

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
 Data File : BF089061.D
 Acq On : 16 Jul 2016 18:12
 Operator : UM/SJ
 Sample : H3989-13
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 U3-B2(0-11)C

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	1.644	4	5	14	rVB	136112	223221	12.25%	1.279%
2	1.770	14	16	21	rVV	549398	892540	48.98%	5.115%
3	1.838	21	22	45	rVB	62006	201659	11.07%	1.156%
4	2.810	104	107	115	rBV	10385	27475	1.51%	0.157%
5	4.810	280	282	290	rBV	113329	196699	10.79%	1.127%
6	5.267	319	322	324	rBV	1562464	1575379	86.45%	9.029%
7	6.330	411	415	417	rBV	1474975	1822226	100.00%	10.443%
8	6.444	422	425	427	rBV	1576582	1798168	98.68%	10.305%
9	6.662	442	444	446	rBB	323307	319544	17.54%	1.831%
10	6.822	456	458	461	rVB	1361916	1194413	65.55%	6.845%
11	7.233	491	494	497	rBV	866489	880892	48.34%	5.048%
12	7.953	554	557	559	rBV	517036	461491	25.33%	2.645%
13	9.028	649	651	654	rVB	1164006	1649795	90.54%	9.455%
14	9.428	684	686	688	rBV	260840	216329	11.87%	1.240%
15	9.702	708	710	712	rBV	458052	407367	22.36%	2.335%
