

Data Path : Z:\HPCHEM1\BNA_F\Data\BF052115\
 Data File : BF079423.D
 Acq On : 22 May 2015 3:21
 Operator : TP/IZ
 Sample : G2289-13
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-31S

Integration Parameters: rteint.p

Integrator: RTE

Soothing : 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-BF043015.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF079423.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.335	10	13	25	rVB2	151487	504828	6.93%	1.430%
2	1.495	25	27	30	rVB	317701	364647	5.00%	1.033%
3	1.610	36	37	46	rVV	823909	1358782	18.65%	3.849%
4	1.724	46	47	78	rVB	3630246	7286083	100.00%	20.641%
5	4.810	315	317	324	rBV	137482	201536	2.77%	0.571%
6	5.347	362	364	367	rBV	1815457	1959340	26.89%	5.551%
7	6.650	475	478	480	rBV	2000499	2113810	29.01%	5.988%
8	6.776	487	489	492	rBV	1607197	2124533	29.16%	6.019%
9	7.073	513	515	517	rBV	321889	369668	5.07%	1.047%
10	7.256	528	531	533	rBV	1710462	1602203	21.99%	4.539%
11	7.770	573	576	578	rBV	1191396	1301141	17.86%	3.686%
12	8.650	650	653	655	rBV	433584	506129	6.95%	1.434%
13	9.999	768	771	773	rBV	2128530	2460356	33.77%	6.970%
14	10.502	813	815	818	rBV	150957	142455	1.96%	0.404%
15	10.811	840	842	845	rVB	477811	536754	7.37%	1.521%
16	11.794	925	928	931	rBV	1587657	1658665	22.76%	4.699%
17	12.651	1001	1003	1004	rBV	615887	598311	8.21%	1.695%
18	12.685	1004	1006	1008	rVV	413302	468810	6.43%	1.328%
19	12.742	1009	1011	1015	rVB	124355	147934	2.03%	0.419%
20	13.314	1060	1061	1064	rVB	80070	75572	1.04%	0.214%
21	13.417	1068	1070	1071	rBV	77038	103934	1.43%	0.294%
22	14.159	1132	1135	1137	rBV	684118	851422	11.69%	2.412%
23	14.434	1156	1159	1161	rBV	782932	851414	11.69%	2.412%
24	14.651	1175	1178	1180	rBV	2559120	2805023	38.50%	7.947%
25	14.857	1191	1196	1198	rVB2	62508	119200	1.64%	0.338%
26	14.982	1205	1207	1212	rBV2	66505	104535	1.43%	0.296%
27	15.657	1264	1266	1269	rVV2	49042	89416	1.23%	0.253%
28	15.828	1278	1281	1286	rBV	116530	220002	3.02%	0.623%
29	15.931	1286	1290	1292	rVV2	758216	1272394	17.46%	3.605%
30	15.965	1292	1293	1295	rVV	310407	296628	4.07%	0.840%
31	17.200	1399	1401	1407	rBV	292941	632822	8.69%	1.793%
32	17.508	1426	1428	1432	rVB	143430	210757	2.89%	0.597%
33	17.577	1432	1434	1437	rBV	268518	322578	4.43%	0.914%
34	17.634	1437	1439	1448	rVB2	560156	791054	10.86%	2.241%
35	18.697	1527	1532	1540	rVB6	29555	125992	1.73%	0.357%
36	18.834	1540	1544	1550	rVB3	22726	75077	1.03%	0.213%
37	18.983	1554	1557	1562	rVB2	113714	243208	3.34%	0.689%

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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-BF043015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

38	19.154	1569	1572	1574	rBV	34504	78157	1.07%	0.221%
39	19.371	1588	1591	1600	rVB	109918	235352	3.23%	0.667%
40	19.589	1608	1610	1619	rVB2	27935	87852	1.21%	0.249%

