

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071516\
 Data File : BF089042.D
 Acq On : 16 Jul 2016 5:33
 Operator : UM/SJ
 Sample : H4048-06
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-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-BF063016.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	1.655	5	6	14	rVB	83866	133655	9.87%	1.042%
2	1.770	14	16	24	rVV	767611	1163052	85.91%	9.064%
3	1.873	24	25	39	rVB	40704	91383	6.75%	0.712%
4	4.821	280	283	288	rVB	120987	157050	11.60%	1.224%
5	5.267	320	322	325	rBV	1046930	1095494	80.92%	8.537%
6	6.330	412	415	417	rVB	1181107	1353844	100.00%	10.550%
7	6.444	423	425	427	rBV	1382436	1214576	89.71%	9.465%
8	6.673	443	445	447	rBV	433123	348795	25.76%	2.718%
9	6.833	456	459	461	rBV	1130324	1011201	74.69%	7.880%
10	7.245	492	495	497	rBV	807854	826581	61.05%	6.442%
11	7.359	503	505	508	rBB	14374	14922	1.10%	0.116%
12	7.965	555	558	560	rBV	379892	434788	32.12%	3.388%
13	9.039	649	652	654	rBV	1542991	1282622	94.74%	9.995%
14	9.439	684	687	689	rBV	442464	430774	31.82%	3.357%
15	9.713	708	711	713	rBB	326941	410630	30.33%	3.200%
16	10.159	748	750	751	rVB	15539	17672	1.31%	0.138%
17	10.491	777	779	782	rBV	581744	530998	39.22%	4.138%
18	10.628	789	791	797	rVB	22997	29988	2.22%	0.234%
19	11.074	828	830	831	rBV	19051	18772	1.39%	0.146%
20	11.176	837	839	842	rVB2	250562	326199	24.09%	2.542%