16	10.251	751	758	761	rBV	17672	23499	1.29%	0.135%
17	10.491	777	779	782	rBV	761353	752126	41.28%	4.310%
18	10.628	789	791	794	rBV	19568	30752	1.69%	0.176%
19	11.074	828	830	831	rBV2	30234	28365	1.56%	0.163%
20	11.188	837	840	843	rBV	265562	517278	28.39%	2.965%
21	11.256	843	846	848	rVV	68370	58032	3.18%	0.333%
22	11.496	865	867	870	rBV2	21176	25739	1.41%	0.148%
23	11.679	881	883	885	rBV	23923	33592	1.84%	0.193%
24	11.714	885	886	887	rVB	40567	27829	1.53%	0.159%
25	11.794	891	893	897	rBV2	59532	77522	4.25%	0.444%
26	11.908	900	903	905	rBV3	13999	22702	1.25%	0.130%
27	11.976	907	909	910	rBV2	19974	23178	1.27%	0.133%
28	12.239	930	932	933	rBV	18188	21732	1.19%	0.125%
29	12.274	933	935	938	rVB3	13398	22156	1.22%	0.127%
30	12.399	943	946	947	rBV	257243	348978	19.15%	2.000%
31	12.617	962	965	967	rBV	355859	398490	21.87%	2.284%
32	12.765	976	978	981	rVB	807229	1150707	63.15%	6.595%
33	12.834	981	984	988	rBV3	22577	60945	3.34%	0.349%
34	12.948	990	994	996	rVV	52634	80154	4.40%	0.459%