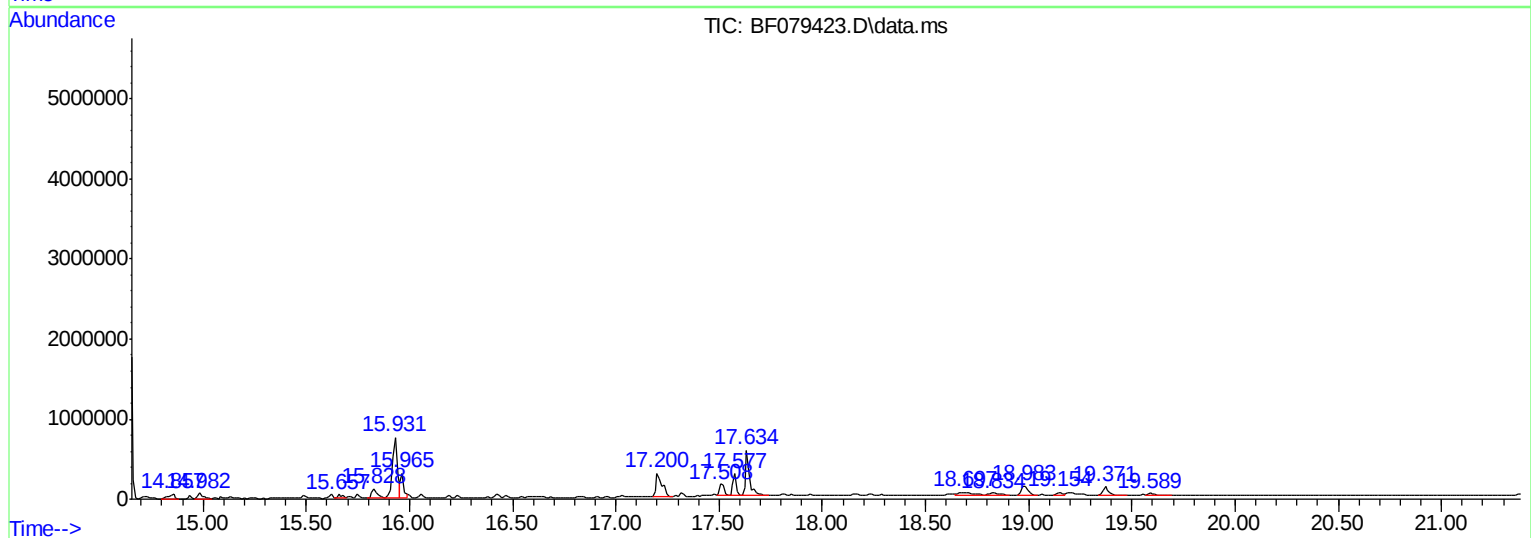
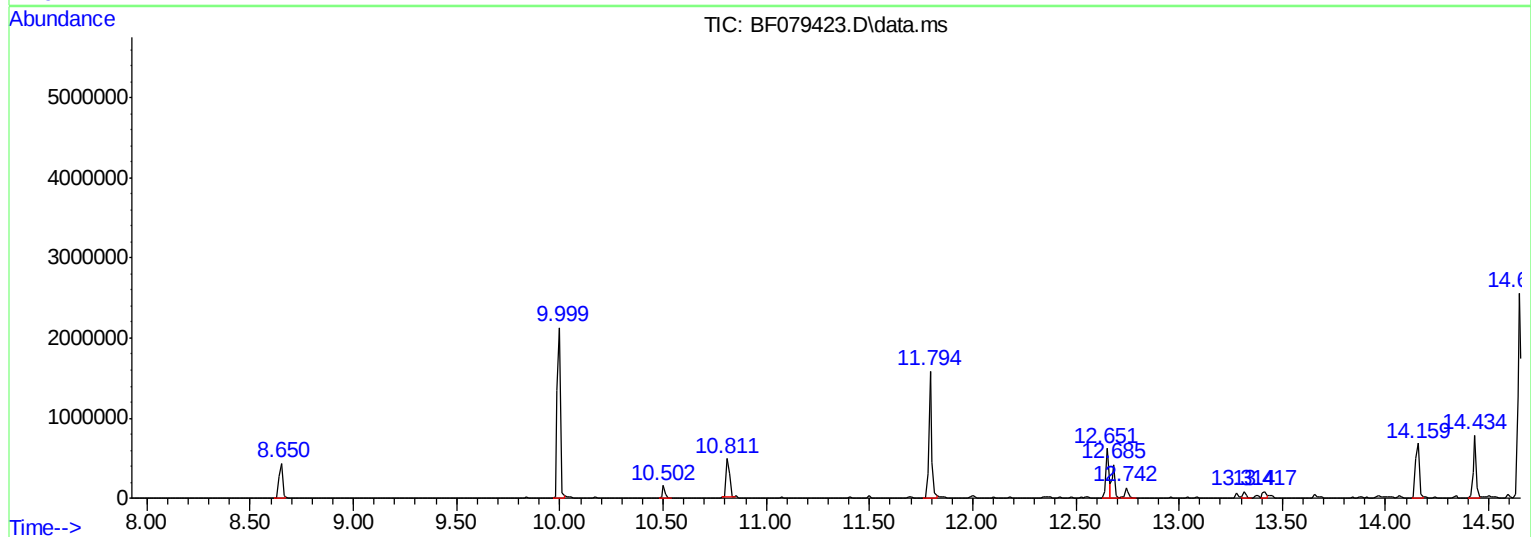
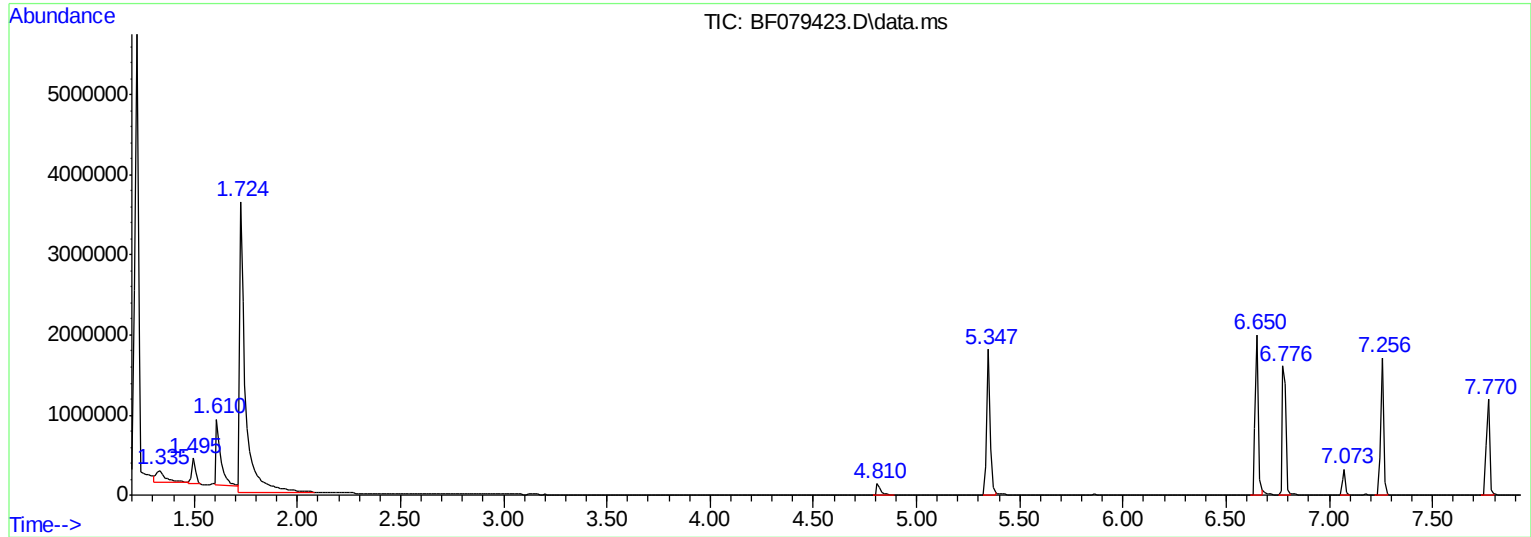
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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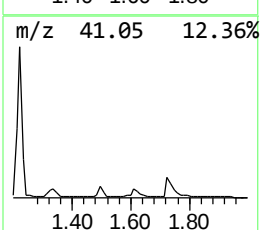
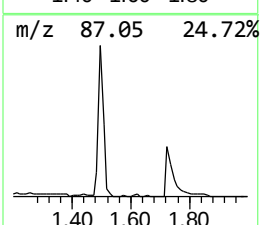
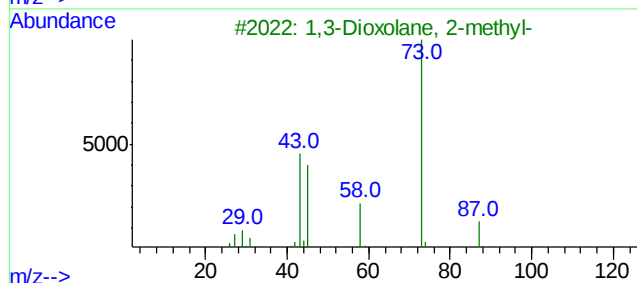
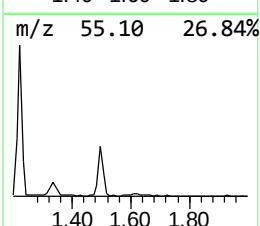
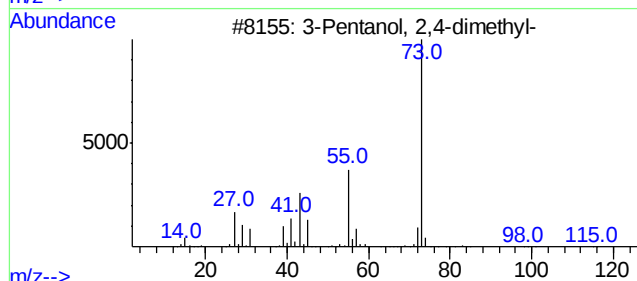
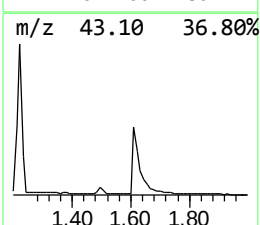
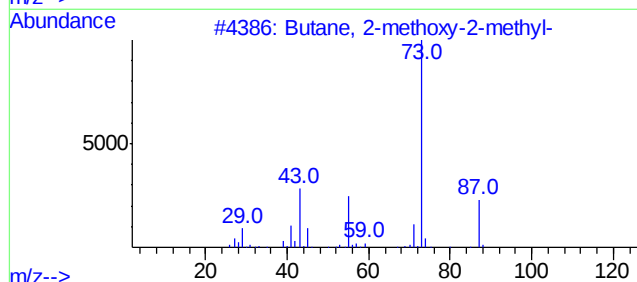
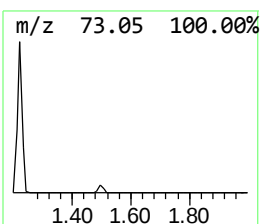
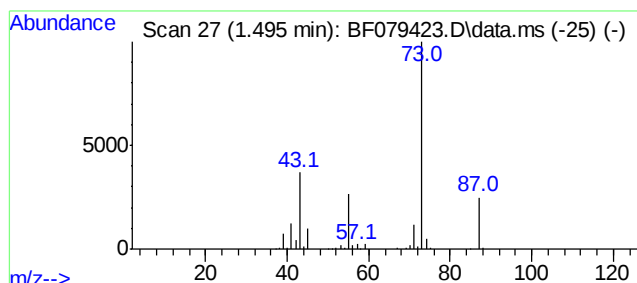
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.495	19.73 ng	364647	1,4-Dichlorobenzene-d4	7.073

