

Data Path : Z:\HPCHEM1\BNA M\DATA\BM122515\
 Data File : BM003806.D
 Acq On : 25 Dec 2015 08:42
 Operator : UM/SJ
 Sample : G4952-06
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-19

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_M\METHODS\8270-BM120915.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	4.804	286	292	306	rBV	76845	104625	4.63%	0.718%
2	5.269	365	371	384	rBB	452115	651336	28.81%	4.467%
3	6.863	636	642	652	rBV	287356	441080	19.51%	3.025%
4	7.216	696	702	711	rBV	793639	1251144	55.33%	8.580%
5	7.681	775	781	788	rBB	186460	283039	12.52%	1.941%
6	8.004	829	836	845	rBB	692873	1134555	50.18%	7.781%
7	8.839	971	978	988	rBV	555129	916288	40.52%	6.284%
8	10.469	1248	1255	1265	rBV	263101	429211	18.98%	2.944%
9	12.151	1533	1541	1548	rBV4	34340	71087	3.14%	0.488%
10	12.398	1579	1583	1592	rVB4	17431	27875	1.23%	0.191%
11	12.951	1670	1677	1683	rBV	1464868	2197712	97.20%	15.072%
12	12.998	1683	1685	1691	rVB5	17820	26362	1.17%	0.181%
13	13.333	1739	1742	1751	rVB3	14200	24595	1.09%	0.169%
14	13.669	1791	1799	1806	rBV6	15503	44591	1.97%	0.306%
15	13.792	1816	1820	1824	rBV	60026	80087	3.54%	0.549%
16	14.233	1887	1895	1899	rBV4	13318	26476	1.17%	0.182%
17	14.333	1907	1912	1919	rVB2	342996	536605	23.73%	3.680%