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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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.017	997	1000	1001	rVV	44347	52903	2.90%	0.303%
36	13.051	1001	1003	1007	rVB2	42402	59741	3.28%	0.342%
37	13.165	1012	1013	1015	rBV	15664	23546	1.29%	0.135%
38	13.314	1024	1026	1028	rBV2	32939	49595	2.72%	0.284%
39	13.565	1045	1048	1049	rBV2	29537	55930	3.07%	0.321%
40	13.680	1055	1058	1061	rBV3	44571	76826	4.22%	0.440%
41	13.805	1066	1069	1074	rBV2	342918	723560	39.71%	4.147%
42	14.811	1154	1157	1161	rVB	162568	317310	17.41%	1.819%
43	15.074	1178	1180	1183	rVB	92267	125672	6.90%	0.720%
44	15.131	1183	1185	1187	rVB	82992	111266	6.11%	0.638%
45	15.188	1187	1190	1193	rBV2	170447	281481	15.45%	1.613%

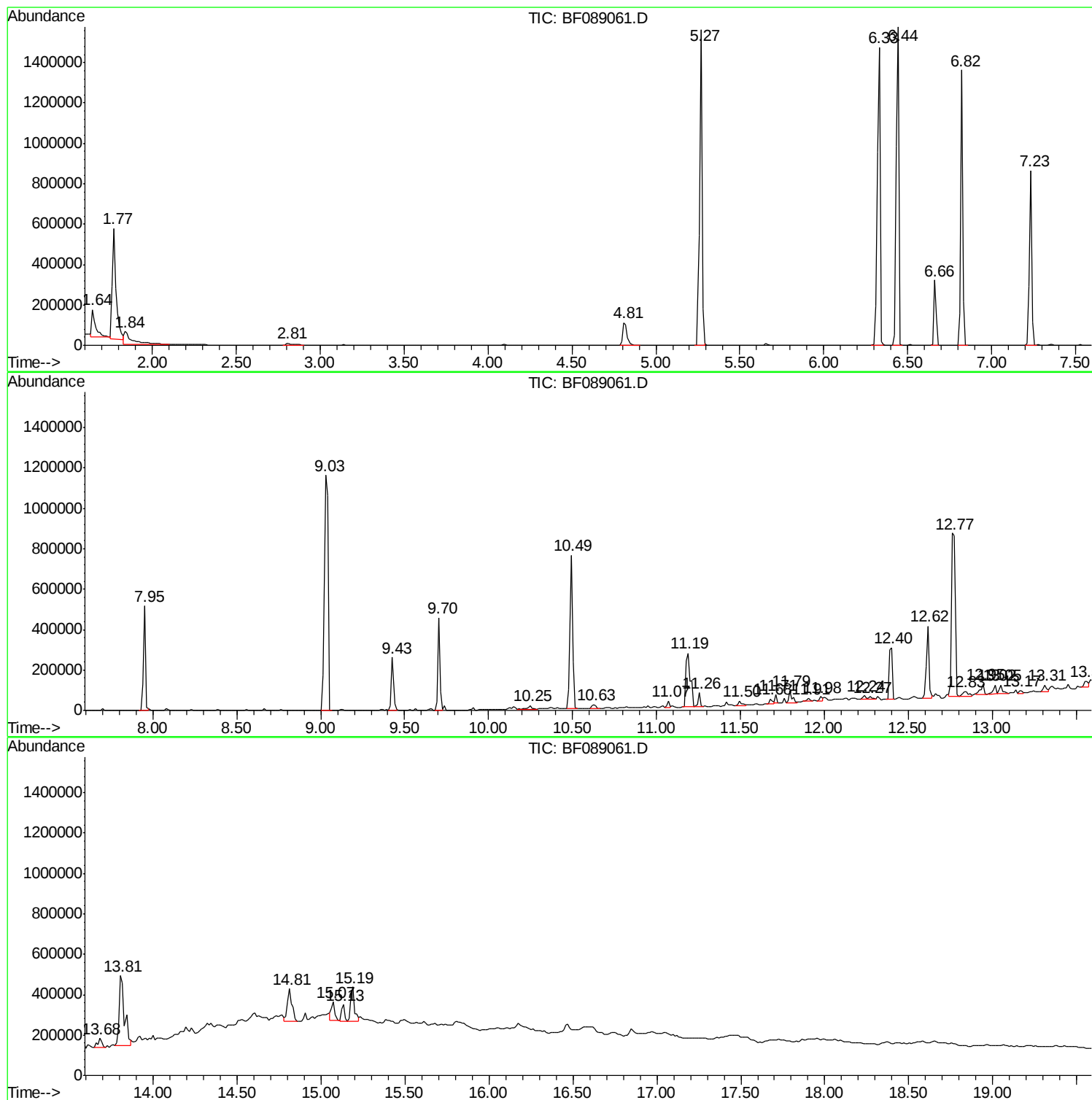
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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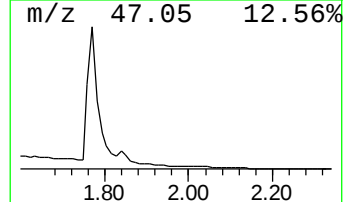
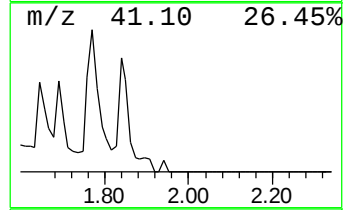
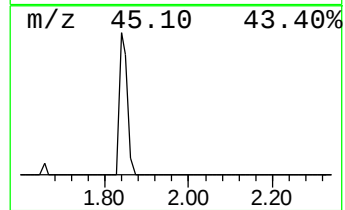
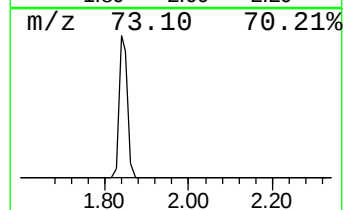
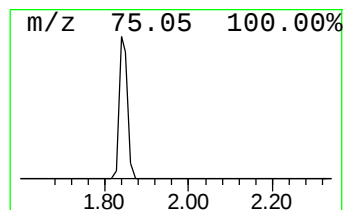