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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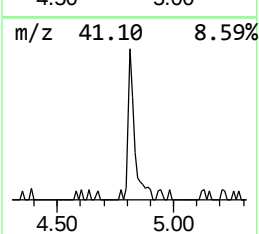
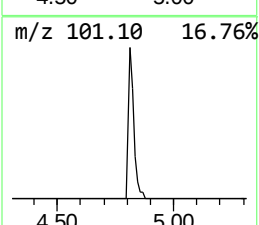
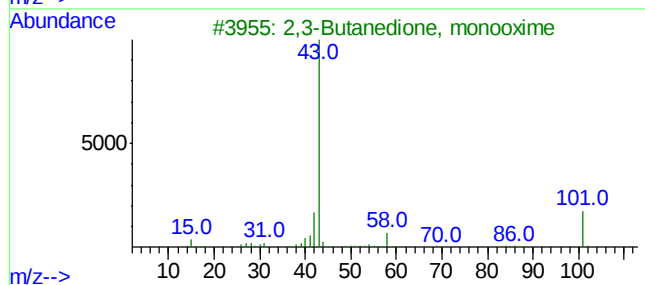
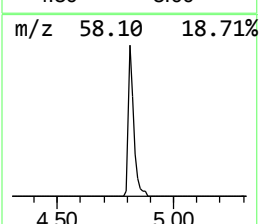
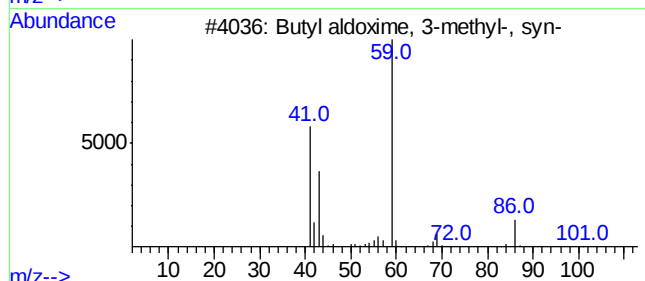
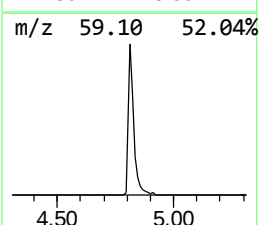
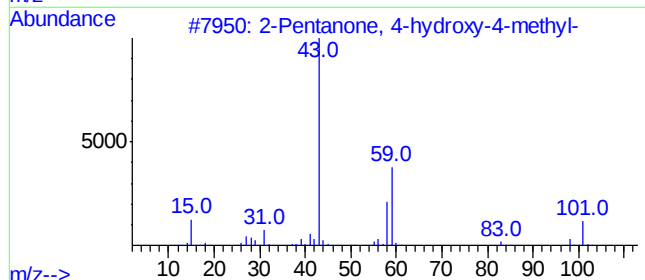
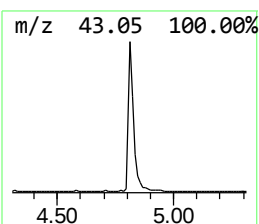
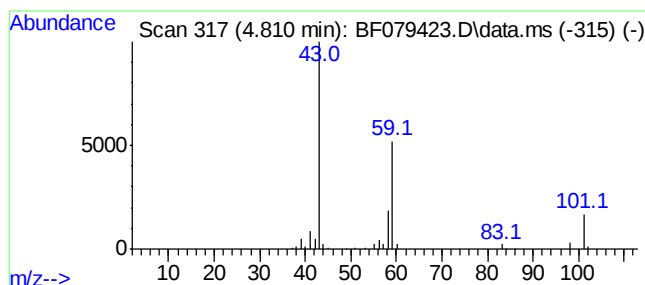
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.810	10.90 ng	201536	1,4-Dichlorobenzene-d4	7.073