18	14.616	1956	1960	1963	rBV	25793	33607	1.49%	0.230%
19	14.651	1963	1966	1970	rVV3	34523	46703	2.07%	0.320%
20	14.716	1970	1977	1987	rVB2	29057	91291	4.04%	0.626%
21	14.821	1987	1995	1998	rBV6	30136	77477	3.43%	0.531%
22	14.886	2003	2006	2011	rVB	62881	88895	3.93%	0.610%
23	15.080	2036	2039	2047	rVB7	25821	45718	2.02%	0.314%
24	15.451	2097	2102	2106	rBV8	11786	26353	1.17%	0.181%
25	15.710	2140	2146	2155	rBV	77972	162115	7.17%	1.112%
26	15.833	2160	2167	2182	rVB	928808	1440796	63.72%	9.881%
27	16.045	2199	2203	2207	rVV3	15550	27716	1.23%	0.190%
28	16.174	2219	2225	2229	rBV8	13723	36073	1.60%	0.247%
29	16.862	2336	2342	2347	rBV4	12797	23371	1.03%	0.160%
30	17.086	2374	2380	2385	rBV2	376457	557033	24.64%	3.820%
31	17.445	2436	2441	2446	rBV	38399	56224	2.49%	0.386%
32	17.980	2528	2532	2536	rBV2	37086	47584	2.10%	0.326%
33	19.356	2763	2766	2771	rBV	26685	35905	1.59%	0.246%
34	19.721	2822	2828	2833	rBV	1818228	2261098	100.00%	15.507%

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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	20.992	3040	3044	3049	rBV	43974	58682	2.60%	0.402%
36	21.286	3088	3094	3099	rBV	474553	617255	27.30%	4.233%
37	23.521	3467	3474	3483	rVB2	315785	600844	26.57%	4.121%

