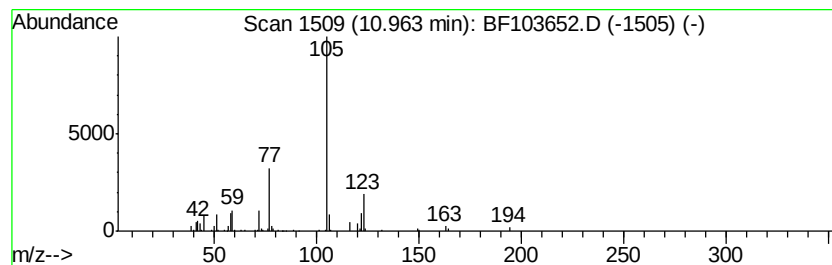
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown10.96 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	5.23 ng	207437	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 1-methylpropyl ester	178	C11H14O2	003306-36-3	47
2		Benzoic acid, 2-methylpropyl ester	178	C11H14O2	000120-50-3	47
3		Butanedioic acid, 2,3-bis(benzoyl-...	358	C18H14O8	017026-42-5	43
4		Benzoic acid, (3-isopropyl-6-met...	283	C17H17NO3	039870-46-7	43
5		Pentanal, 5-(benzoyloxy)-	206	C12H14O3	055162-83-9	43



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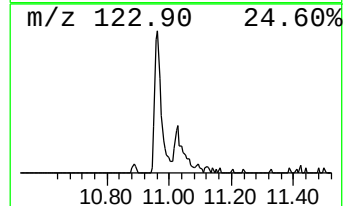
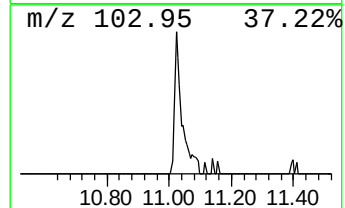
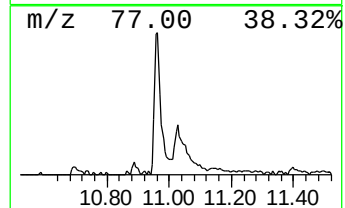
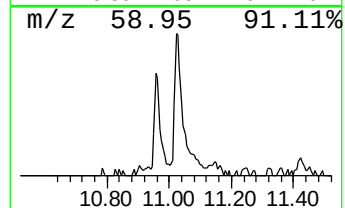
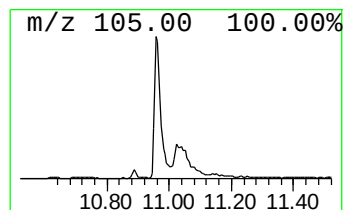
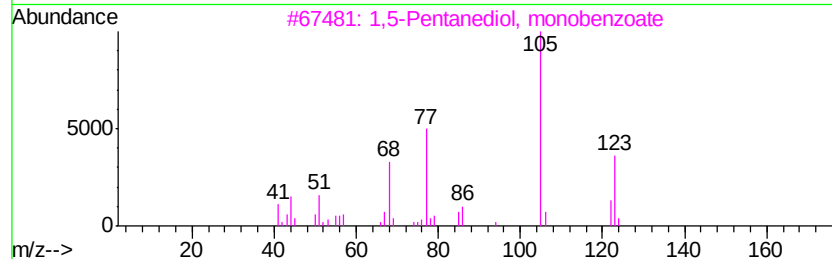