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	59
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO		005780-40-5	23
3	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	16
4	Acetone	58	C3H6O		000067-64-1	12
5	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	10



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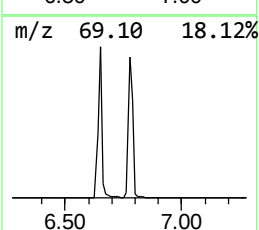
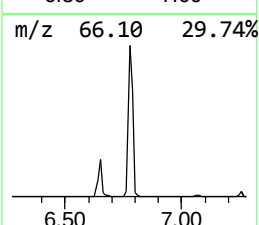
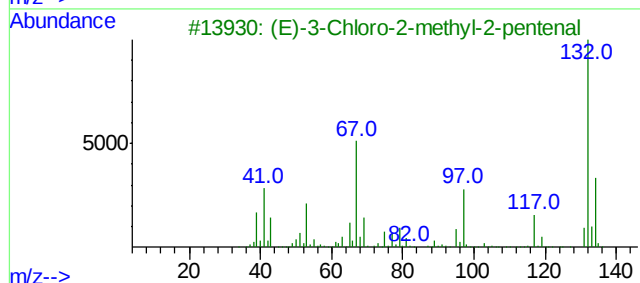
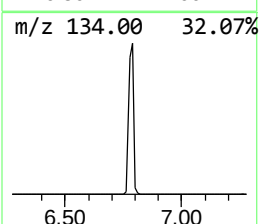
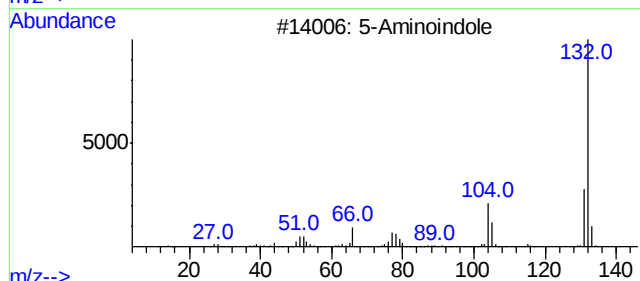
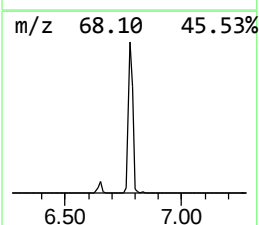
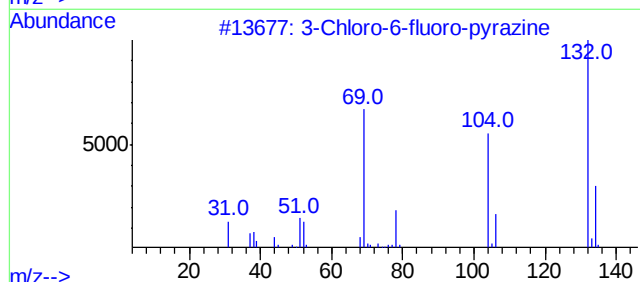
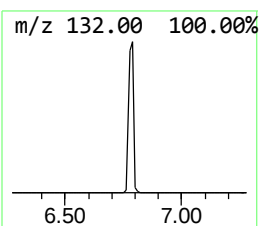
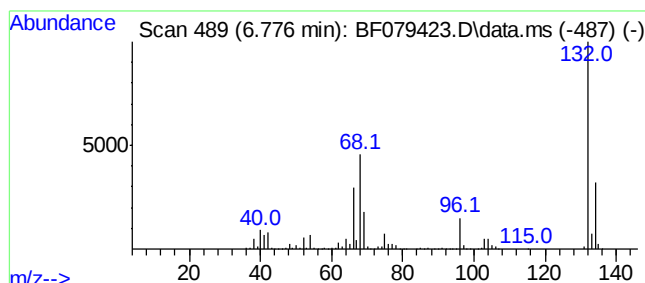
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.776 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.776	114.94 ng	2124530	1,4-Dichlorobenzene-d4	7.073