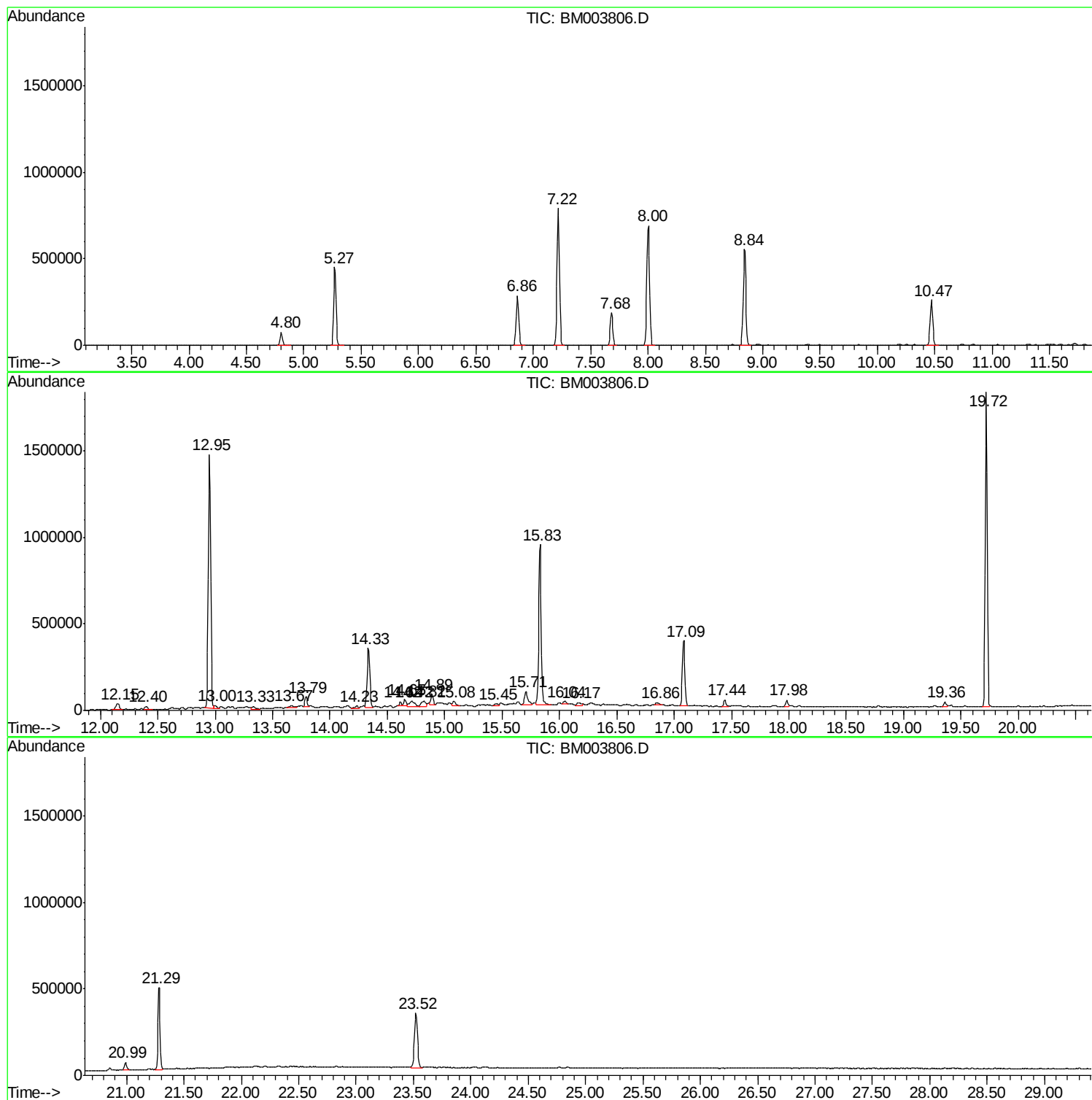
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM120915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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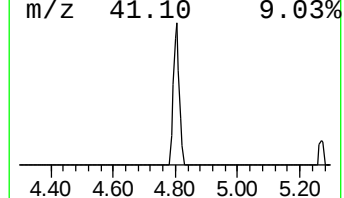
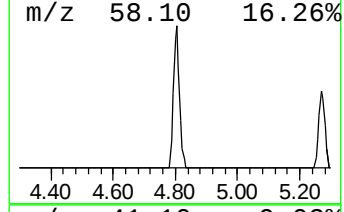
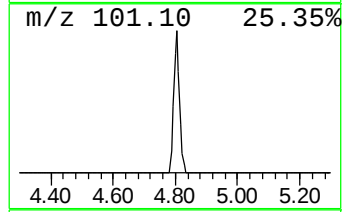
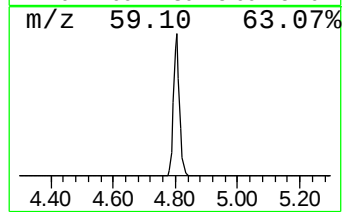
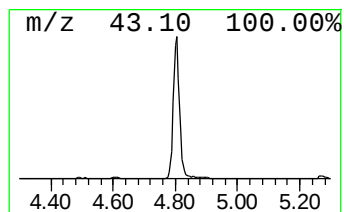
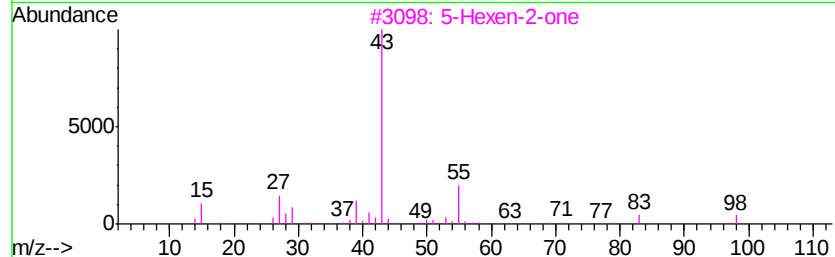
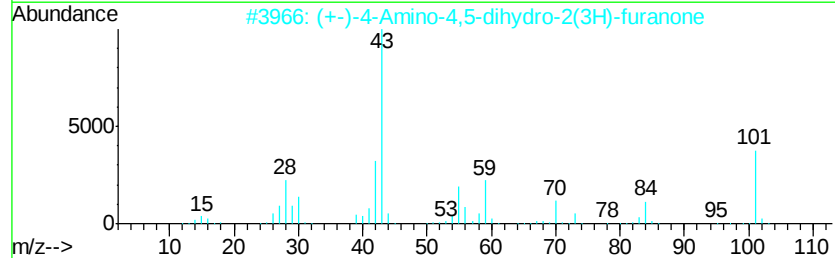
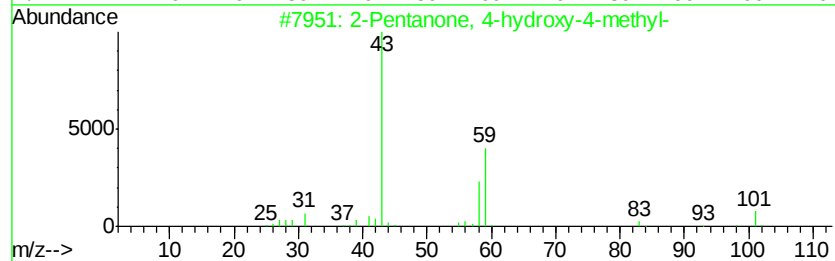
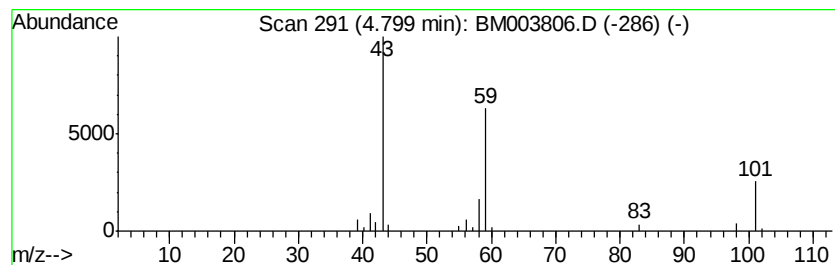
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	7.39 ng	104625	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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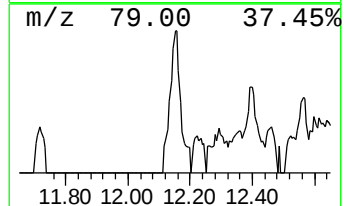
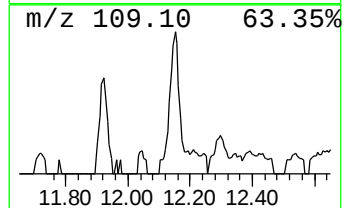
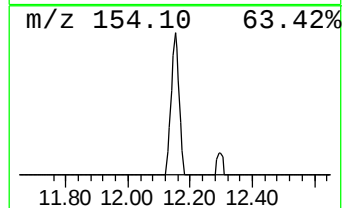
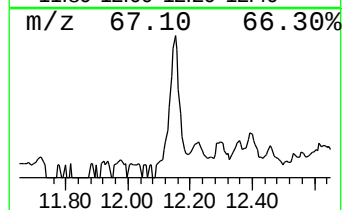
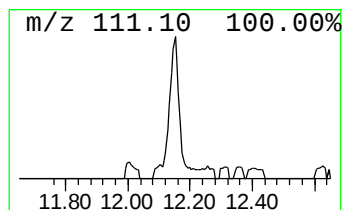
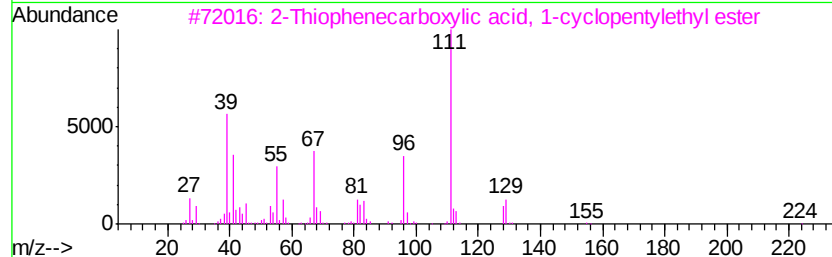
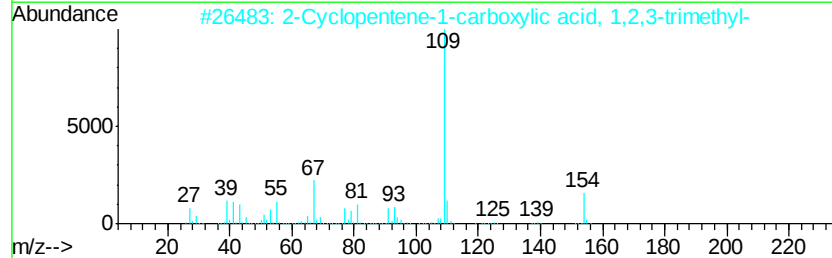
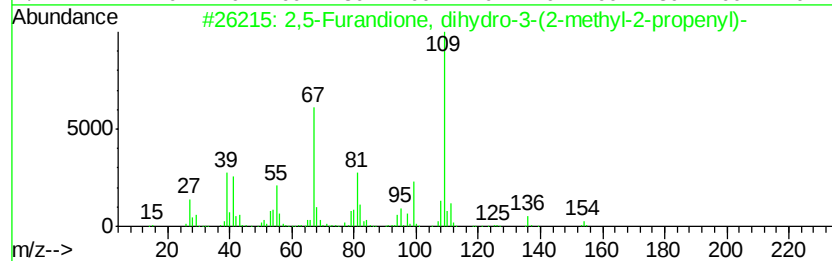
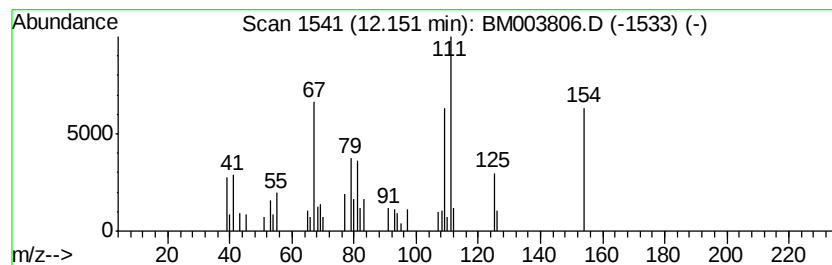
