

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
 Data File : BF094967.D
 Acq On : 8 May 2017 4:06
 Operator : SJ/MA
 Sample : I2947-10
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04-0-2.0

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-BF050217.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	3.325	229	236	248	rBV	63807	142400	5.49%	0.630%
2	5.037	523	527	544	rBV	126421	256465	9.90%	1.135%
3	5.666	630	634	658	rBV	1424539	2147608	82.87%	9.501%
4	7.260	900	905	921	rBV	1632979	2288134	88.29%	10.123%
5	7.384	921	926	946	rVB	1901602	2591678	100.00%	11.465%
6	7.719	979	983	994	rBV	481533	577695	22.29%	2.556%
7	7.960	1019	1024	1037	rBV	1639996	1956192	75.48%	8.654%
8	8.619	1131	1136	1164	rBV	1141318	1501316	57.93%	6.642%
9	9.742	1322	1327	1341	rBV	565224	782290	30.18%	3.461%
10	11.513	1623	1628	1647	rBV	2063683	2553427	98.52%	11.296%
11	12.207	1741	1746	1758	rBV	240033	336287	12.98%	1.488%
12	12.571	1803	1808	1819	rBV2	546030	805741	31.09%	3.565%
13	13.413	1947	1951	1955	rBV	48565	52914	2.04%	0.234%
14	13.860	2023	2027	2041	rBV	890627	1450836	55.98%	6.418%
15	14.183	2078	2082	2093	rBV	41054	62355	2.41%	0.276%
16	14.971	2211	2216	2232	rVB	554018	743265	28.68%	3.288%
17	15.936	2376	2380	2390	rBV	111357	152375	5.88%	0.674%
18	17.024	2561	2565	2570	rBV2	42842	57246	2.21%	0.253%
19	17.065	2570	2572	2581	rVV2	27625	40196	1.55%	0.178%
20	17.142	2581	2585	2589	rVB	91495	85262	3.29%	0.377%
21	17.295	2606	2611	2622	rBV	1772205	2021158	77.99%	8.942%
22	18.065	2738	2742	2745	rBV	58782	55562	2.14%	0.246%
23	18.600	2827	2833	2834	rBV3	18020	33779	1.30%	0.149%
24	18.636	2835	2839	2857	rVB	517216	734365	28.34%	3.249%
25	19.330	2951	2957	2962	rBV5	16496	26892	1.04%	0.119%
26	19.418	2965	2972	2974	rBV6	12641	27119	1.05%	0.120%
27	19.771	3028	3032	3037	rBV	42761	46906	1.81%	0.208%
28	19.912	3052	3056	3060	rBV2	24380	43840	1.69%	0.194%
29	20.053	3077	3080	3084	rBV3	24276	27953	1.08%	0.124%
30	20.124	3087	3092	3098	rBV9	13582	39799	1.54%	0.176%
31	20.300	3118	3122	3132	rBV	458734	604177	23.31%	2.673%