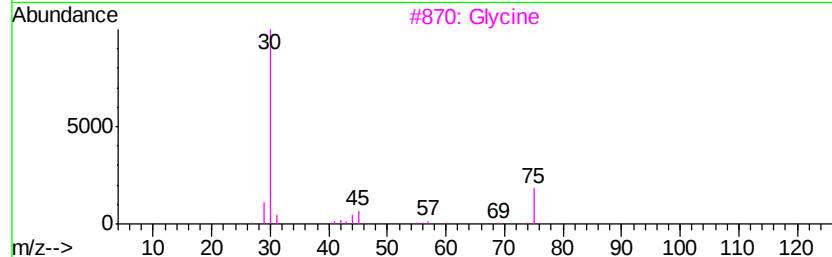
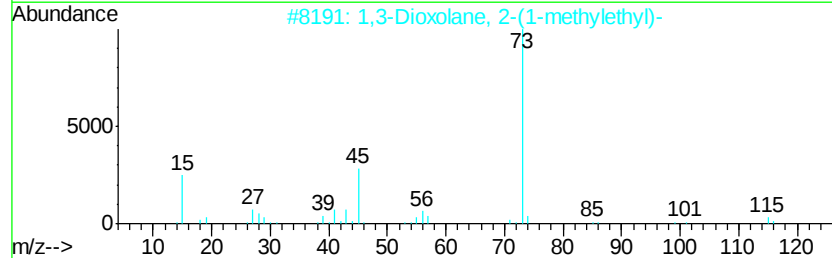
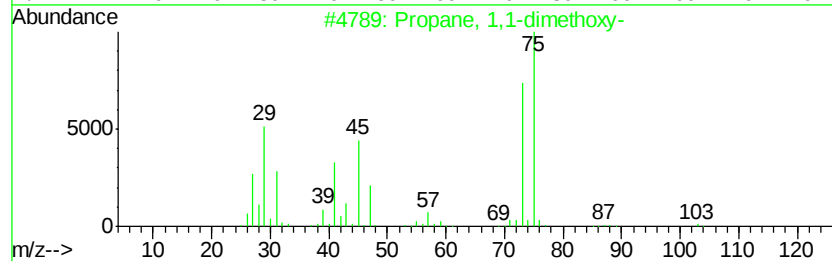
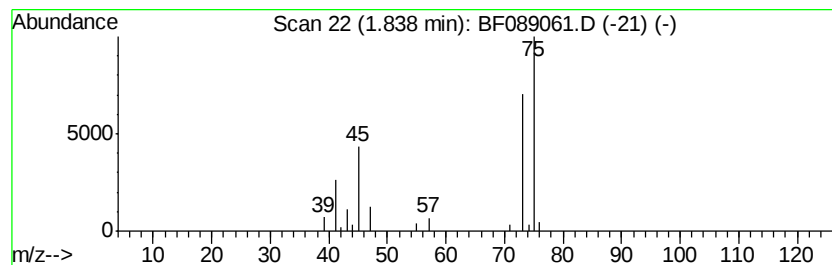
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown1.84 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.84	12.62 ng	201659	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
3		Glycine	75	C2H5NO2	000056-40-6	7
4		Methanamine, N,N-dimethyl-, N-oxide	75	C3H9NO	001184-78-7	5
5		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	4



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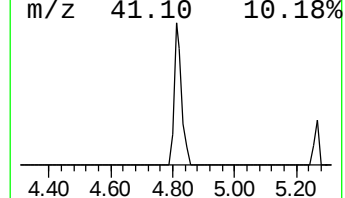
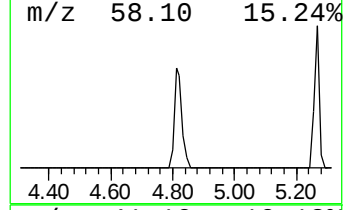
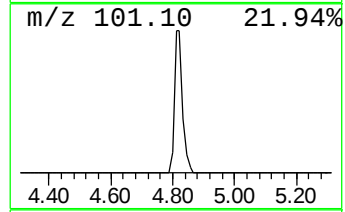
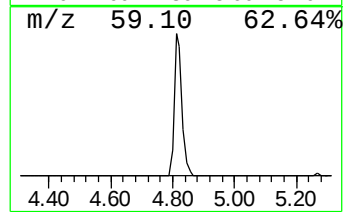
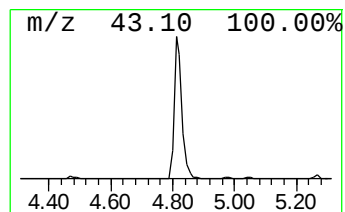
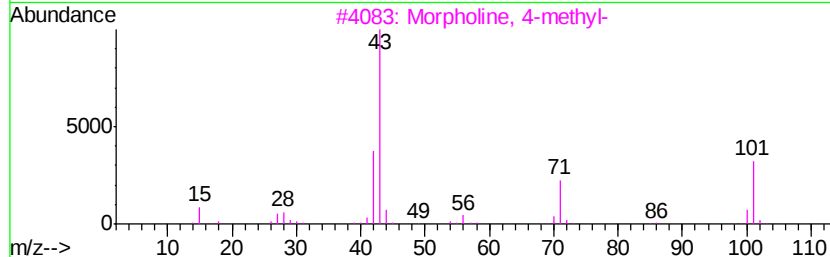
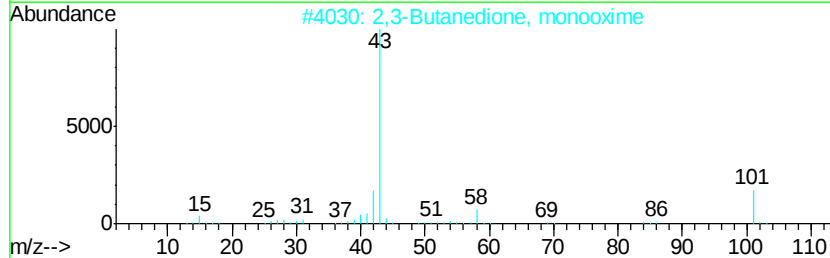
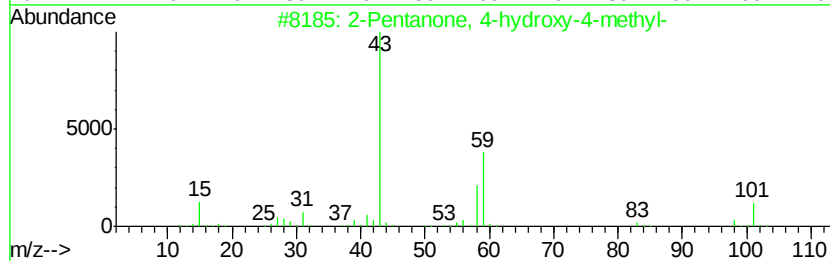
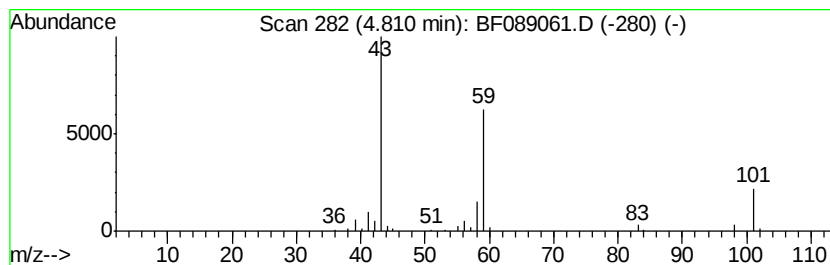