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.15 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	3.31 ng	71087	Napthalene-d8	10.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Furandione, dihydro-3-(2-met...	154	C8H10O3	018908-20-8	35
2		2-Cyclopentene-1-carboxylic acid...	154	C9H14O2	006894-69-5	35
3		2-Thiophenecarboxylic acid, 1-cv...	224	C12H16O2S	1000278-88-4	32
4		Cyclooctene, 3-(2-propenyl)-	150	C11H18	061141-59-1	25
5		2,4,6-Trimethyl-1,5-diazabicyclo...	126	C7H14N2	1000283-21-2	22



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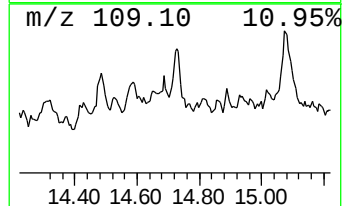
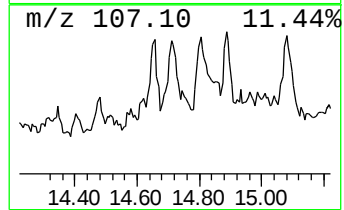
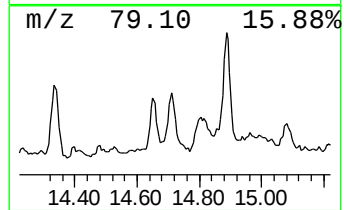
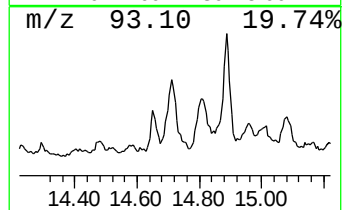
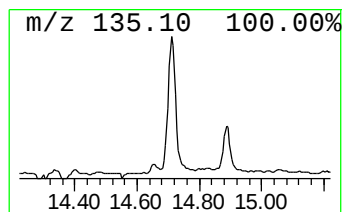
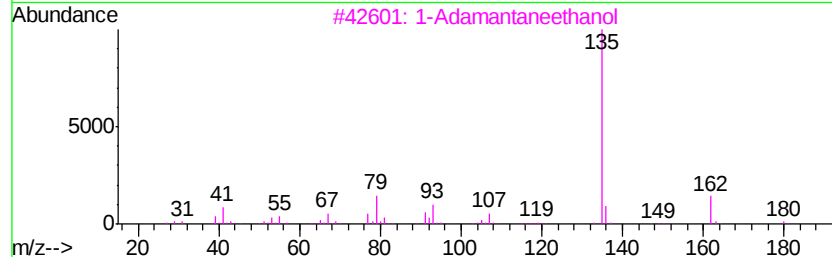
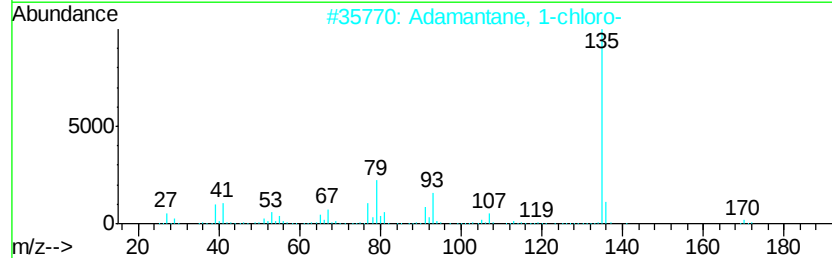
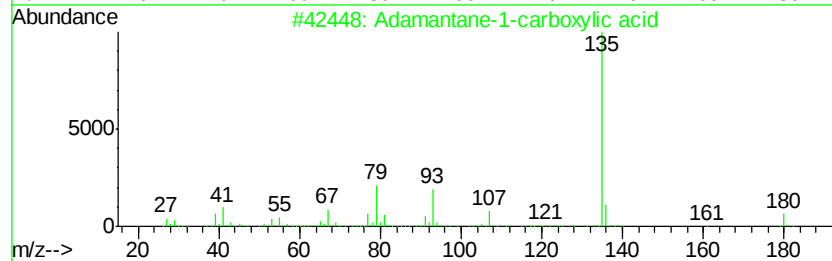
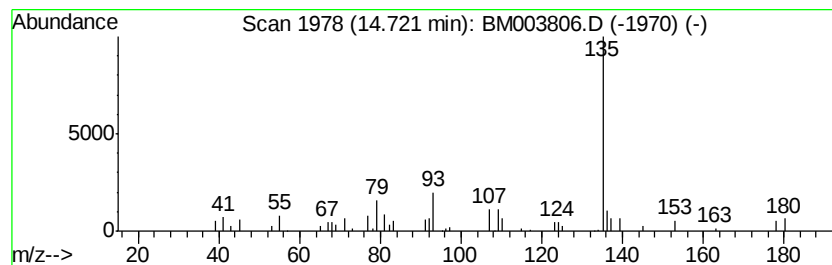
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Adamantane-1-carboxylic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.40 ng	91291	Acenaphthene-d10	14.33

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane-1-carboxylic acid	180	C11H16O2	000828-51-3	87
2	Adamantane, 1-chloro-	170	C10H15Cl	000935-56-8	72
3	1-Adamantaneethanol	180	C12H20O	006240-11-5	72
4	N-Adamantan-1-ylmethyl-2-chloro-...	348	C18H21ClN2O3	227327-87-9	72