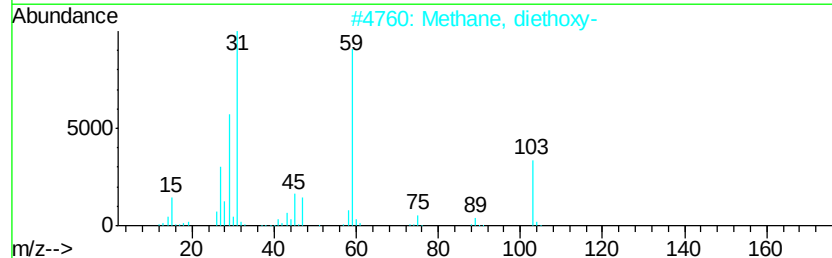
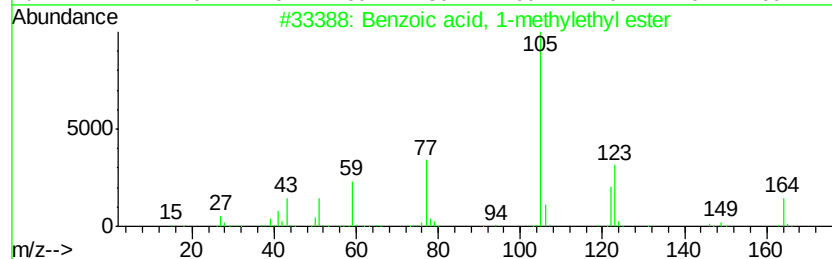
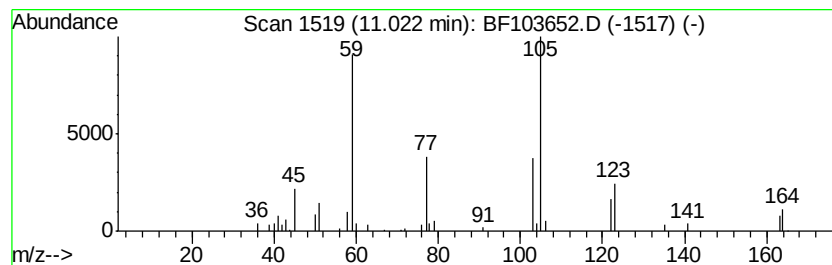
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown11.02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	3.07 ng	121684	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzoic acid, 1-methylethyl ester	164	C10H12O2	000939-48-0	38
2		Methane, diethoxy-	104	C5H12O2	000462-95-3	38
3		1,5-Pentanediol, monobenzoate	208	C12H16O3	055162-82-8	27
4		n-Propyl benzoate	164	C10H12O2	002315-68-6	27
5		Pentanal, 5-(benzoyloxy)-	206	C12H14O3	055162-83-9	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031418\
Data File : BF103652.D
Acq On : 14 Mar 2018 20:26
Operator : SJ/JU
Sample : J1909-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-3-RO-COMP

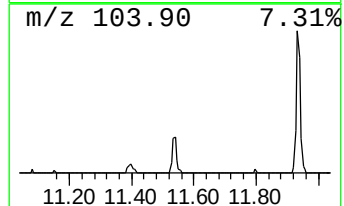