21	12.765	975	978	980	rBV	953260	809803	59.82%	6.311%
22	13.245	1017	1020	1022	rBV	180573	219451	16.21%	1.710%
23	13.679	1055	1058	1063	rBV	37951	56918	4.20%	0.444%
24	13.805	1066	1069	1071	rBV	333352	305503	22.57%	2.381%
25	13.920	1077	1079	1083	rBV	6777	15014	1.11%	0.117%
26	14.320	1110	1114	1118	rBV3	8970	17522	1.29%	0.137%
27	14.422	1120	1123	1125	rBV	12219	22775	1.68%	0.177%
28	14.502	1127	1130	1131	rVV	18355	29180	2.16%	0.227%
29	14.582	1134	1137	1139	rVV	37951	51663	3.82%	0.403%
30	14.662	1142	1144	1146	rVV	41666	56406	4.17%	0.440%
31	14.742	1149	1151	1153	rVV	38447	42629	3.15%	0.332%
32	14.777	1153	1154	1156	rVB	16881	16356	1.21%	0.127%
33	14.834	1156	1159	1160	rBV	26647	31918	2.36%	0.249%
34	15.165	1185	1188	1191	rBV	170262	190456	14.07%	1.484%

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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

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35	16.251	1280	1283	1288	rBV2	6129	17441	1.29%	0.136%
36	16.708	1320	1323	1329	rVB	28473	56037	4.14%	0.437%

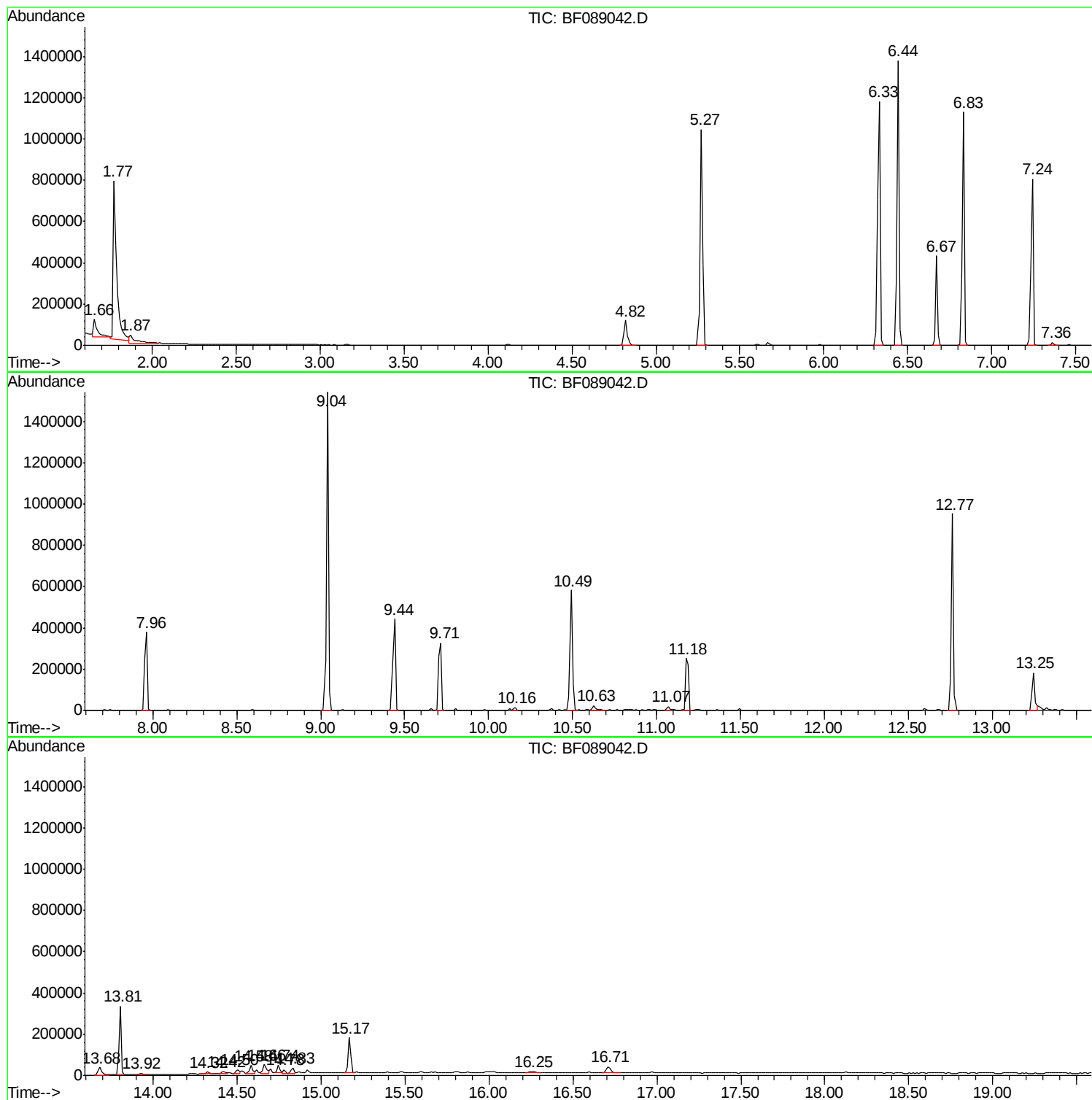
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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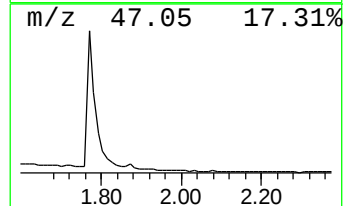
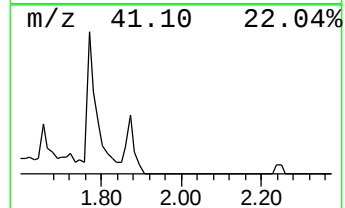
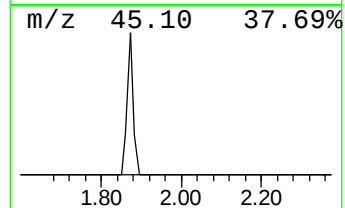
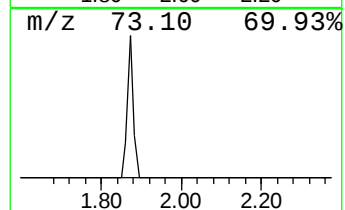
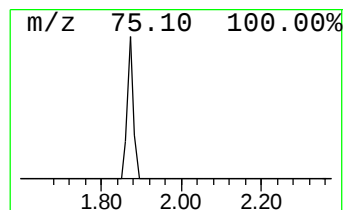