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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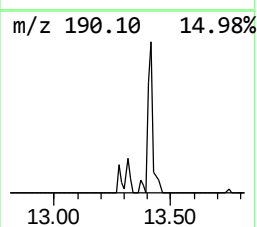
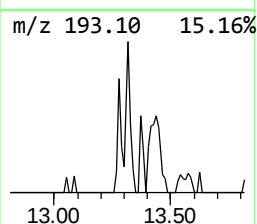
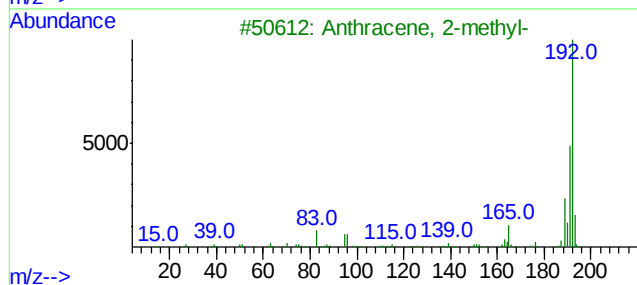
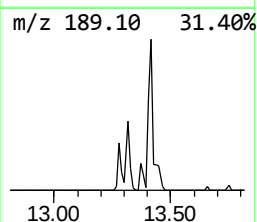
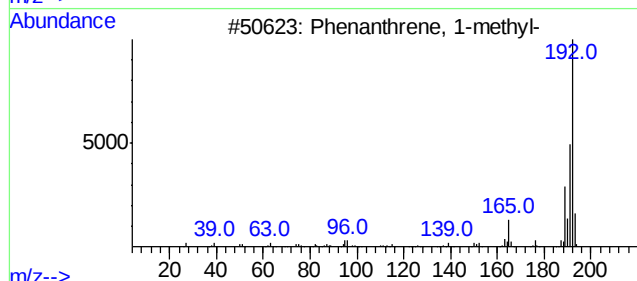
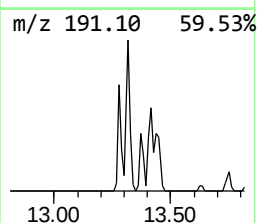
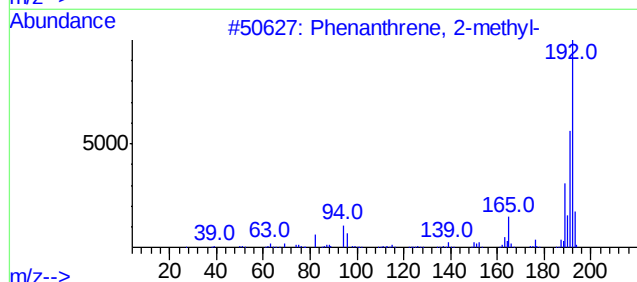
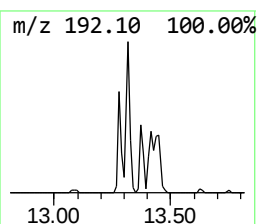
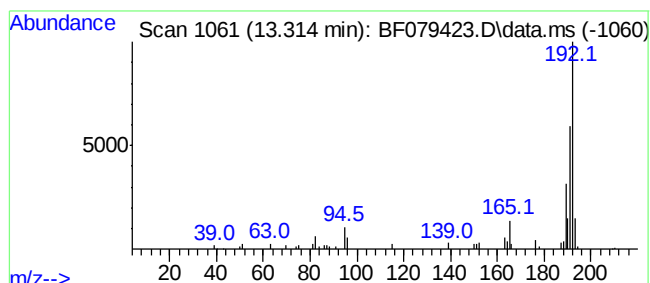
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Phenanthrene, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.314	2.53 ng	75572	Phenanthrene-d10	12.651

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97	
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97	
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95	
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95	
5	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	95	