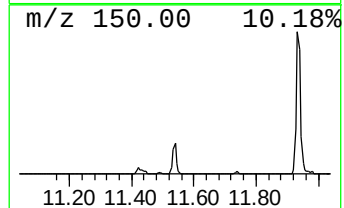
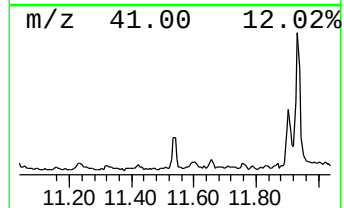
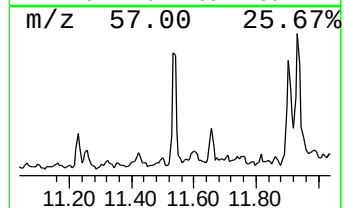
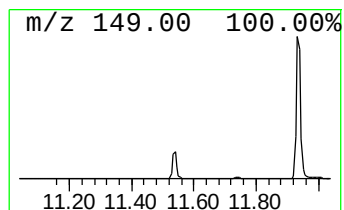
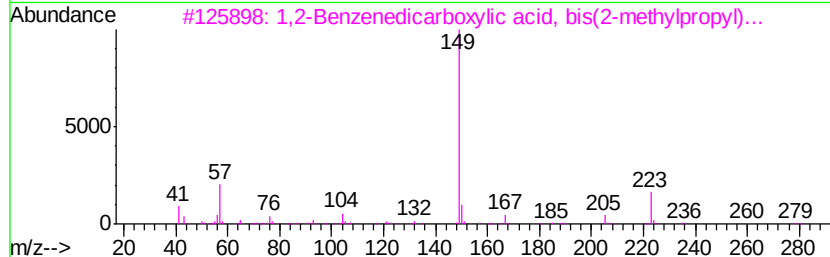
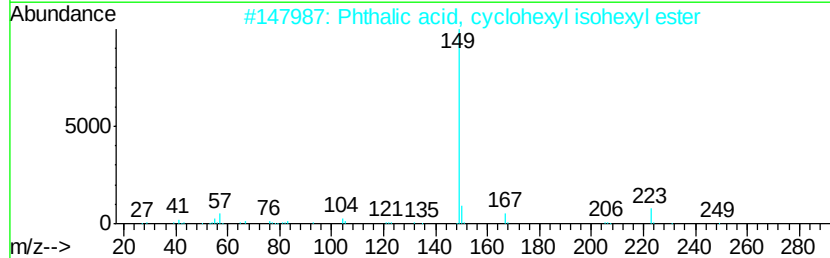
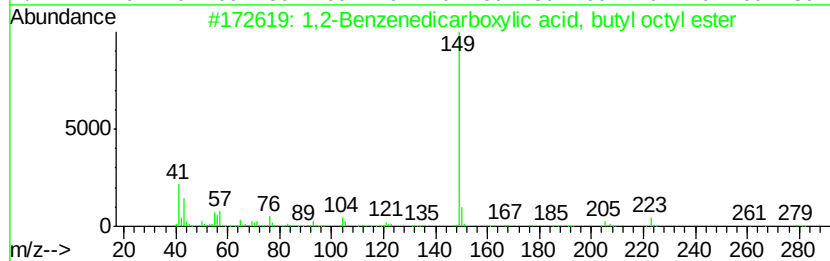
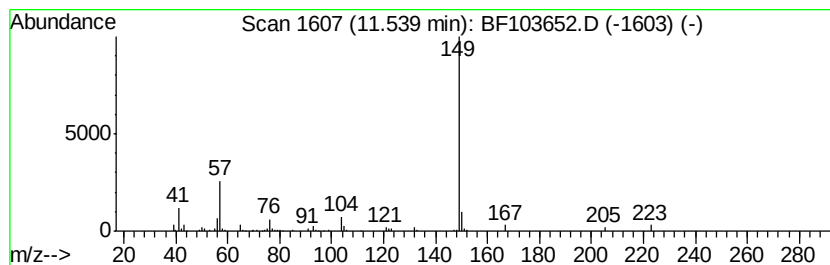
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,2-Benzenedicarboxylic aci... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.77 ng	109861	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	83
2		Phthalic acid, cyclohexyl isohex...	304	C18H24O4	1000315-34-0	83
3		1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	83
4		Phthalic acid, hex-2-yn-4-yl iso...	302	C18H22O4	1000315-19-9	78
5		Phthalic acid, hept-3-yl isobuty...	320	C19H28O4	1000356-98-6	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031418\