5	Trichloroacetic acid, 1-adamanty...	310	C13H17Cl3O2	1000282-92-0	72



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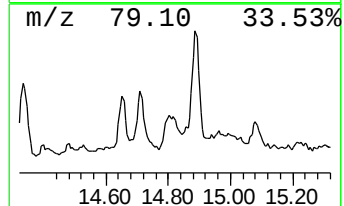
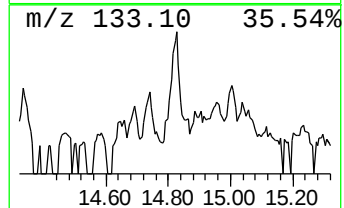
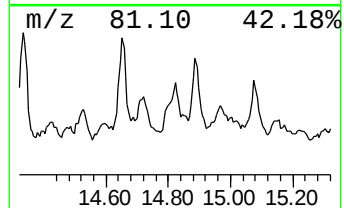
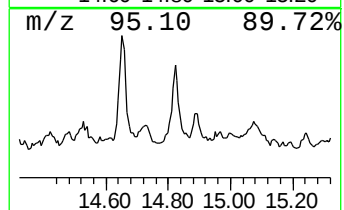
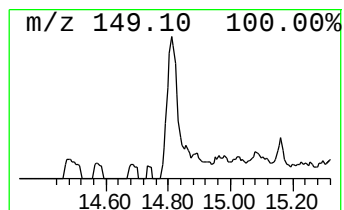
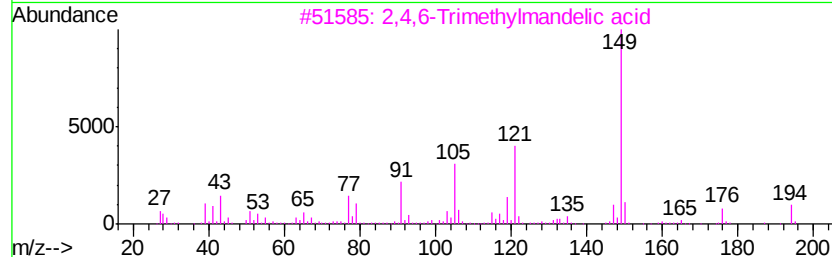
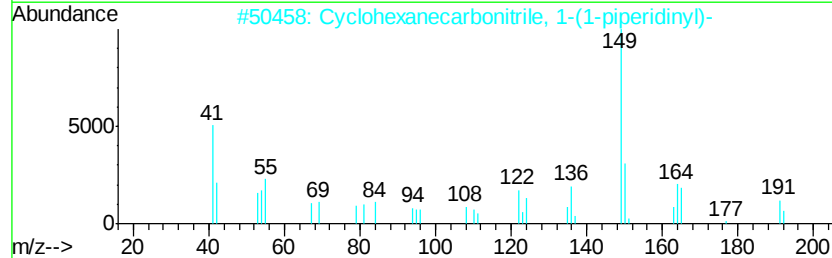
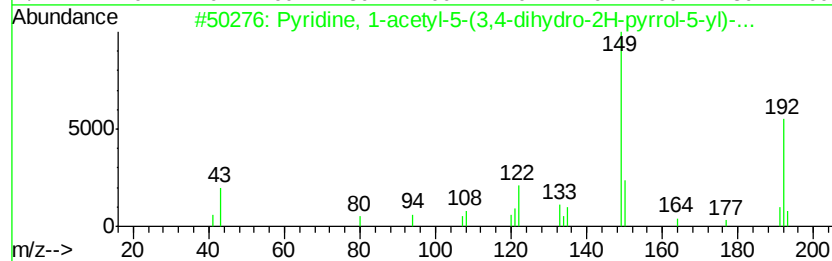
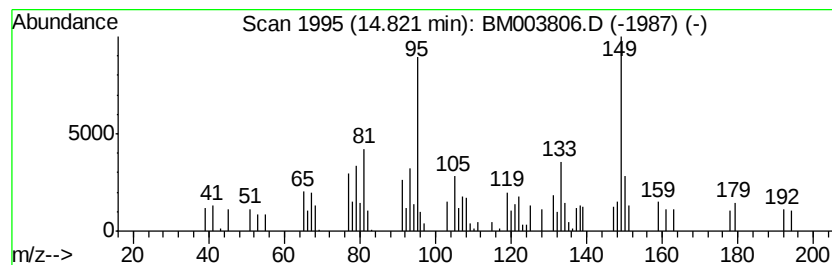
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown14.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	2.89 ng	77477	Acenaphthene-d10	14.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyridine, 1-acetyl-5-(3,4-dihydr...	192 C11H16N2O	054966-57-3 46
2		Cyclohexanecarbonitrile, 1-(1-pi...	192 C12H20N2	003867-15-0 35
3		2,4,6-Trimethylmandelic acid	194 C11H14O3	020797-56-2 27
4		1,3-Dioxolane, 2-phenyl-	150 C9H10O2	000936-51-6 22
5		Pyridine, 1-oxide	95 C5H5NO	000694-59-7 18



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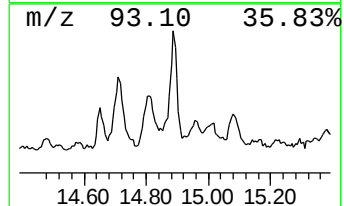
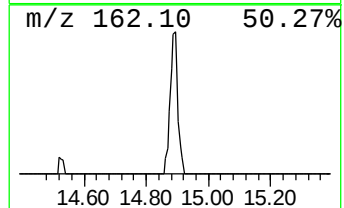
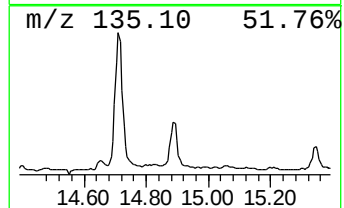
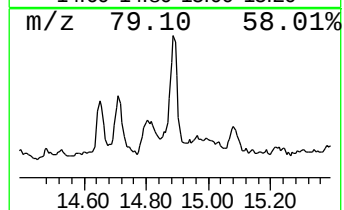