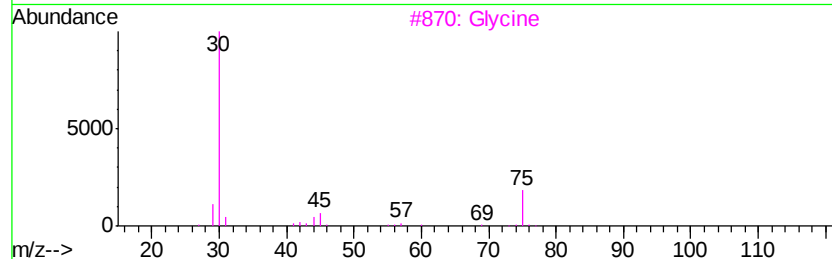
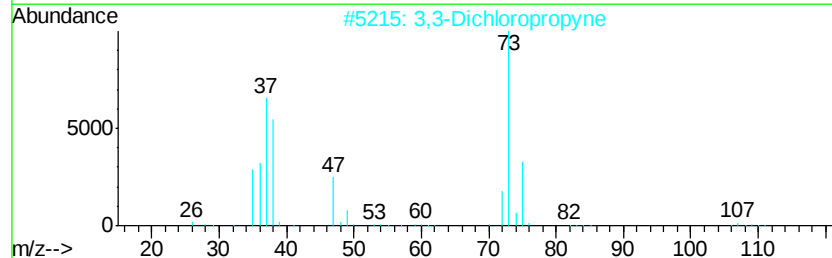
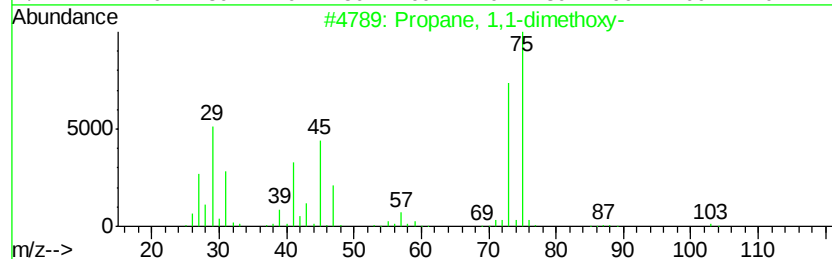
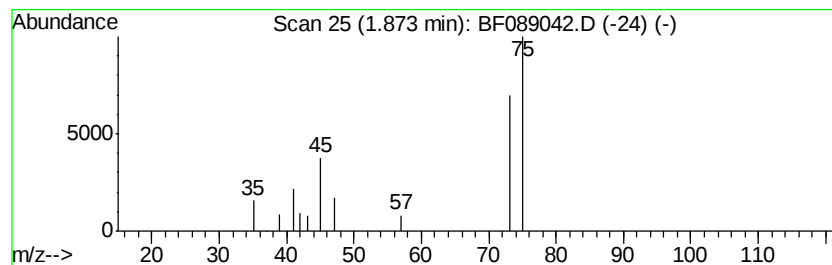
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.87	5.24 ng	91383	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2			3,3-Dichloropropyne	108	C3H2Cl2	025523-14-2	9
3			Glycine	75	C2H5NO2	000056-40-6	7
4			Ethylamine	45	C2H7N	000075-04-7	3
5			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	2



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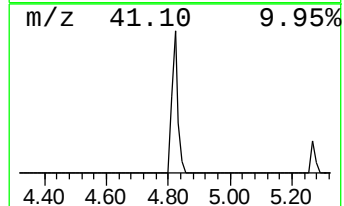
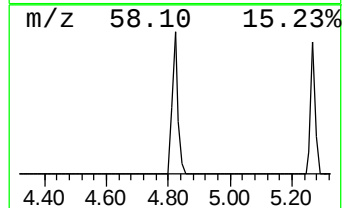
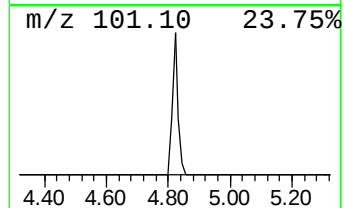
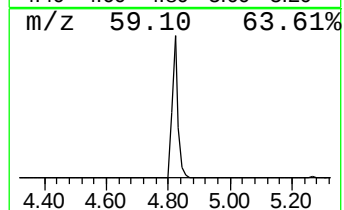
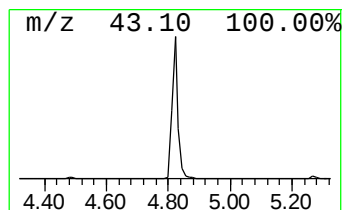
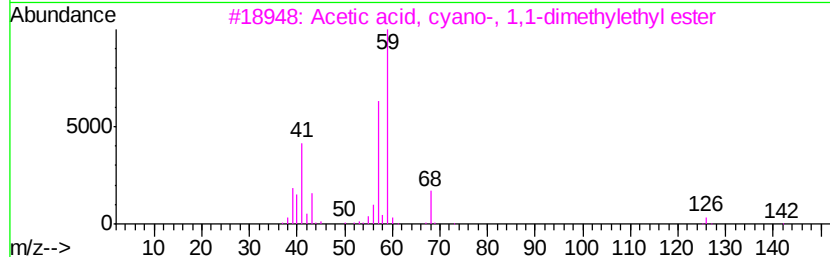
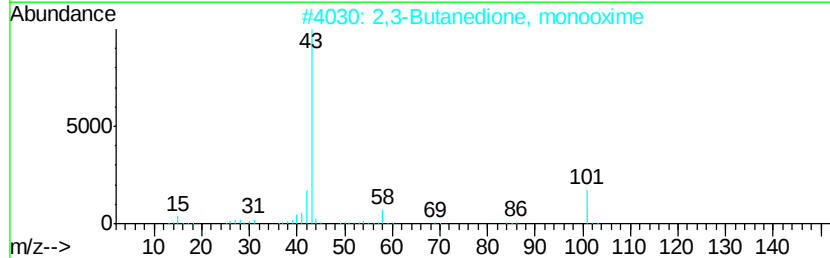
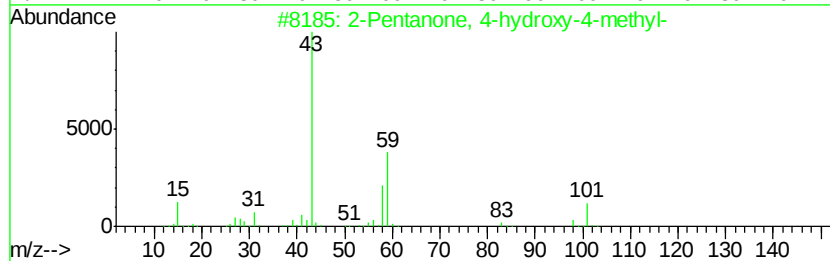
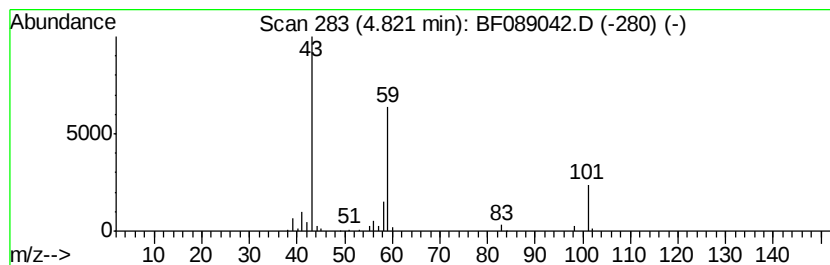
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	9.01 ng	157050	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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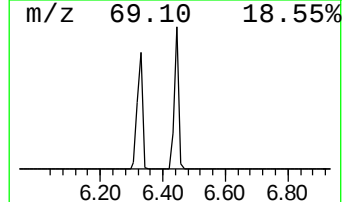
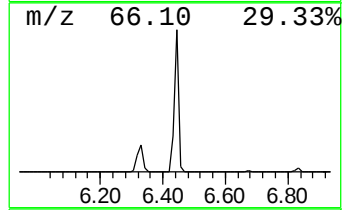
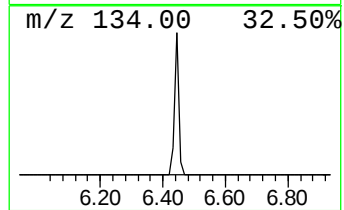
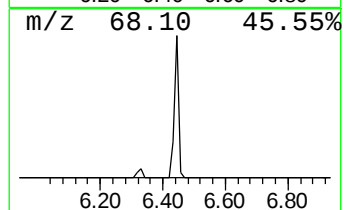
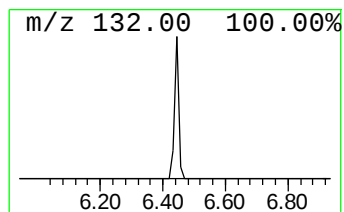
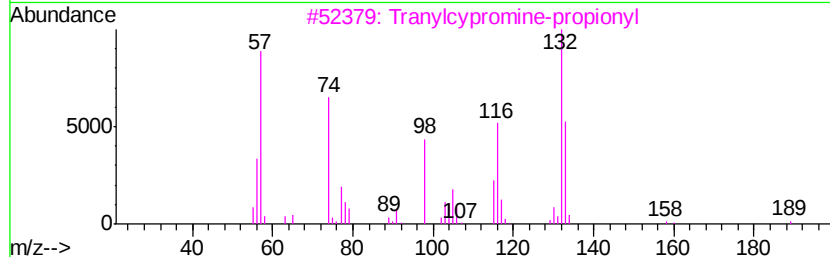
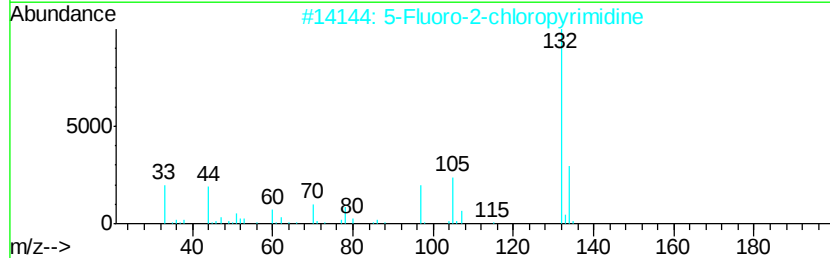
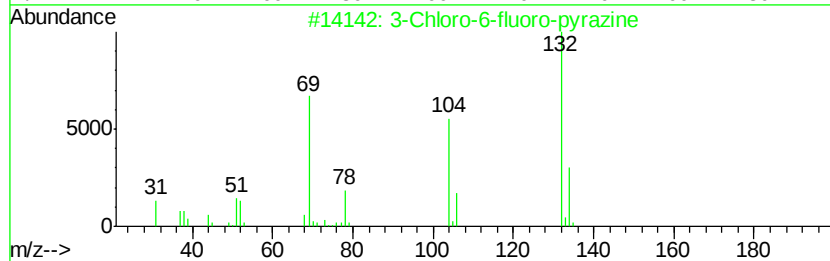