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	12.31 ng	196699	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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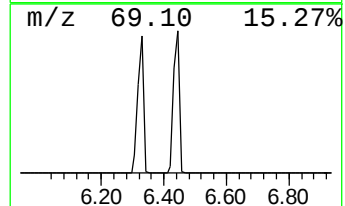
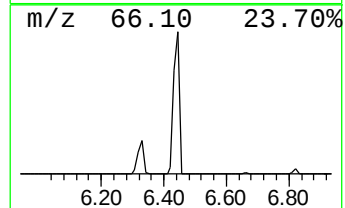
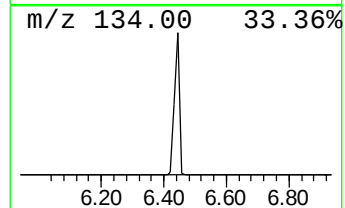
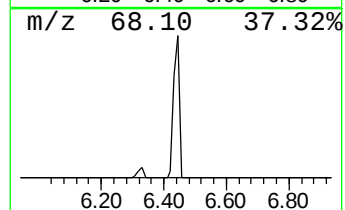
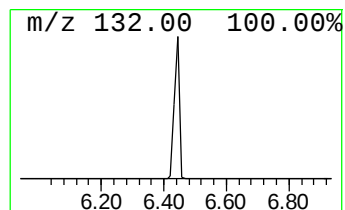
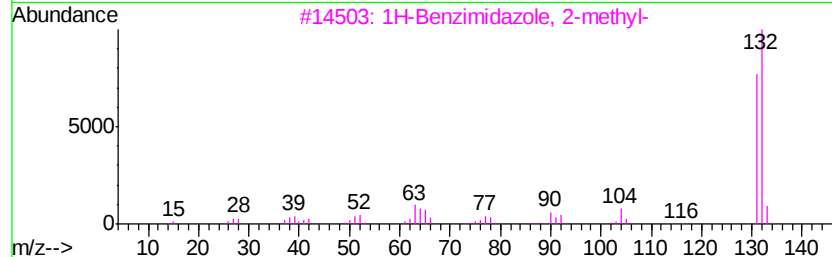
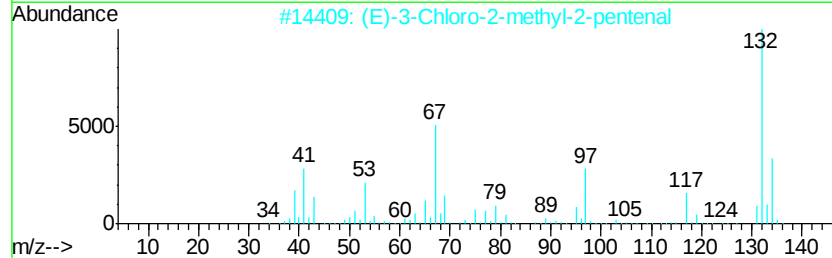
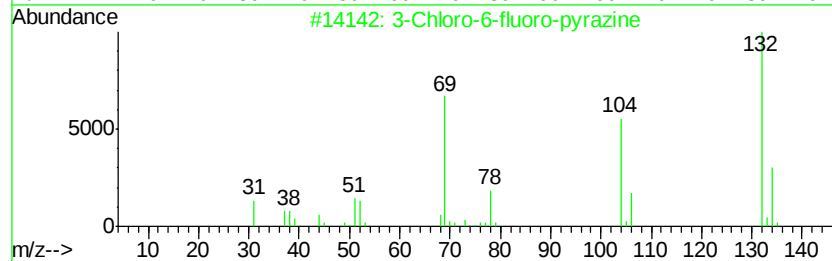
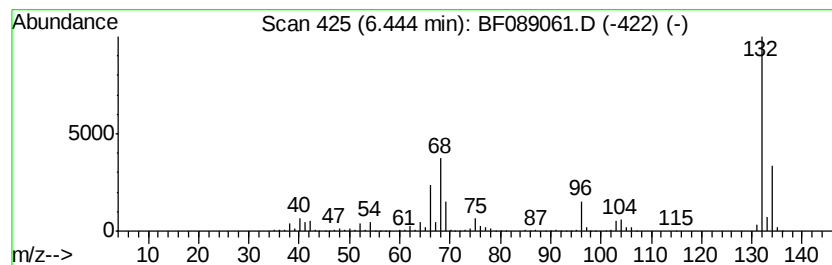
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	112.55 ng	1798170	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	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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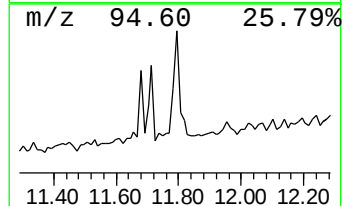
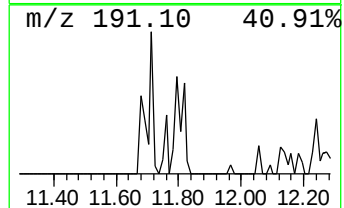
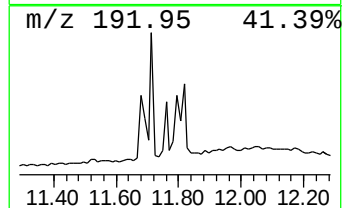
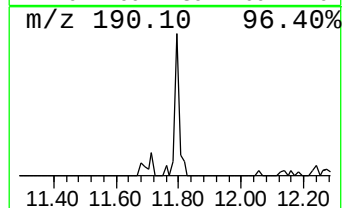
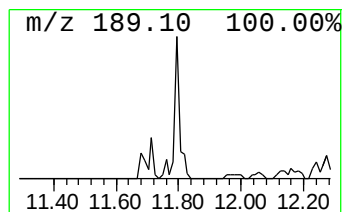
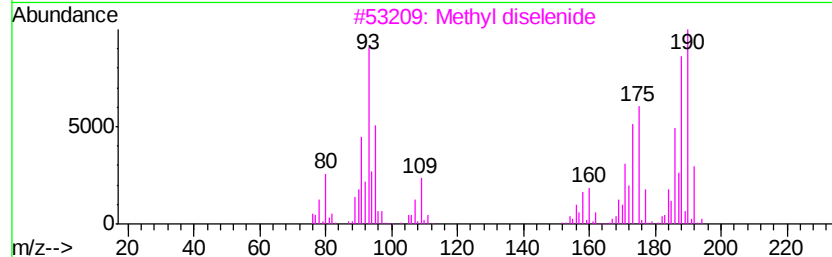
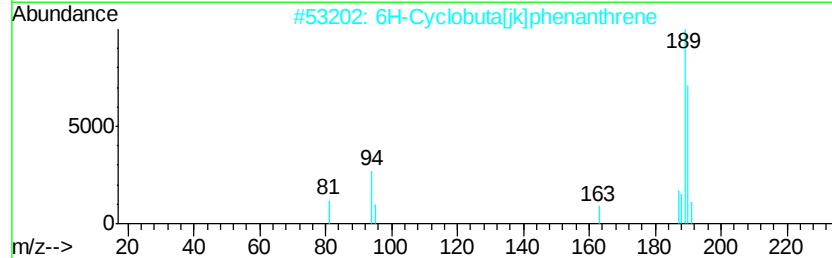
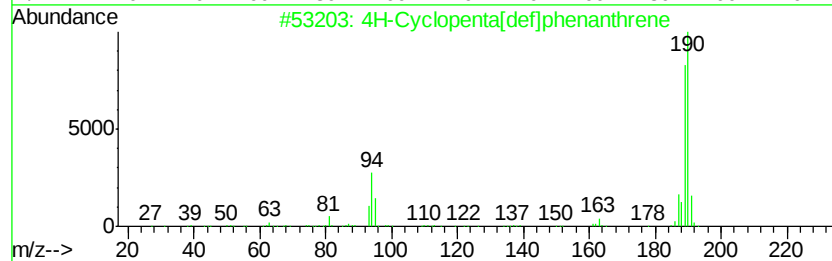
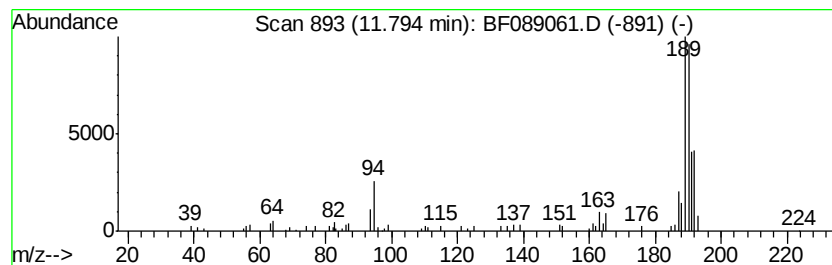