Data File : BF103652.D
Acq On : 14 Mar 2018 20:26
Operator : SJ/JU
Sample : J1909-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

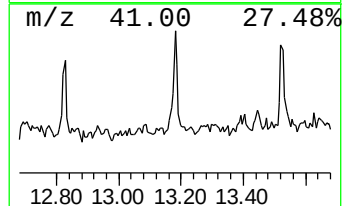
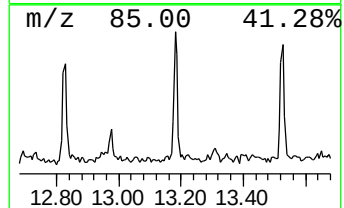
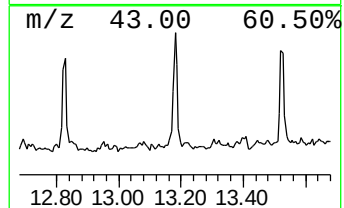
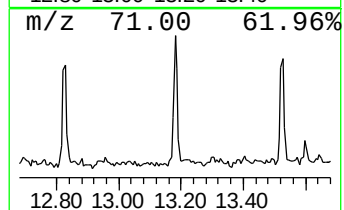
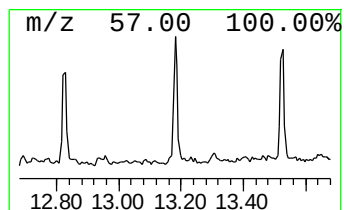
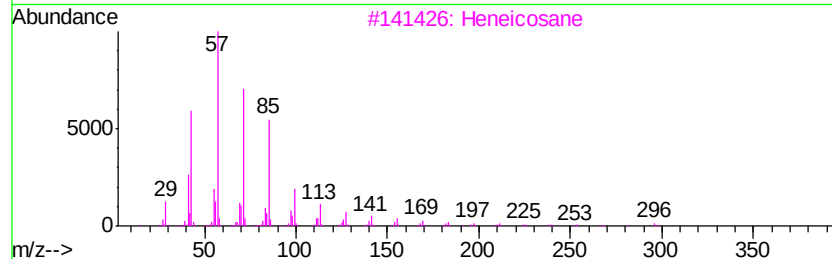
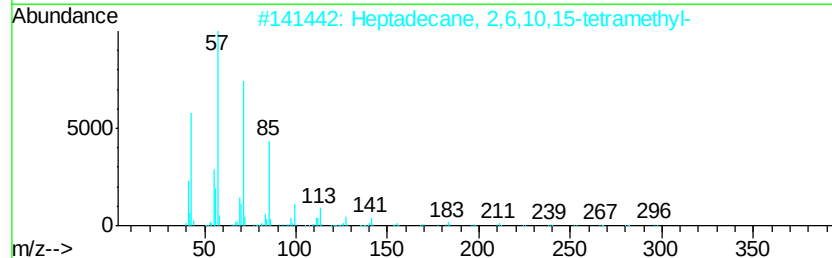
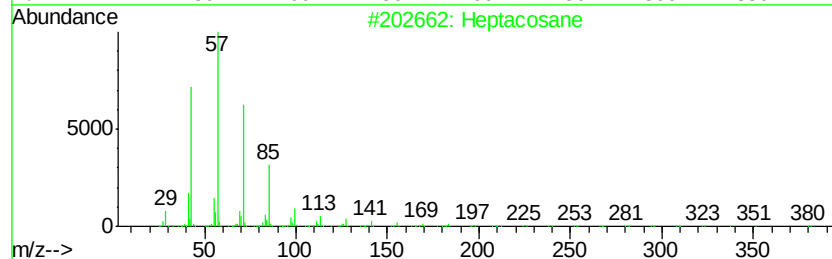
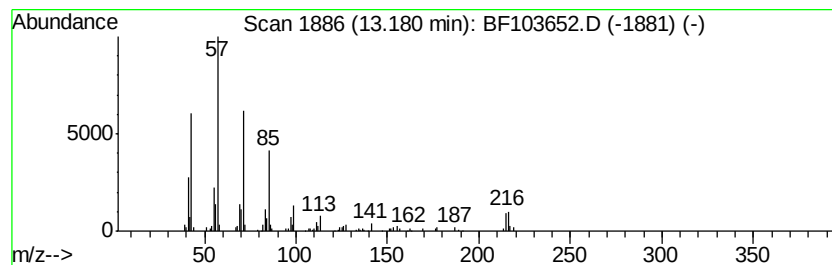
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	2.93 ng	120481	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	83
2	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	80
3	Heneicosane	296 C21H44	000629-94-7	80
4	Octacosane	394 C28H58	000630-02-4	80
5	2-methyloctacosane	408 C29H60	1000376-72-8	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031418\