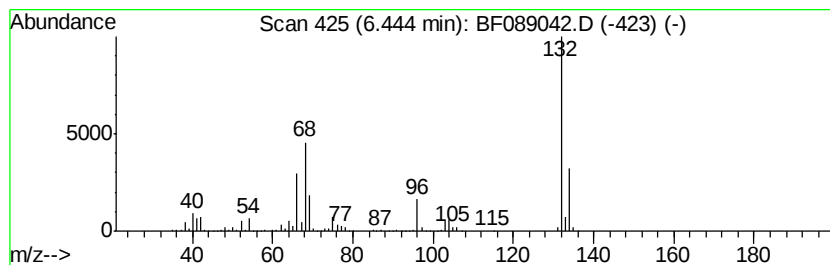
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	69.64 ng	1214580	1,4-Dichlorobenzene-d4	6.67

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		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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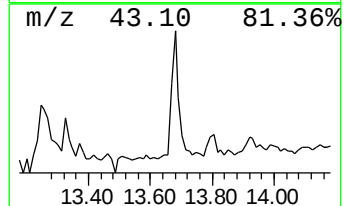
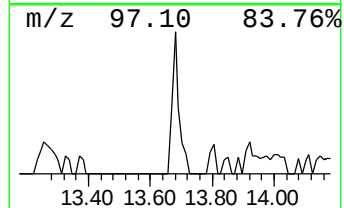
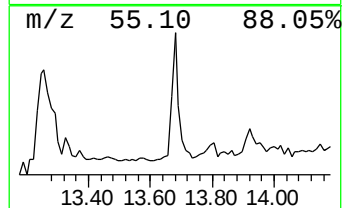
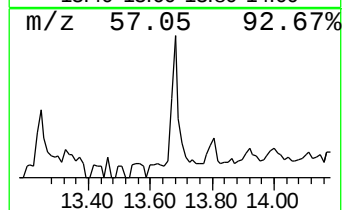
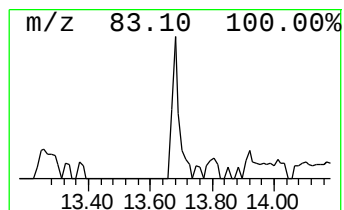
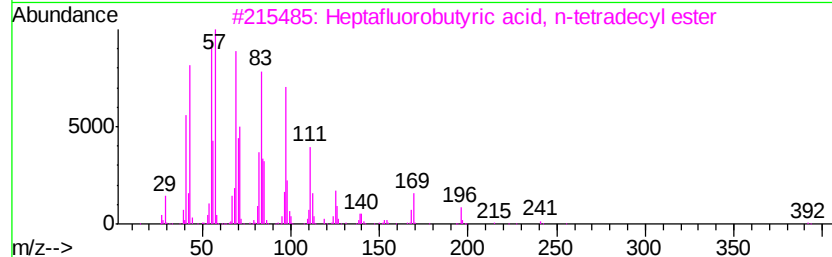
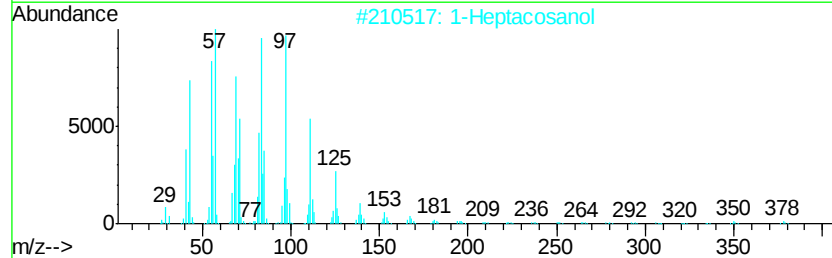
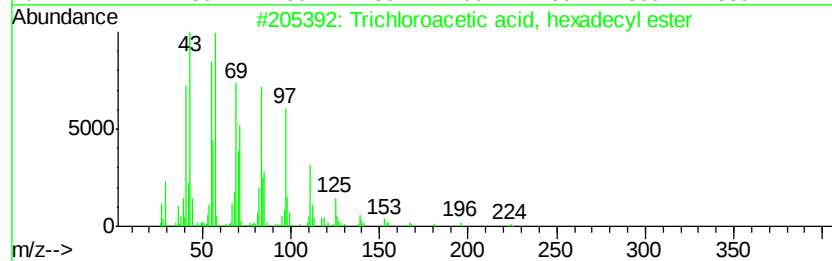
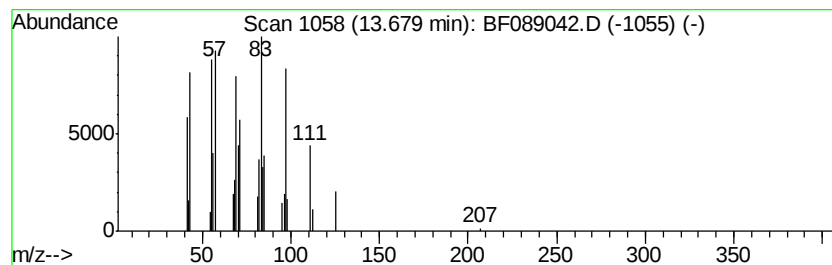
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	3.73 ng	56918	Chrysene-d12	13.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		1-Heptacosanol	396	C27H56O	002004-39-9	91
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
4		Behenic alcohol	326	C22H46O	000661-19-8	90
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	90



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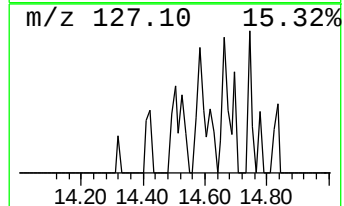
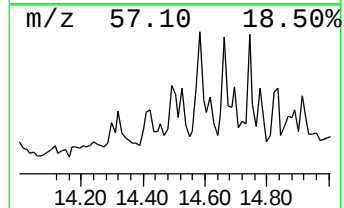
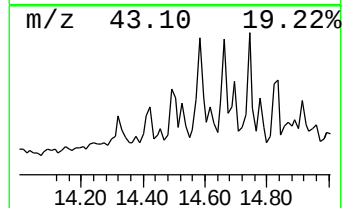
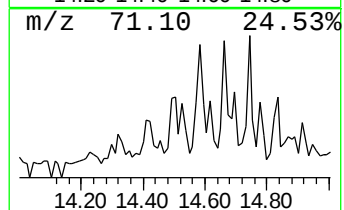
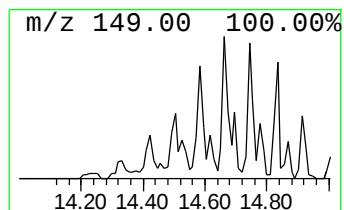
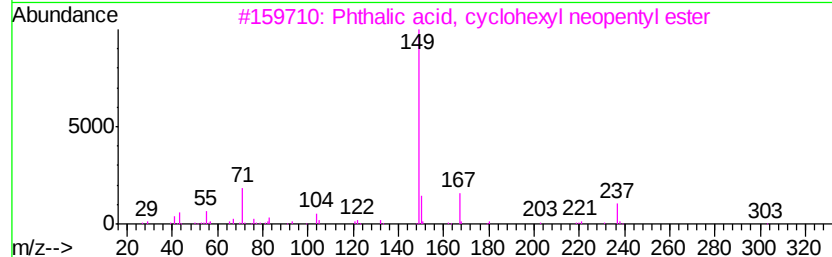
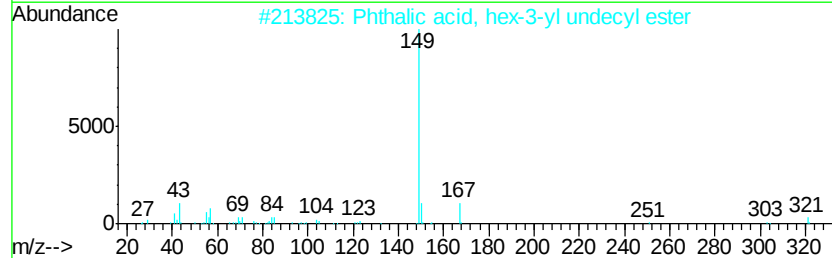