32	20.771	3198	3202	3213	rVB4	43575	88675	3.42%	0.392%
33	21.194	3272	3274	3279	rBV5	19590	29900	1.15%	0.132%
34	21.688	3354	3358	3363	rBV7	19398	37682	1.45%	0.167%

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Instrument :
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ClientSampleId :
SB-04-0-2.0

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.930	3562	3569	3574	rBV9	20198	45210	1.74%	0.200%
36	23.277	3619	3628	3639	rBV4	57625	157490	6.08%	0.697%

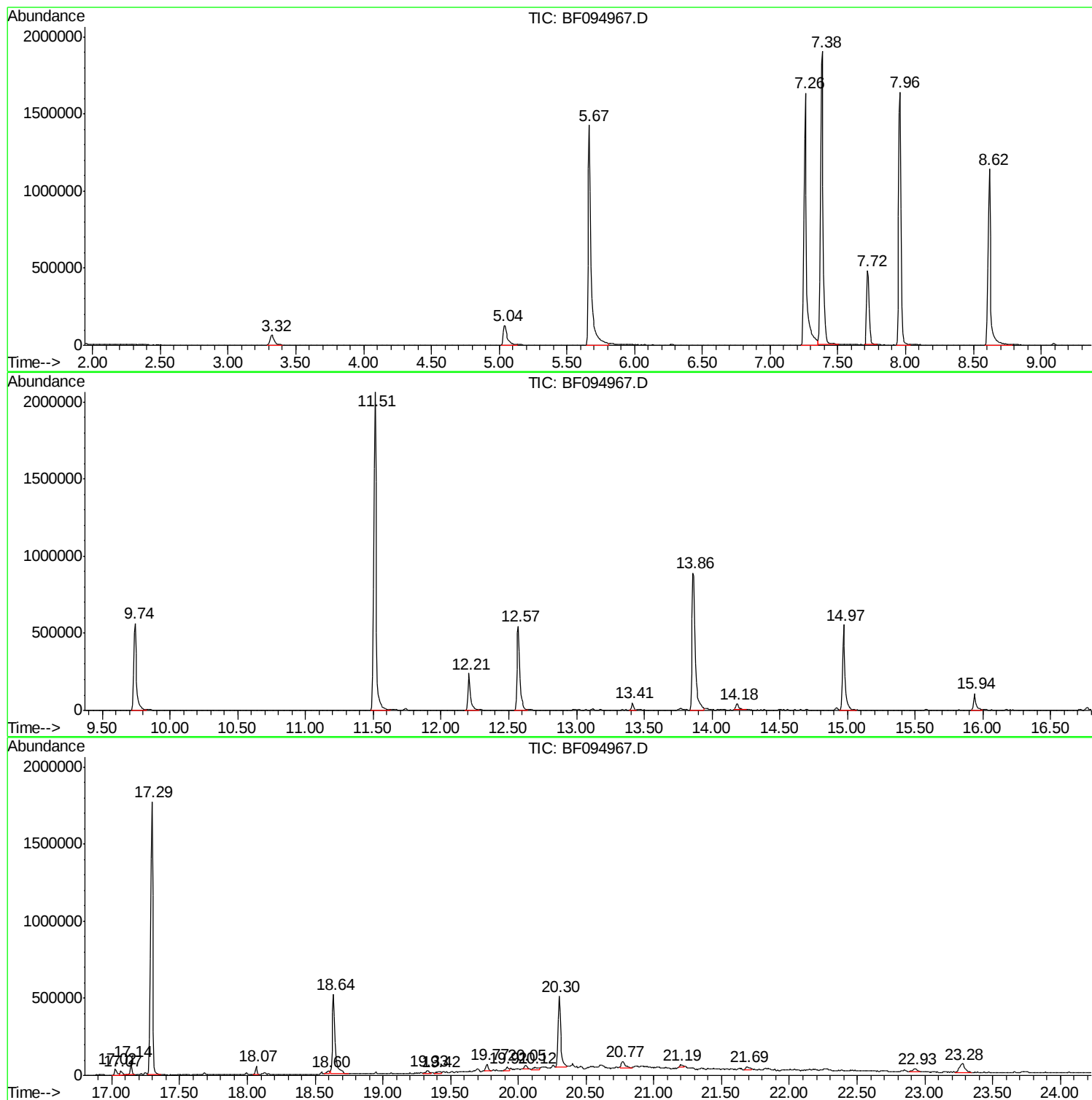
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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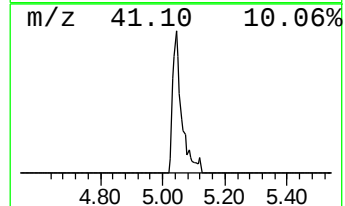
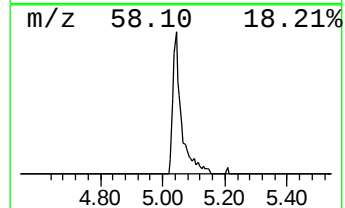
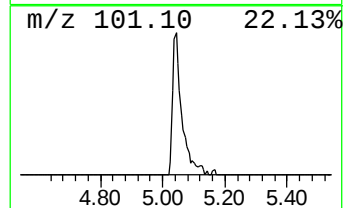
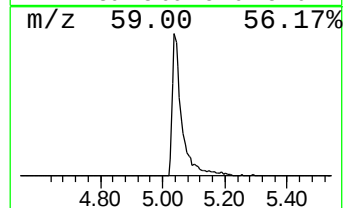
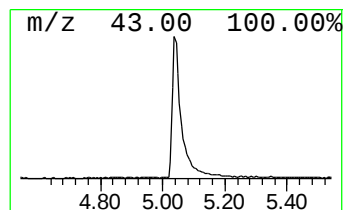
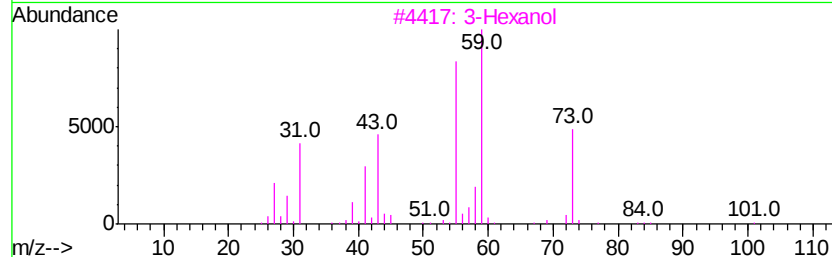
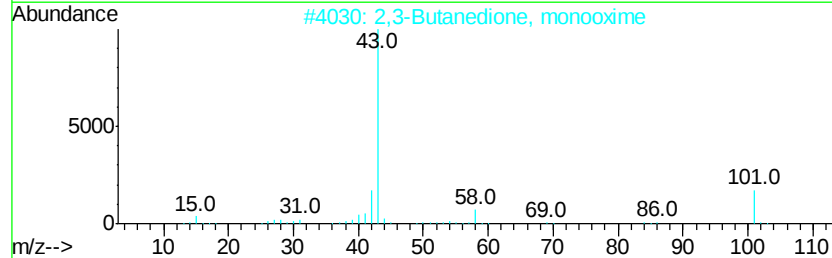
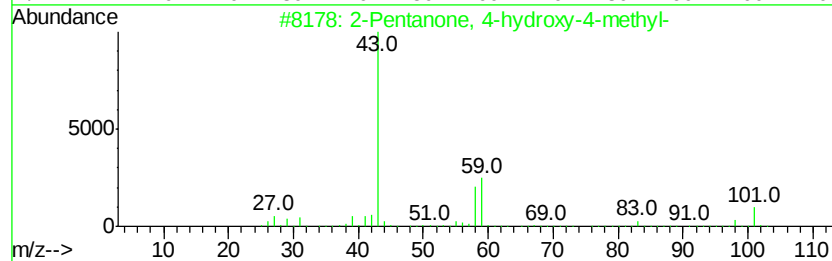
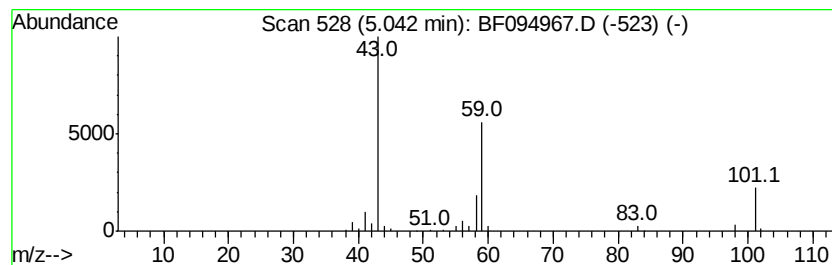