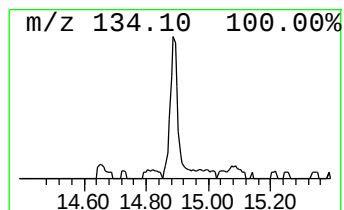
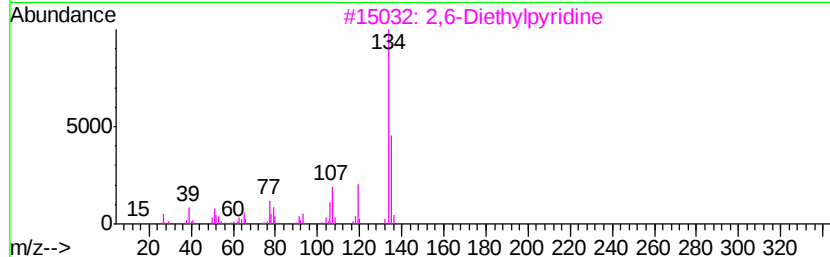
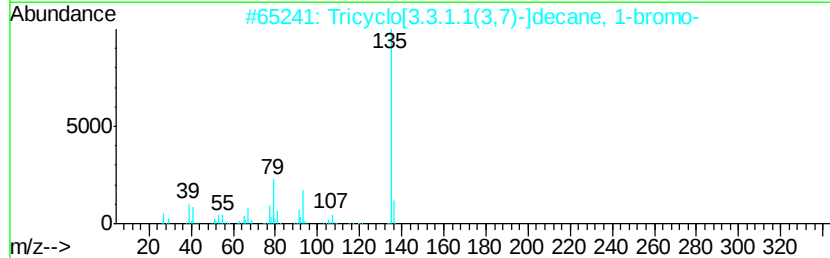
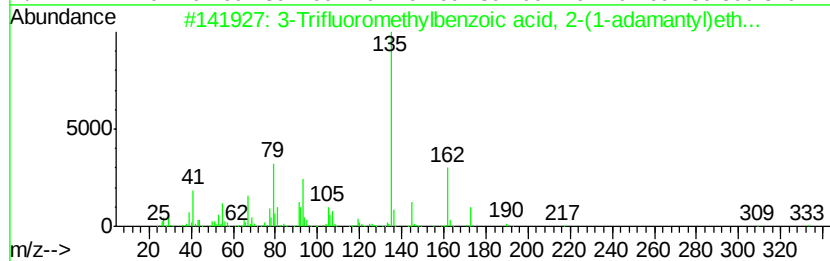
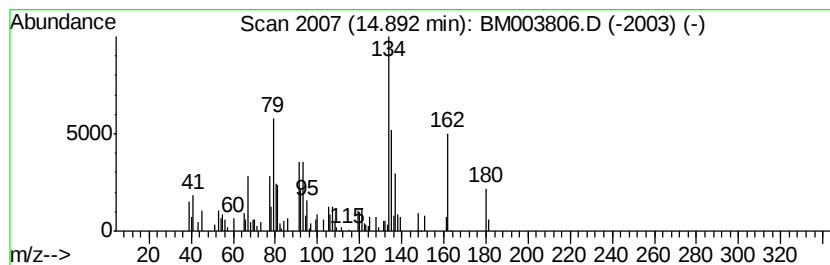
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ClientSampled :
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Peak Number 7 unknown14.89 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.89	3.31 ng	88895	Acenaphthene-d10	14.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Trifluoromethylbenzoic acid, 2...	352	C20H23F3O2	1000282-87-7	35
2	Tricyclo[3.3.1.1(3,7)]decane, 1...	214	C10H15Br	000768-90-1	30
3	2,6-Diethylpvridine	135	C9H13N	000935-28-4	30
4	Phosphonic dichloride, 1-adamantyl-	252	C10H15Cl2OP	1000294-15-7	27
5	2-[1-(Adamantan-1-ylamino)-2,2,2...	295	C15H16F3N3	1000275-90-9	27



Data Path : Z:\HPCHEM1\BNA M\DATA\BM122515\
Data File : BM003806.D
Acq On : 25 Dec 2015 08:42
Operator : UM/SJ
Sample : G4952-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampled :
MW-19

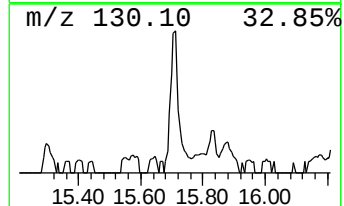
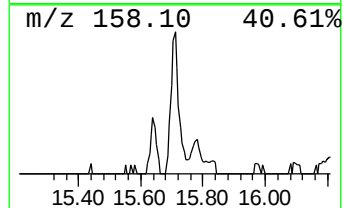
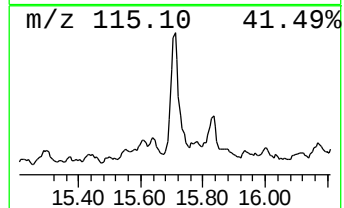
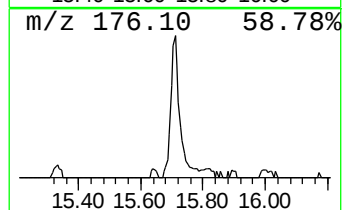
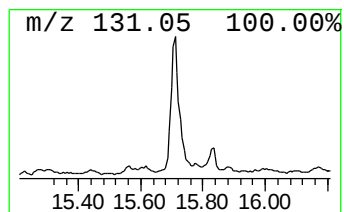