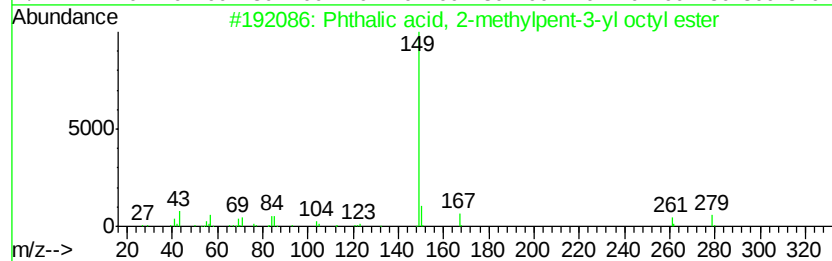
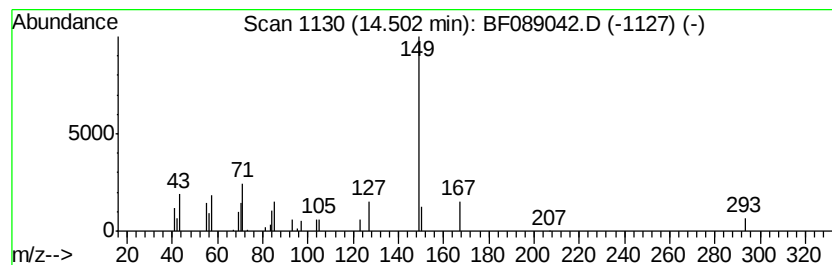
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Peak Number 8 Phthalic acid, 2-methylpent... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	3.06 ng	29180	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 2-methylpent-3-yl...	362	C22H34O4	1000356-91-3	59
2		Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	59
3		Phthalic acid, cyclohexyl neopen...	318	C19H26O4	1000315-54-2	59
4		Phthalic acid, 2-methylpent-3-yl...	432	C27H44O4	1000356-91-8	59
5		Phthalic acid, hexyl 4-methylpen...	334	C20H30O4	1000356-87-6	59



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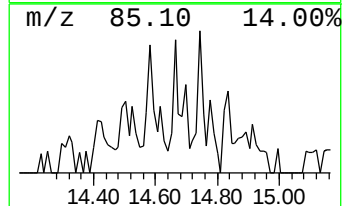
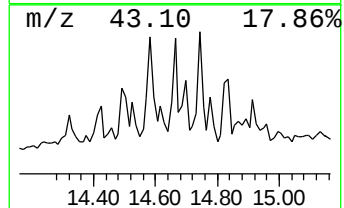
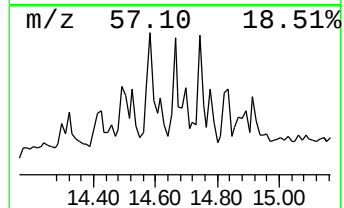
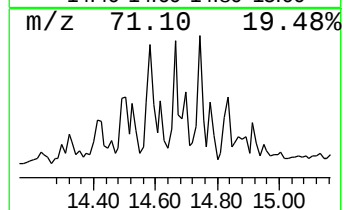
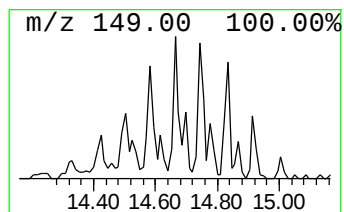
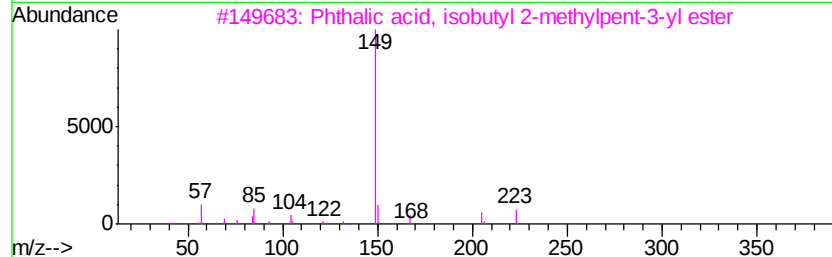
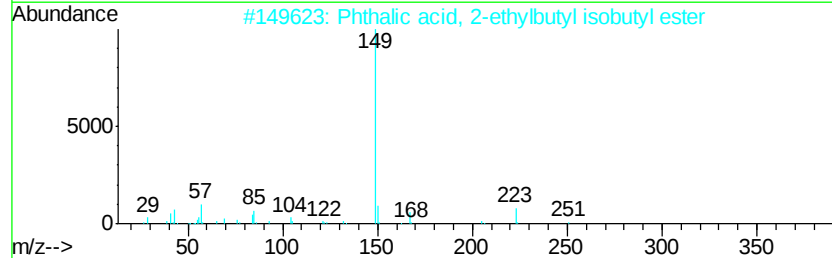
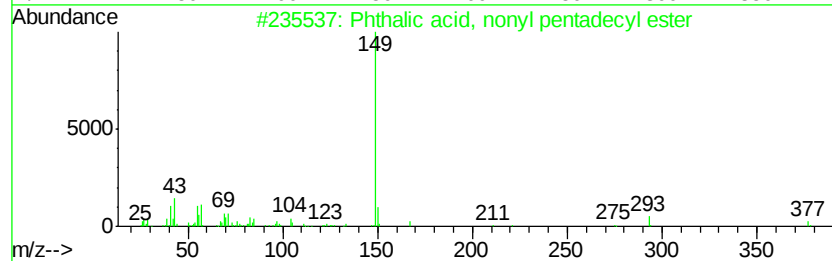
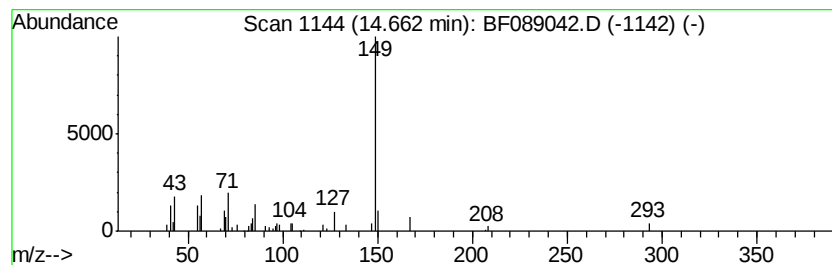
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Phthalic acid, nonyl pentad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	5.92 ng	56406	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	58
2		Phthalic acid, 2-ethylbutyl isob...	306	C18H26O4	1000356-88-9	53
3		Phthalic acid, isobutyl 2-methyl...	306	C18H26O4	1000356-90-7	53