Data File : BF103652.D
Acq On : 14 Mar 2018 20:26
Operator : SJ/JU
Sample : J1909-01
Misc :
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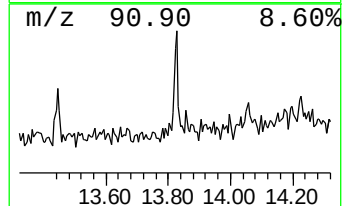
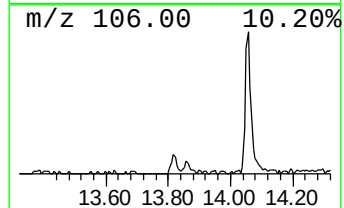
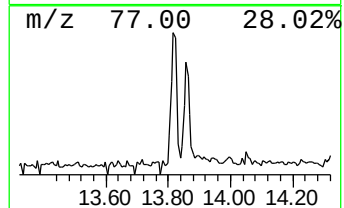
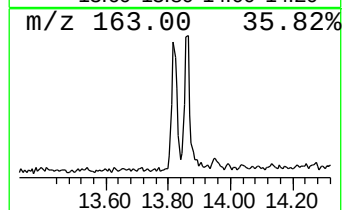
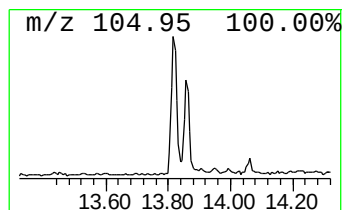
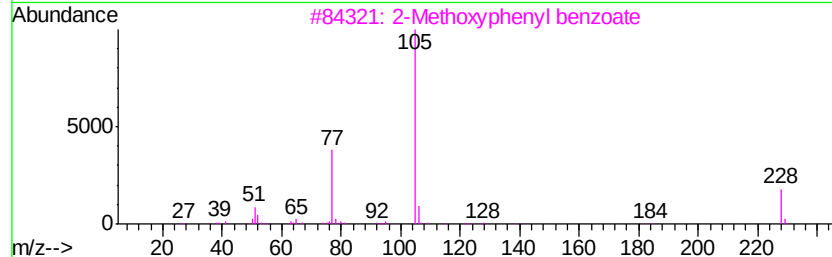
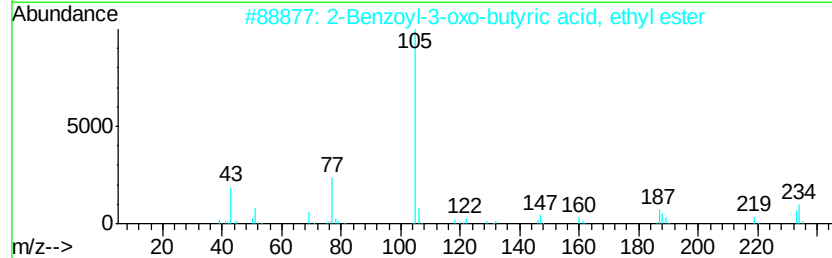
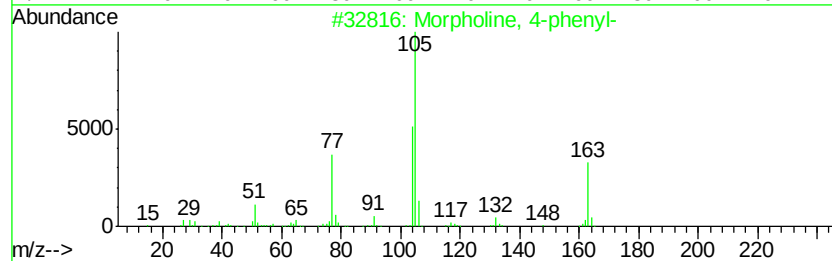
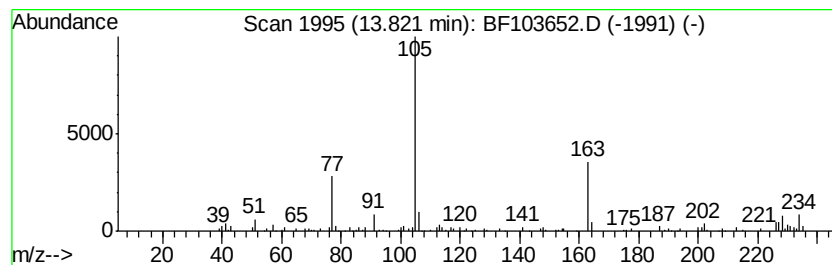
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Morpholine, 4-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	2.48 ng	101976	Chrysene-d12	14.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2	2-Benzoyl-3-oxo-butyric acid, et...	234	C13H14O4	1000317-59-7	49