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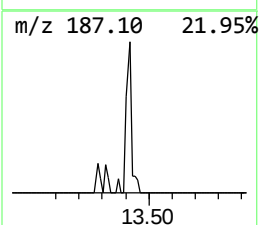
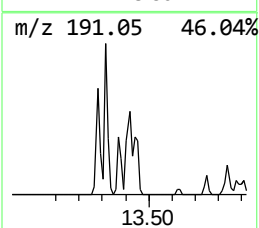
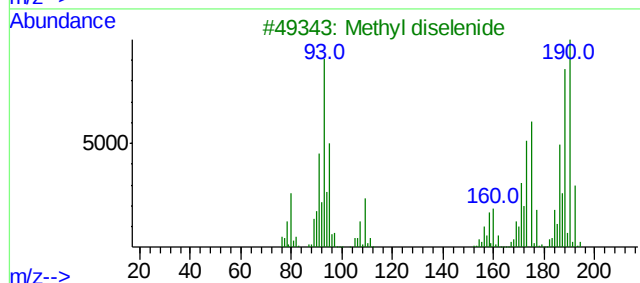
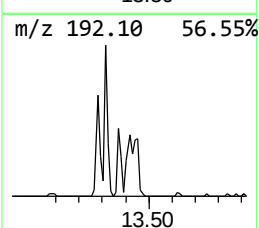
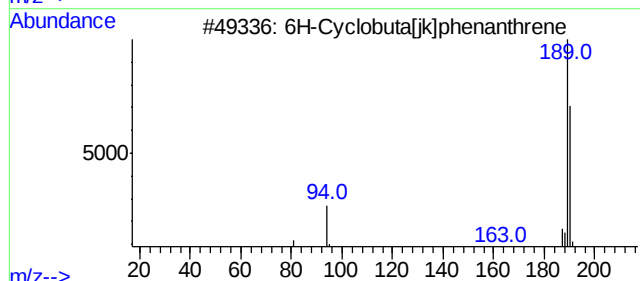
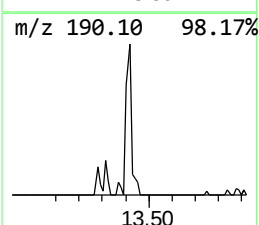
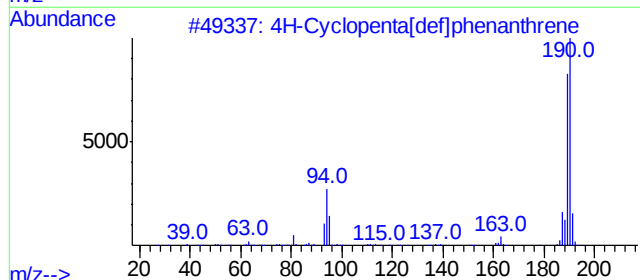
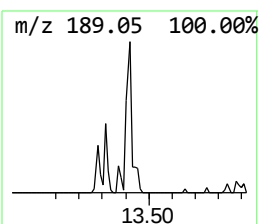
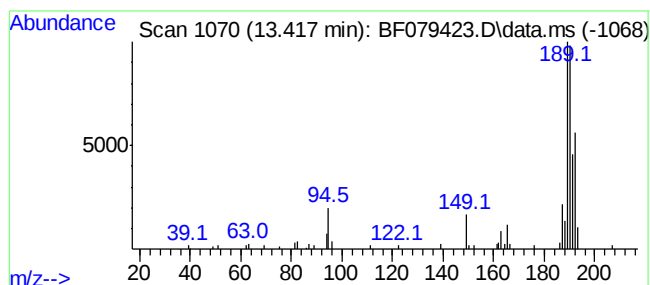
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.416	3.47 ng	103934	Phenanthrene-d10	12.651

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62	
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58	
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43	
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30	
5	Benzene, 1,1'-(1,2-propadienyld...	192	C15H12	014251-57-1	25	



Data Path : Z:\HPCHEM1\BNA_F\Data\BF052115\
Data File : BF079423.D
Acq On : 22 May 2015 3:21
Operator : TP/IZ
Sample : G2289-13
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-31S