4		Phthalic acid, decyl 3,4-dimethyl...	410	C26H34O4	1000309-82-4	53
5		Phthalic acid, hexyl octadecyl e...	502	C32H54O4	1000309-06-2	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071516\
Data File : BF089042.D
Acq On : 16 Jul 2016 5:33
Operator : UM/SJ
Sample : H4048-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-COMP

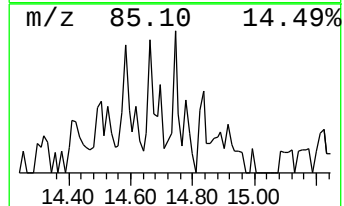
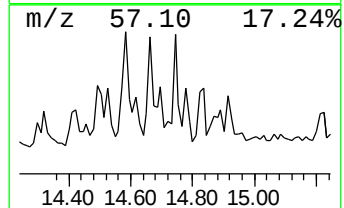
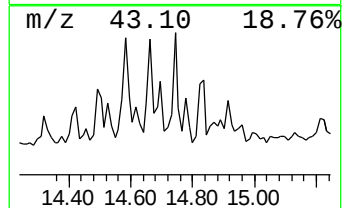
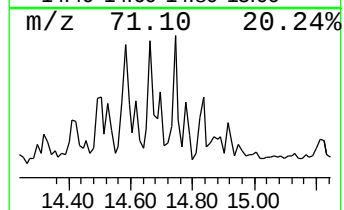
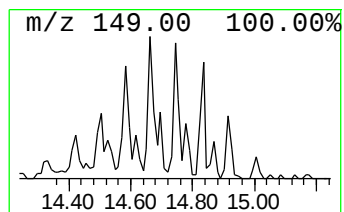
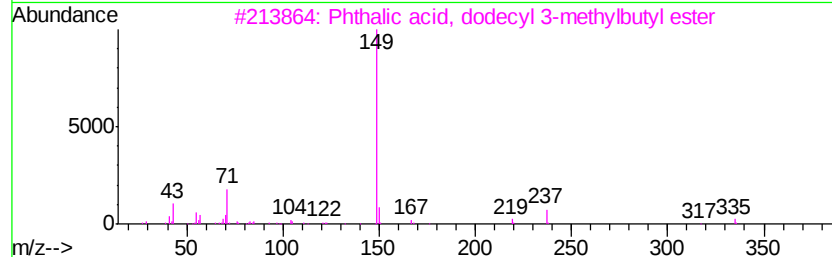
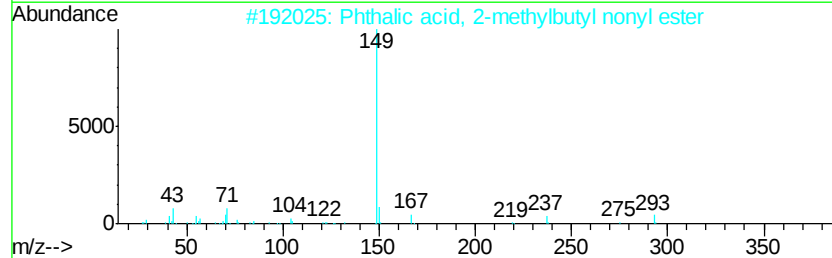
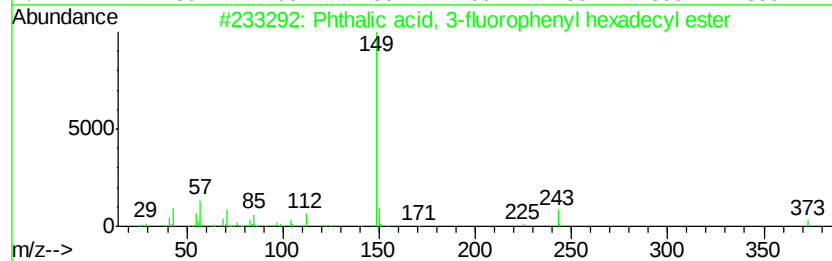
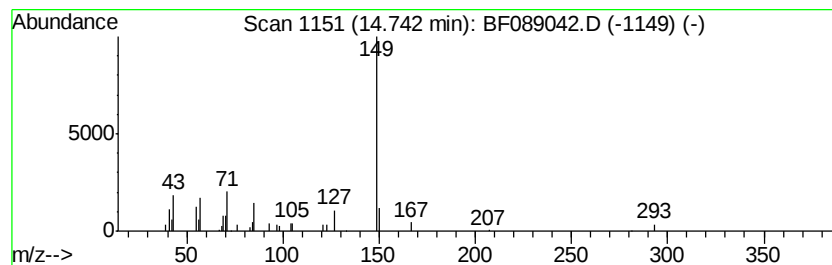
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phthalic acid, 3-fluorophen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	4.48 ng	42629	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, 3-fluorophenyl he...	484	C30H41F04	1000356-66-4	64
2		Phthalic acid, 2-methylbutyl non...	362	C22H34O4	1000322-81-7	64
3		Phthalic acid, dodecyl 3-methylb...	404	C25H40O4	1000356-81-3	64
4		1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	000146-50-9	59
5		Phthalic acid, 2-fluorophenyl pe...	470	C29H39F04	1000356-50-2	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071516\
Data File : BF089042.D
Acq On : 16 Jul 2016 5:33
Operator : UM/SJ