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.00 ng	77522	Phenanthrene-d10	11.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
2		6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	58
3		Methyl diselenide	190	C2H6Se2	007101-31-7	55
4		Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	38
5		6,7-Methylenedioxy-4(3H)-quinazo...	190	C9H6N2O3	028310-11-4	35



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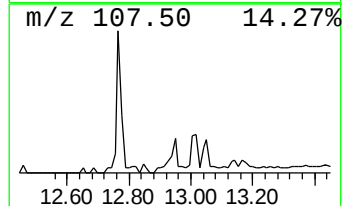
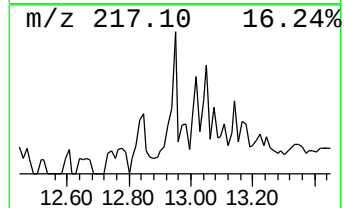
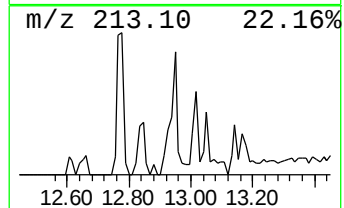
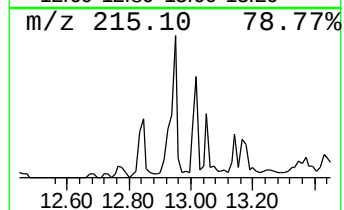
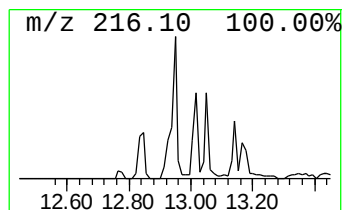
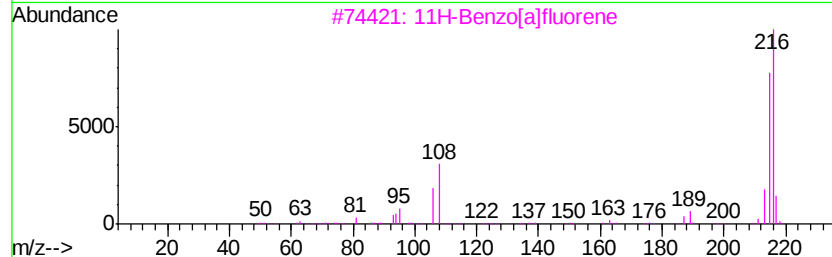
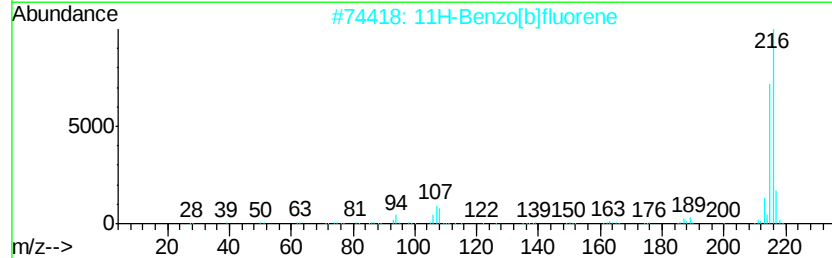
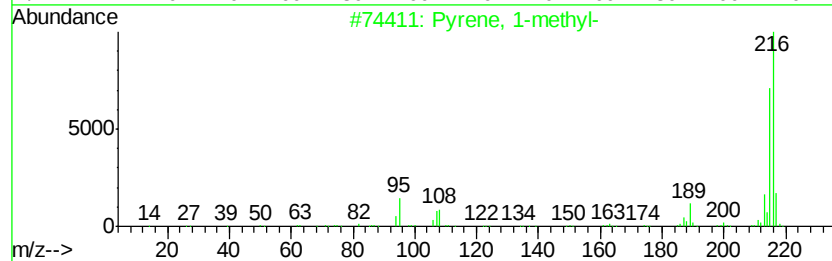
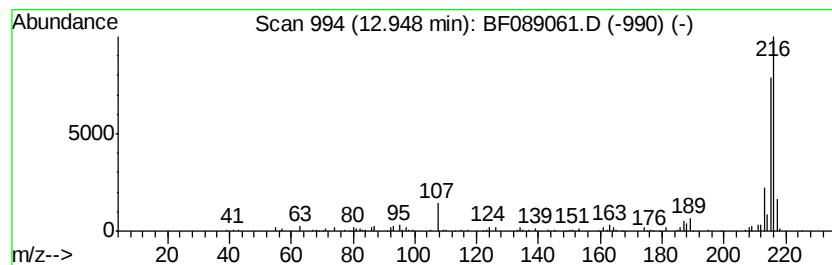
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pyrene, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.95	2.22 ng	80154	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089061.D
Acq On : 16 Jul 2016 18:12
Operator : UM/SJ