3	2-Methoxyphenyl benzoate	228	C14H12O3	000531-37-3	47
4	Propan-1-one, 3-(5-methyl-3-isox...	230	C13H14N2O2	186956-50-3	46
5	Azetidine, 1-benzoyl-3-ethenyl-	187	C12H13NO	118973-03-8	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031418\
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Acq On : 14 Mar 2018 20:26
Operator : SJ/JU
Sample : J1909-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

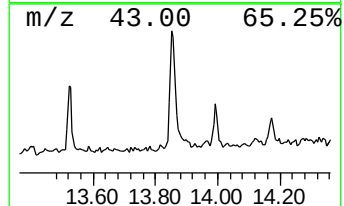
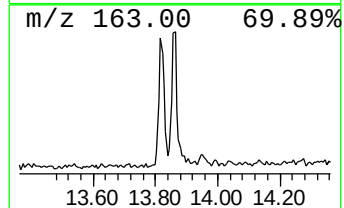
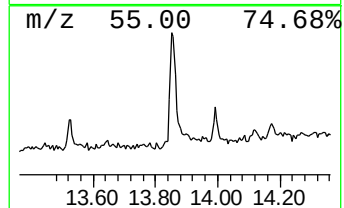
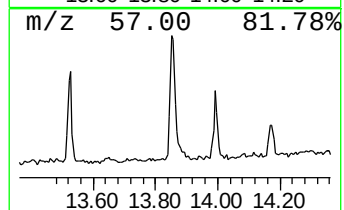
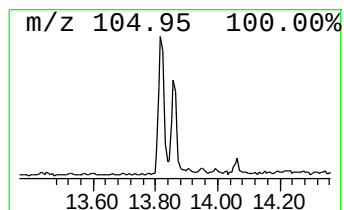
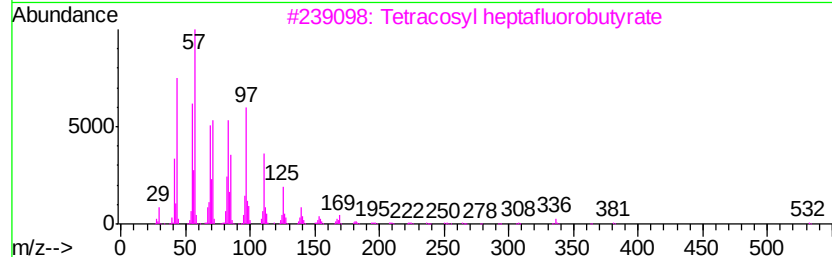
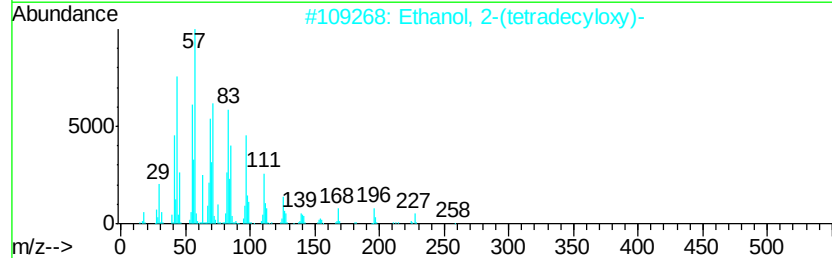
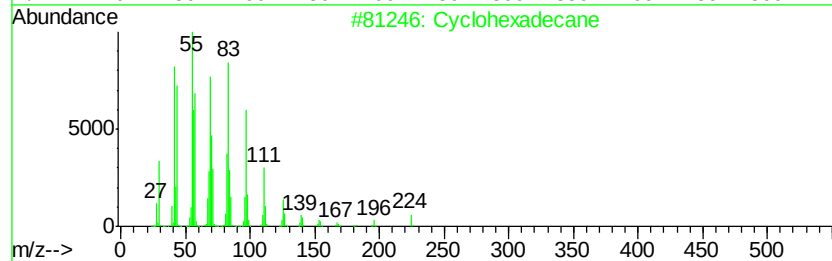
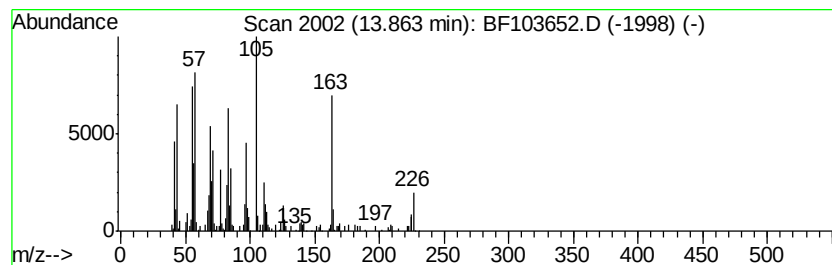