Sample : H4048-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-COMP

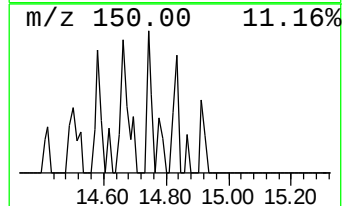
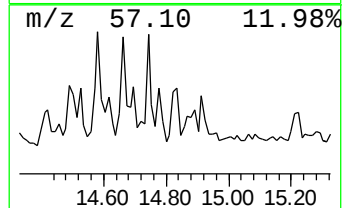
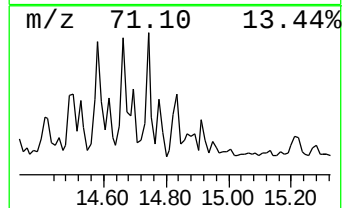
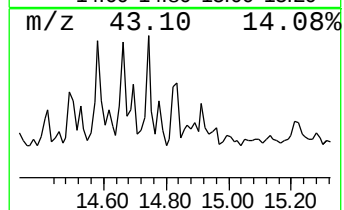
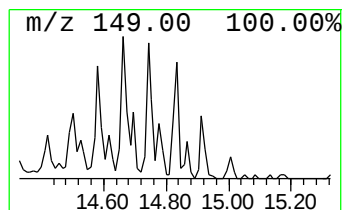
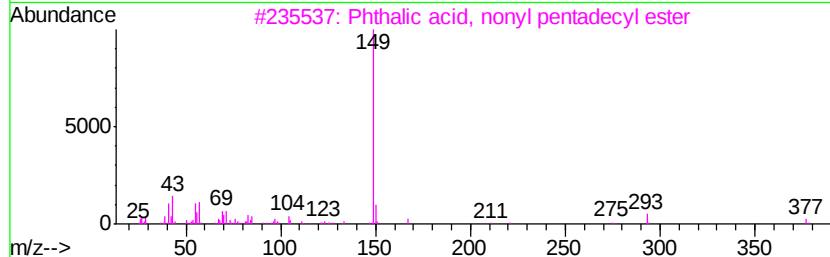
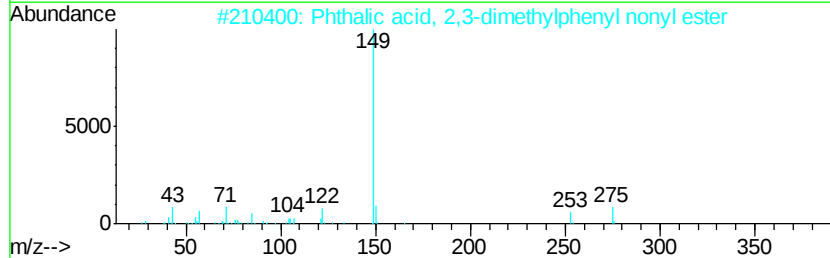
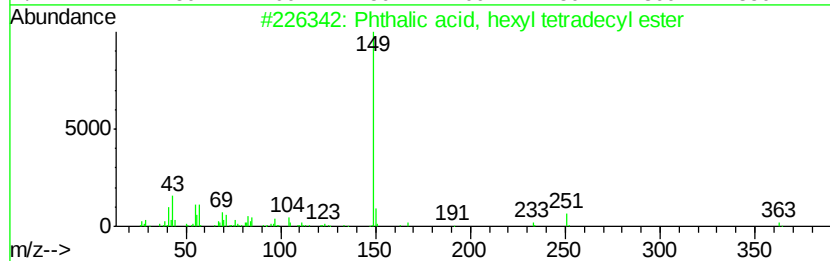
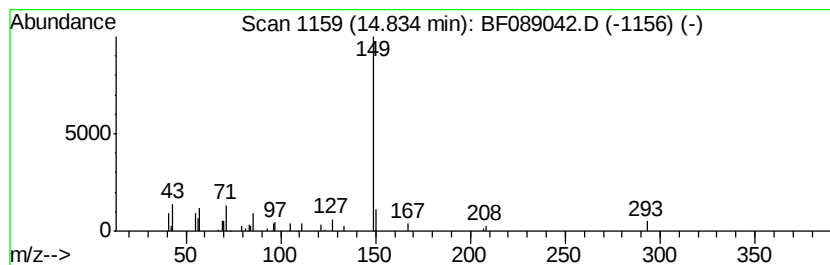
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phthalic acid, hexyl tetrad... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.35 ng	31918	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, hexyl tetradecyl ...	446	C28H46O4	1000308-91-4	72
2		Phthalic acid, 2,3-dimethylphenyl...	396	C25H32O4	1000357-09-1	64
3		Phthalic acid, nonyl pentadecyl ...	502	C32H54O4	1000308-92-7	64
4		1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	64
5		Phthalic acid, 2-ethylbutyl hept...	348	C21H32O4	1000356-89-2	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071516\
Data File : BF089042.D
Acq On : 16 Jul 2016 5:33
Operator : UM/SJ
Sample : H4048-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-07-COMP

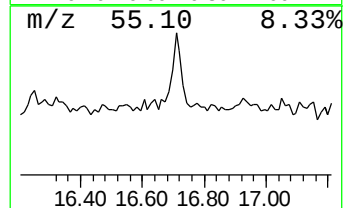
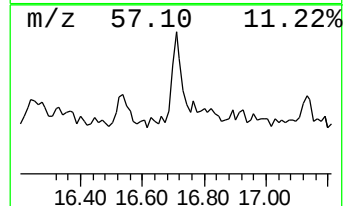
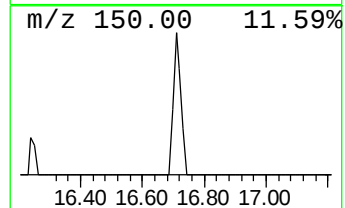
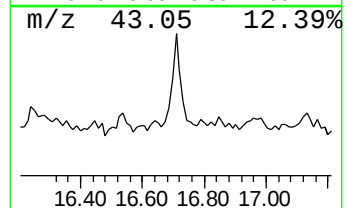
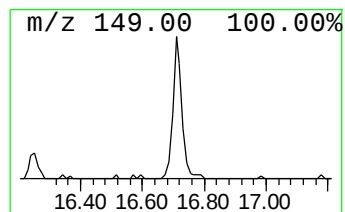
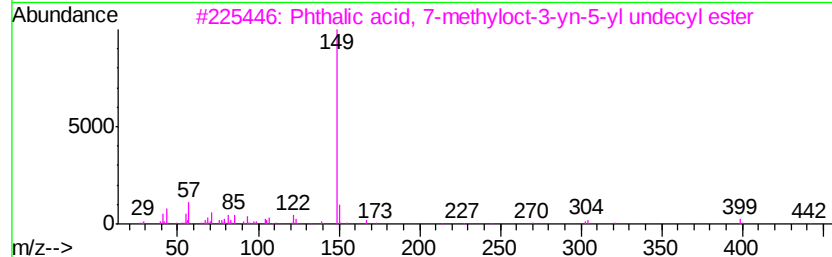