Sample : H3989-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
U3-B2(0-11)C

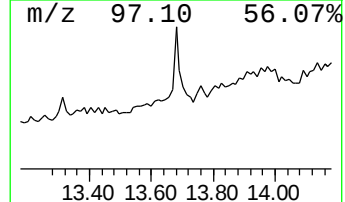
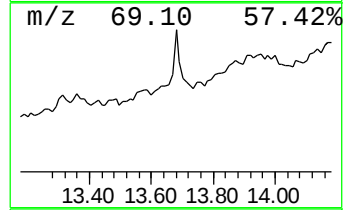
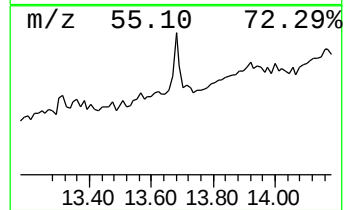
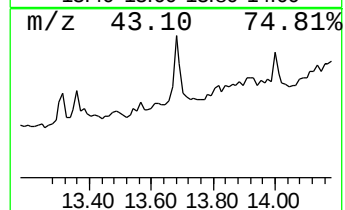
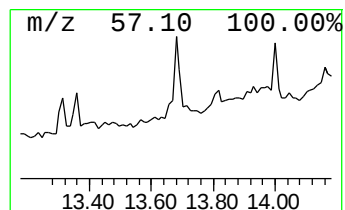
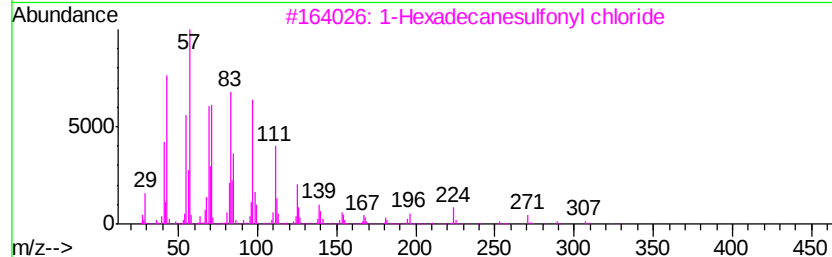
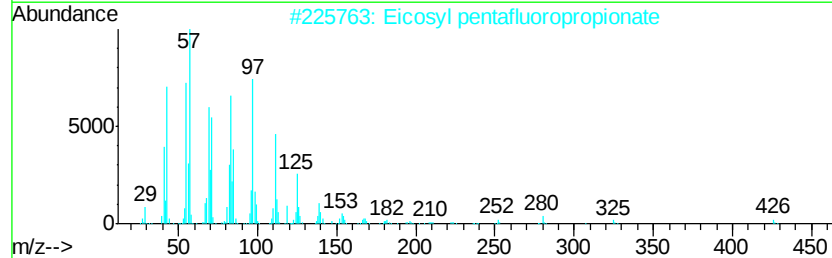
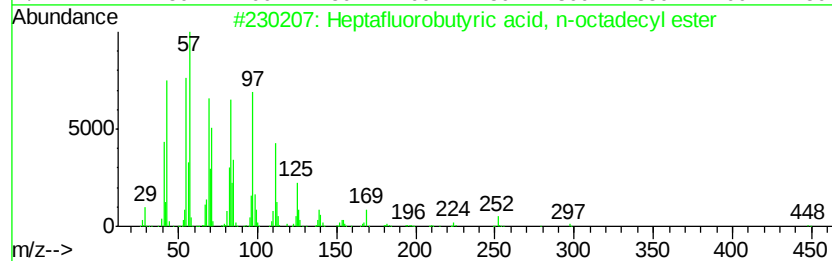
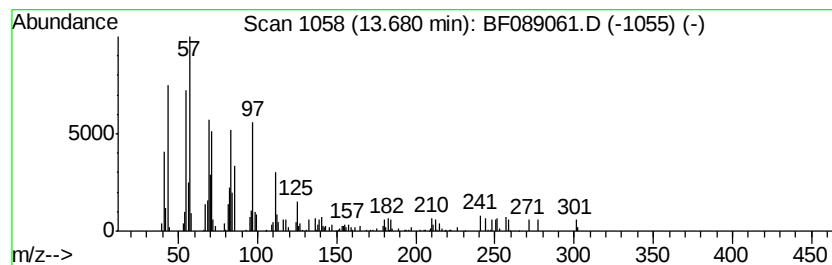
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	2.12 ng	76826	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-octadecyl...	466	C22H37F7O2	000400-57-7	90
2		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	90
3		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
4		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90



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Acq On : 16 Jul 2016 18:12
Operator : UM/SJ
Sample : H3989-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
U3-B2(0-11)C

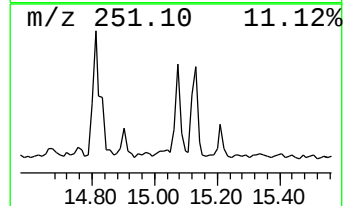
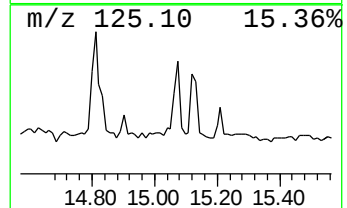