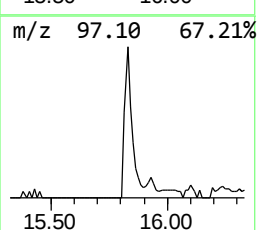
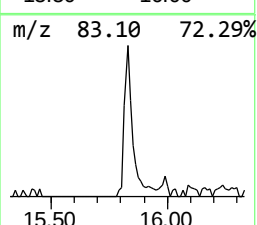
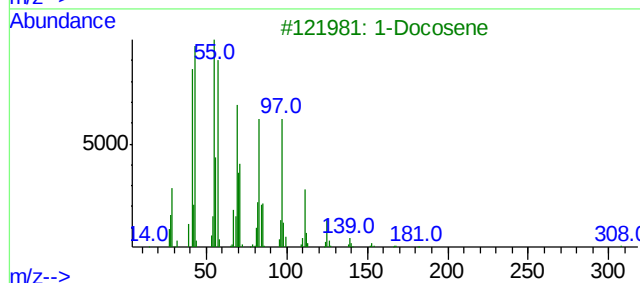
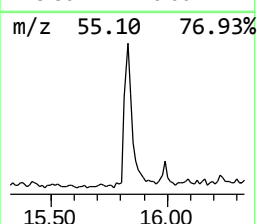
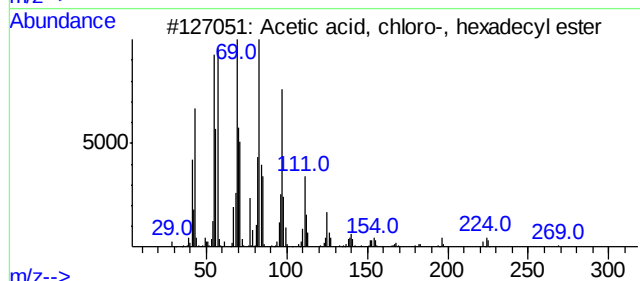
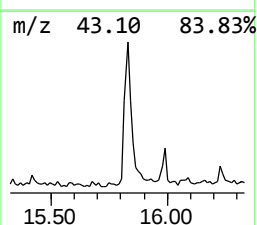
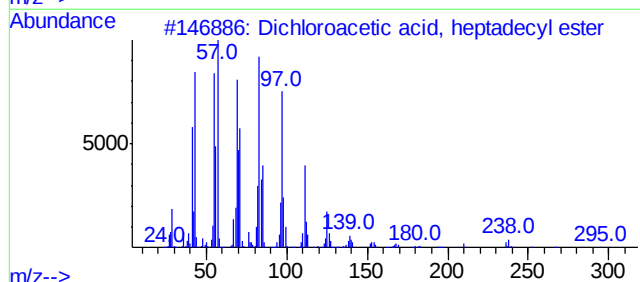
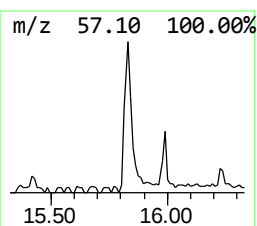
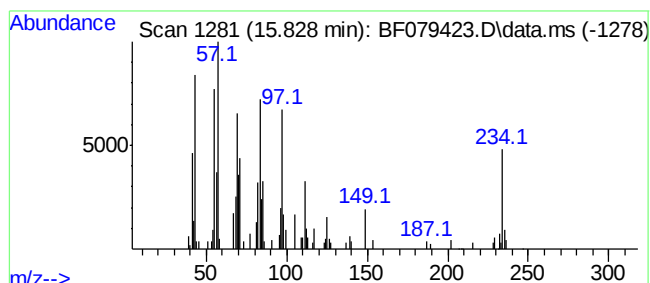
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dichloroacetic acid, heptad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.828	3.46 ng	220002	Chrysene-d12	15.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	76
3	1-Docosene	308	C22H44	001599-67-3	76
4	1-Hexacosanol	382	C26H54O	000506-52-5	70
5	1-Tetracosanol	354	C24H50O	000506-51-4	70



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Sample : G2289-13
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ALS Vial : 20 Sample Multiplier: 1

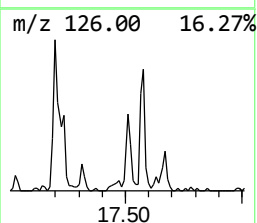
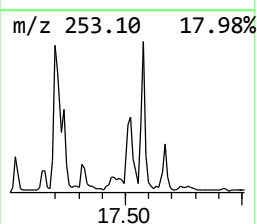
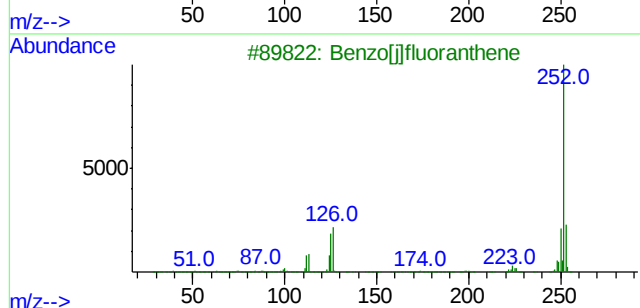
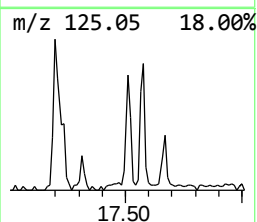
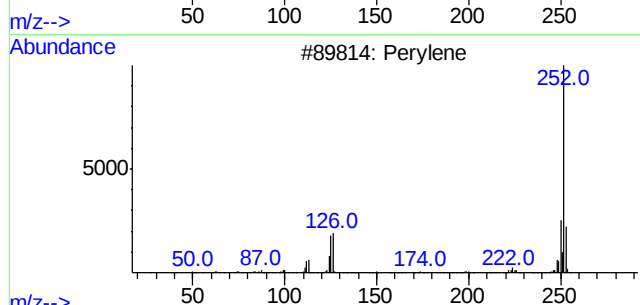
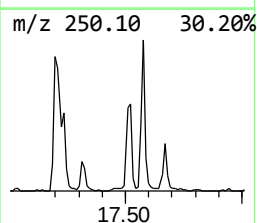
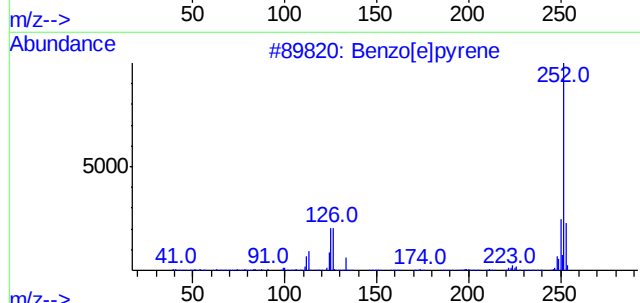
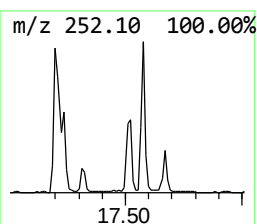
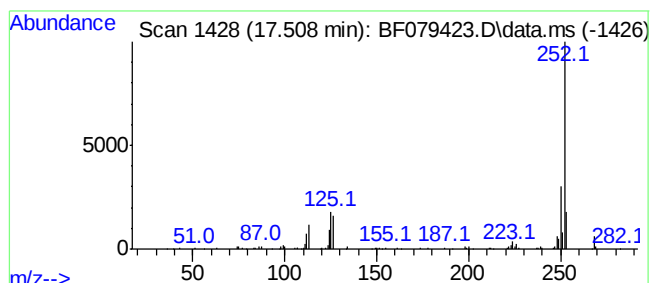
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.508	5.33 ng	210757	Perylene-d12	17.634	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	98
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	89