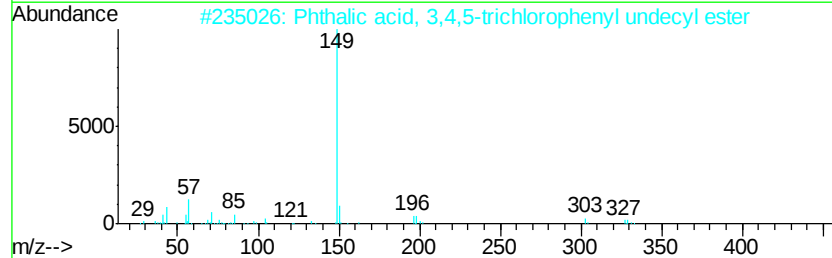
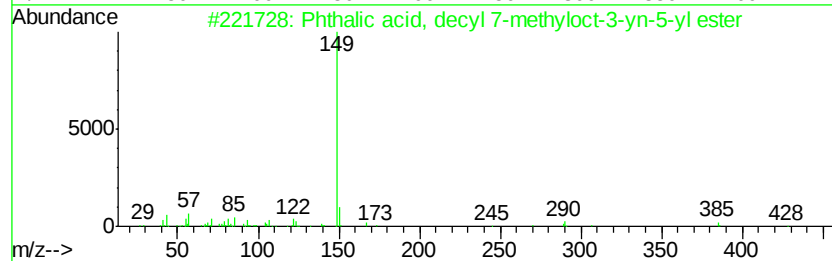
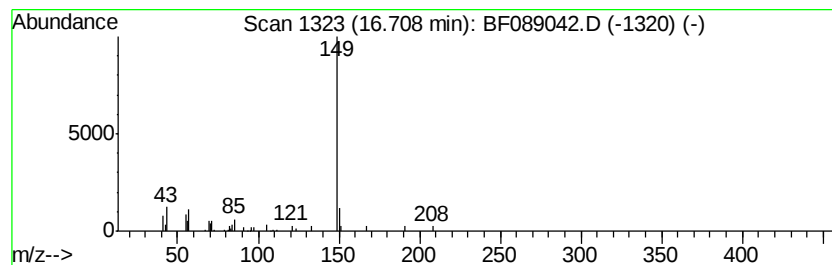
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Phthalic acid, decyl 7-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	5.88 ng	56037	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, decyl 7-methyloct...	428	C27H40O4	1000315-43-2	78
2		Phthalic acid, 3,4,5-trichloroph...	498	C25H29Cl3O4	1000357-07-4	78
3		Phthalic acid, 7-methyloct-3-yn-...	442	C28H42O4	1000315-43-3	78
4		Phthalic acid, dodecyl ethyl ester	362	C22H34O4	1000308-93-4	72
5		Phthalic acid, 5-methylhex-2-yl ...	502	C32H54O4	1000371-07-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071516\
Data File : BF089042.D
Acq On : 16 Jul 2016 5:33
Operator : UM/SJ
Sample : H4048-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
Propane, 1,1-dime...	1.87	5.2	ng	91383	1	6.67	348795	20.0
2-Pentanone, 4-hy...	4.82	9.0	ng	157050	1	6.67	348795	20.0
unknown6.44	6.44	69.6	ng	1214580	1	6.67	348795	20.0
Trichloroacetic a...	13.68	3.7	ng	56918	5	13.81	305503	20.0
Phthalic acid, 2-...	14.50	3.1	ng	29180	6	15.17	190456	20.0
Phthalic acid, no...	14.66	5.9	ng	56406	6	15.17	190456	20.0
Phthalic acid, 3-...	14.74	4.5	ng	42629	6	15.17	190456	20.0
Phthalic acid, he...	14.83	3.4	ng	31918	6	15.17	190456	20.0
Phthalic acid, de...	16.71	5.9	ng	56037	6	15.17	190456	20.0