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	6.81 ng	280146	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 98
2		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 90
3		Tetracosyl heptafluorobutyrte	550 C28H49F7O2	1000351-83-7 90
4		Dotriacontyl pentafluoropropionate	612 C35H65F5O2	1000351-81-4 90
5		Tricosyl heptafluorobutyrate	536 C27H47F7O2	1000351-83-4 90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031418\
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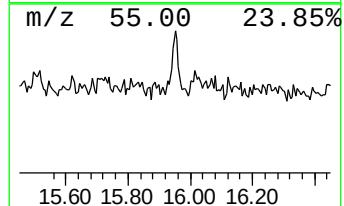
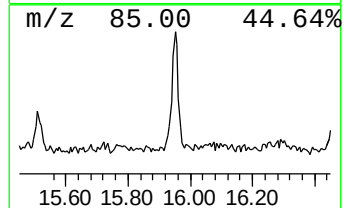
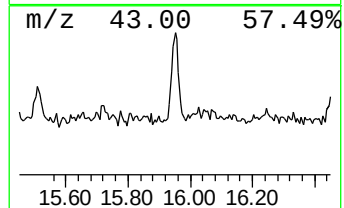
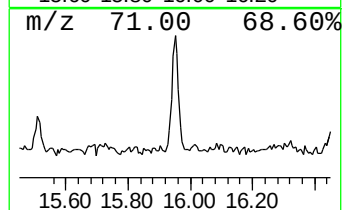
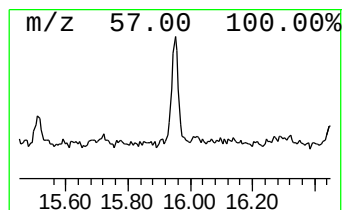
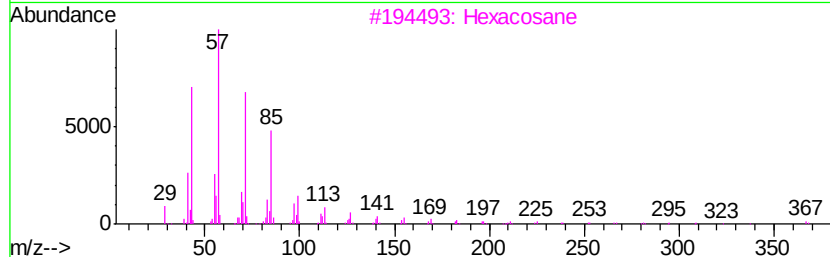
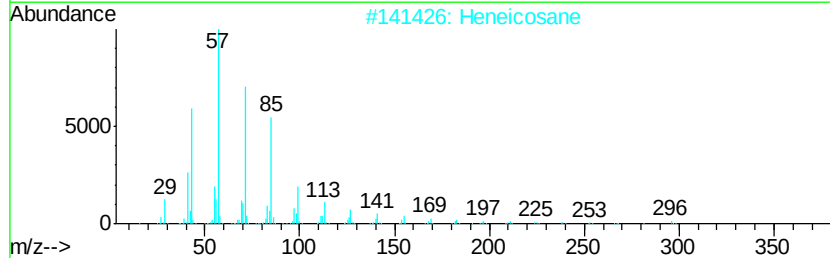
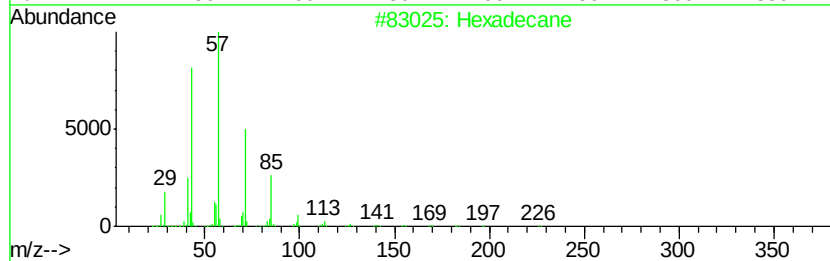
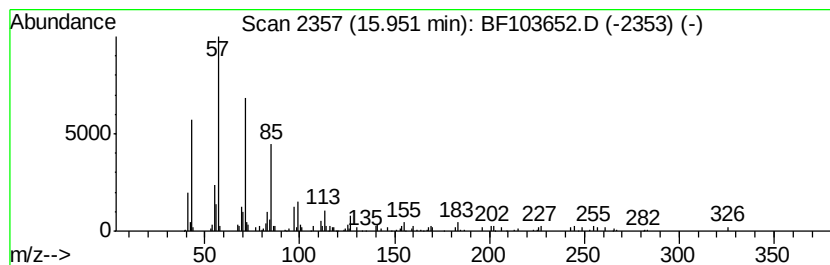
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.94 ng	117684	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Eicosane	282	C20H42	000112-95-8	90
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031418\
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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
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unknown6.63	6.63	75.8	ng	2990040	1	6.86	788871	20.0
Tributyl phosphate	10.51	4.9	ng	223026	3	9.90	909896	20.0
unknown10.96	10.96	5.2	ng	207437	4	11.40	792723	20.0
unknown11.02	11.02	3.1	ng	121684	4	11.40	792723	20.0
1,2-Benzenedicarb...	11.54	2.8	ng	109861	4	11.40	792723	20.0
Heptacosane	13.18	2.9	ng	120481	5	14.06	822645	20.0
Morpholine, 4-phe...	13.82	2.5	ng	101976	5	14.06	822645	20.0
Cyclohexadecane	13.86	6.8	ng	280146	5	14.06	822645	20.0
Hexadecane	15.95	3.9	ng	117684	6	15.57	596945	20.0