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-31S

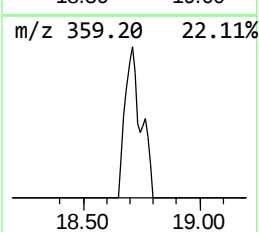
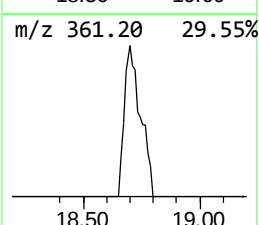
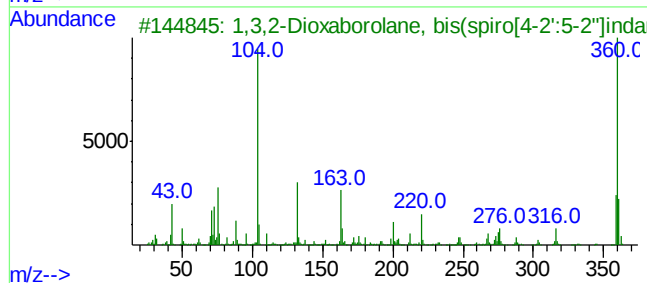
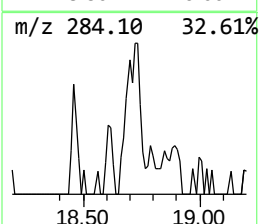
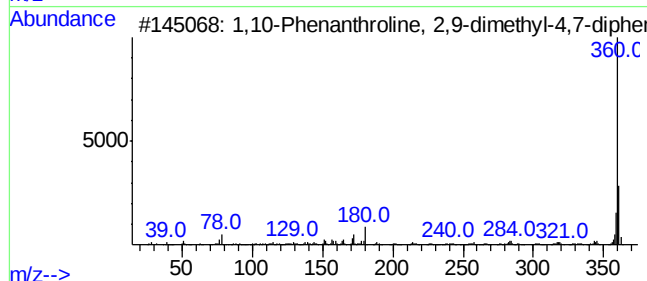
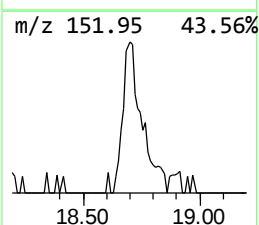
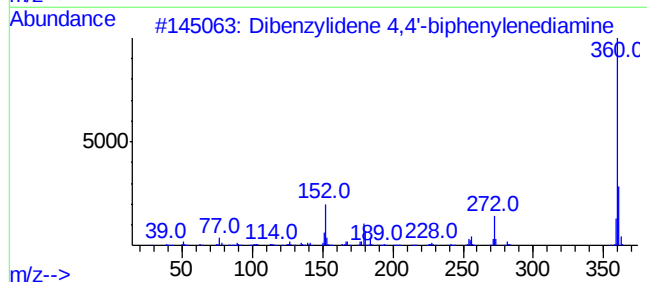
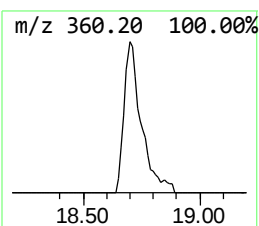
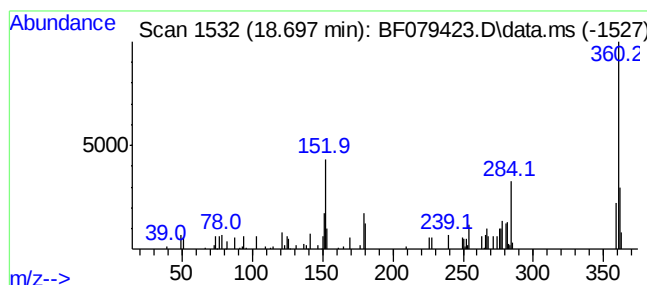
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Dibenzylidene 4,4'-biphenyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.697	3.19 ng	125992	Perylene-d12	17.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	64
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	46
3	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
4	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
5	[2-(4-Methoxy-phenyl)-2H-benzo[g...	360	C22H20N2O3	1000188-59-8	35



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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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
Butane, 2-metho...	1.495	19.7	ng	364647	1	7.073	369668	20.0
2-Pentanone, 4-...	4.810	10.9	ng	201536	1	7.073	369668	20.0
unknown6.776	6.776	114.9	ng	2124530	1	7.073	369668	20.0
Phenanthrene, 2...	13.314	2.5	ng	75572	4	12.651	598311	20.0
4H-Cyclopenta[d...	13.416	3.5	ng	103934	4	12.651	598311	20.0
Dichloroacetic ...	15.828	3.5	ng	220002	5	15.931	1272390	20.0
Benzo[e]pyrene	17.508	5.3	ng	210757	6	17.634	791054	20.0
Dibenzylidene 4...	18.697	3.2	ng	125992	6	17.634	791054	20.0