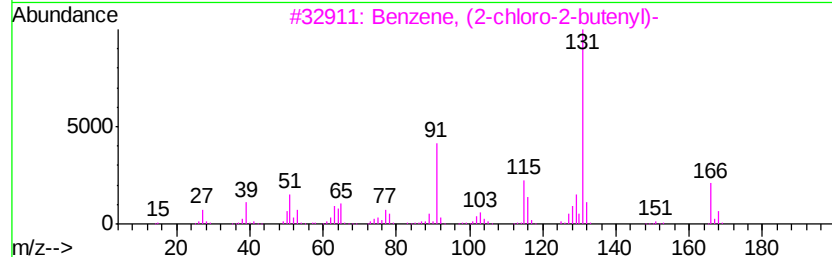
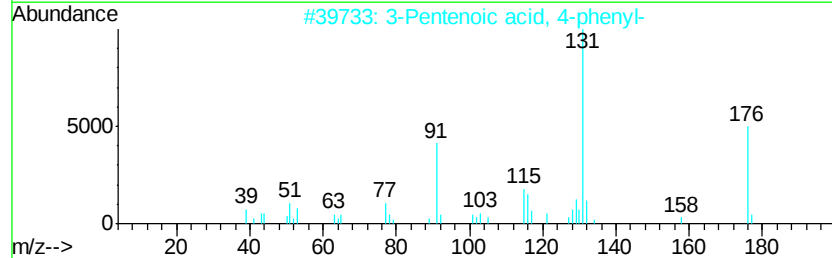
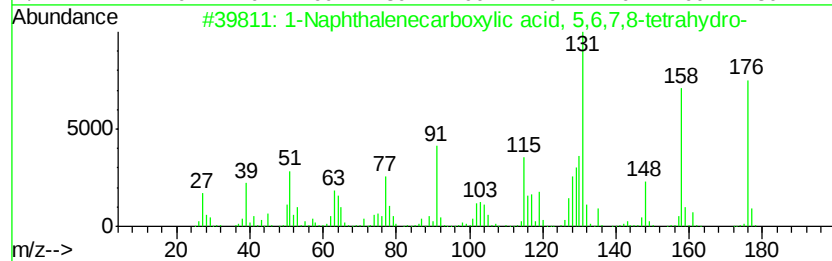
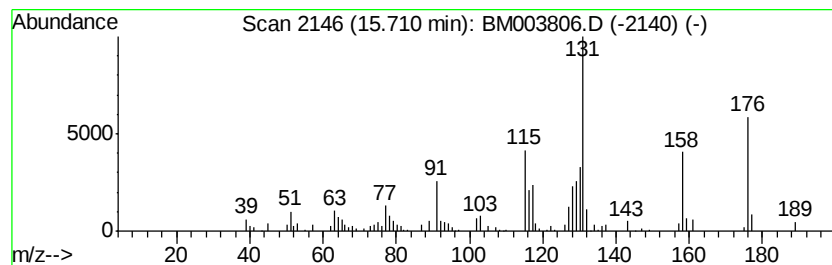
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Naphthalenecarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	5.82 ng	162115	Phenanthrene-d10	17.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	95
2		3-Pentenoic acid, 4-phenyl-	176	C11H12O2	053774-19-9	43
3		Benzene, (2-chloro-2-butenyl)-	166	C10H11Cl	054411-12-0	35
4		Cinnamic acid, .alpha.,.beta.-di...	176	C11H12O2	1000151-56-4	35
5		Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	32



Data Path : Z:\HPCHEM1\BNA M\DATA\BM122515\
Data File : BM003806.D
Acq On : 25 Dec 2015 08:42
Operator : UM/SJ
Sample : G4952-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-19

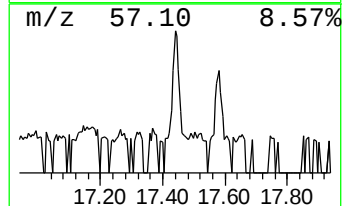
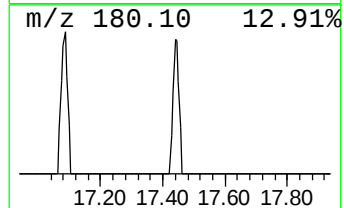
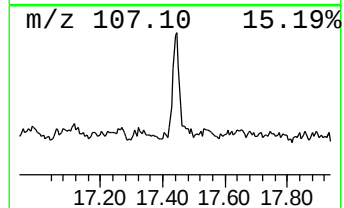
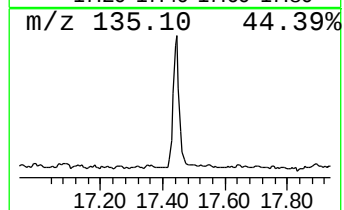
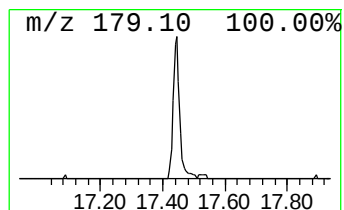
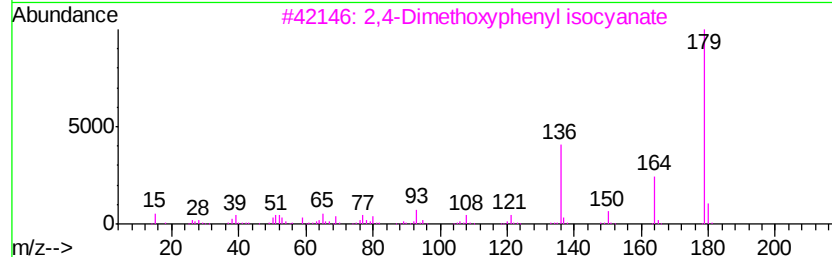
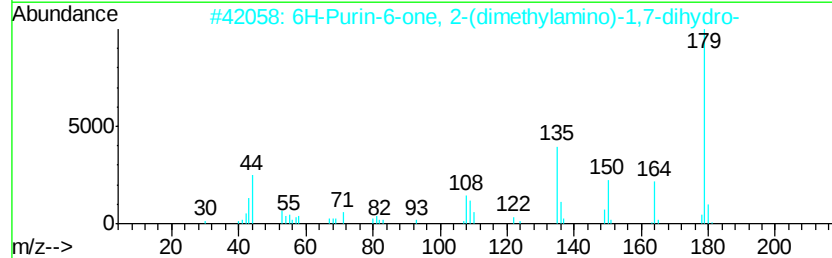
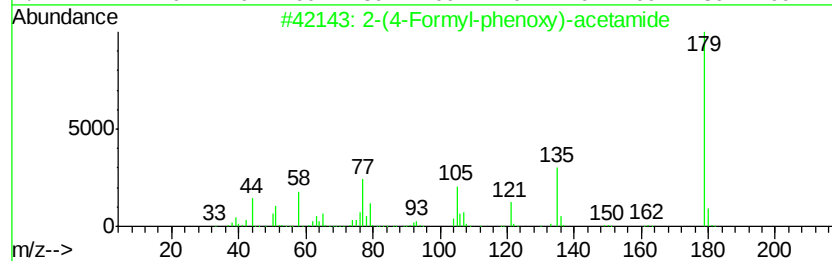
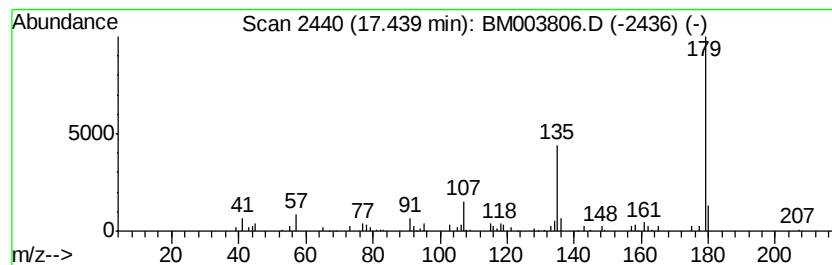