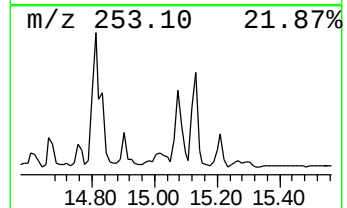
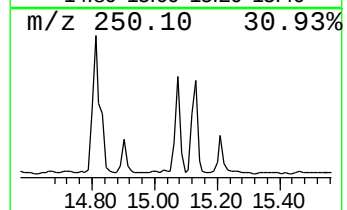
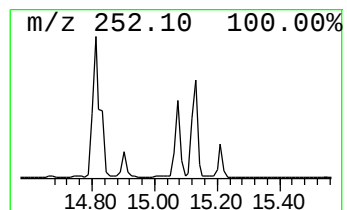
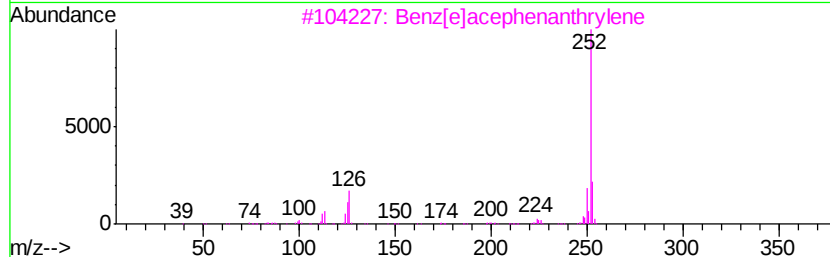
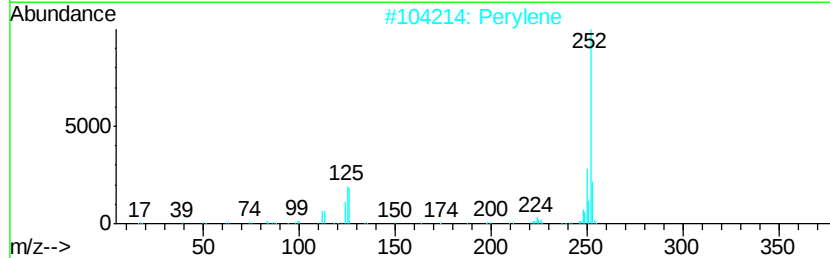
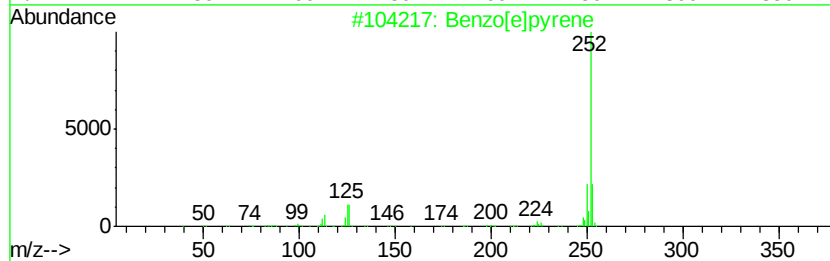
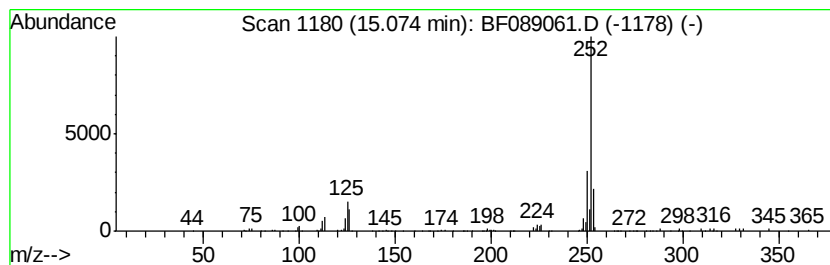
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	8.93 ng	125672	Perylene-d12	15.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2		Perylene	252	C20H12	000198-55-0	94
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	93
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
U3-B2(0-11)C

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
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2-Pentanone, 4-hy...	4.81	12.3	ng	196699	1	6.66	319544	20.0
unknown6.44	6.44	112.6	ng	1798170	1	6.66	319544	20.0
4H-Cyclopenta[def...	11.79	3.0	ng	77522	4	11.19	517278	20.0
Pyrene, 1-methyl-	12.95	2.2	ng	80154	5	13.82	723560	20.0
Heptafluorobutyri...	13.68	2.1	ng	76826	5	13.82	723560	20.0
Benzo[e]pyrene	15.07	8.9	ng	125672	6	15.19	281481	20.0