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM120915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-(4-Formyl-phenoxy)-acetamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	2.02 ng	56224	Phenanthrene-d10	17.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-(4-Formyl-phenoxy)-acetamide	179	C9H9NO3	135857-20-4	53
2		6H-Purin-6-one, 2-(dimethylamino...	179	C7H9N5O	001445-15-4	45
3		2,4-Dimethoxyphenyl isocyanate	179	C9H9NO3	084370-87-6	43
4		4,2-Cresotic acid, 6-methoxy-, b...	538	C29H30O10	019314-74-0	38
5		4-Butylbenzoic acid, octadecyl e...	430	C29H50O2	1000292-33-0	37



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM122515\
Data File : BM003806.D
Acq On : 25 Dec 2015 08:42
Operator : UM/SJ
Sample : G4952-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-19

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM120915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	7.4	ng	104625	1	7.68	283039	20.0
unknown12.15	12.15	3.3	ng	71087	2	10.47	429211	20.0
Adamantane-1-carb...	14.72	3.4	ng	91291	3	14.33	536605	20.0
unknown14.82	14.82	2.9	ng	77477	3	14.33	536605	20.0
unknown14.89	14.89	3.3	ng	88895	3	14.33	536605	20.0
1-Naphthalenecarb...	15.71	5.8	ng	162115	4	17.08	557033	20.0
2-(4-Formyl-pheno...	17.44	2.0	ng	56224	4	17.08	557033	20.0