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	8.88 ng	256465	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		3-Hexanol	102	C6H14O	000623-37-0	28
4		Guanidine	59	CH5N3	000113-00-8	9
5		Butane	58	C4H10	000106-97-8	9



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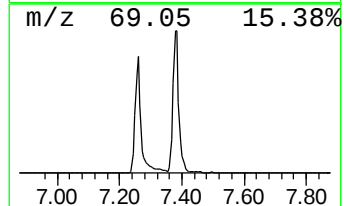
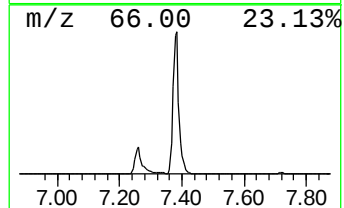
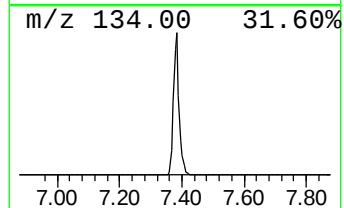
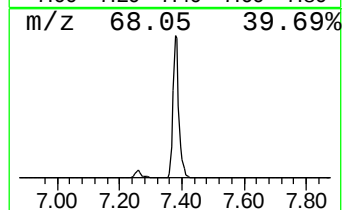
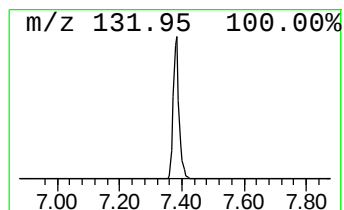
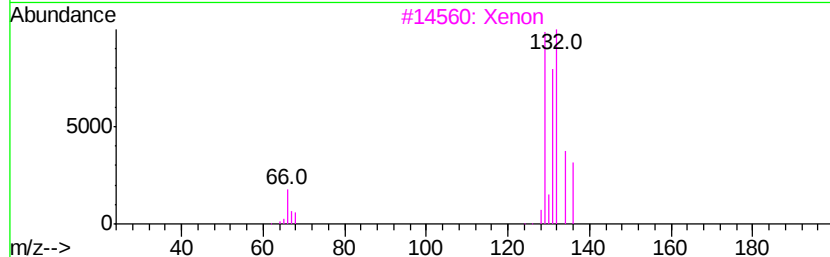
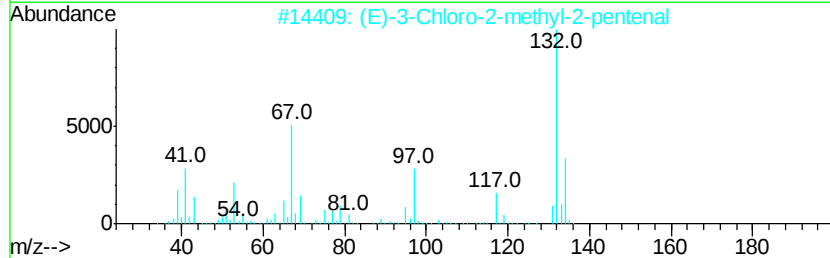
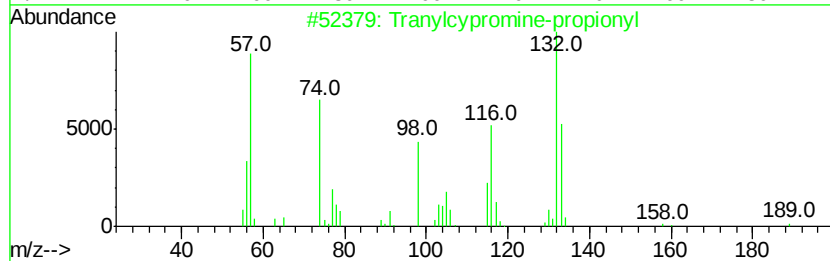
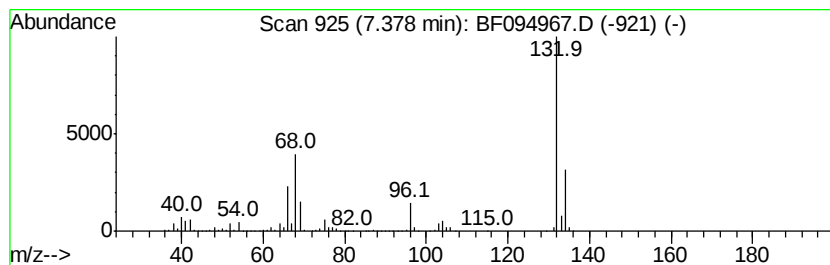
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	89.72 ng	2591680	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Xenon	132	Xe	007440-63-3	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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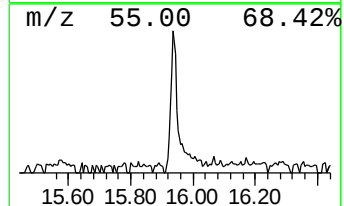
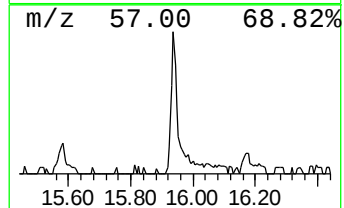
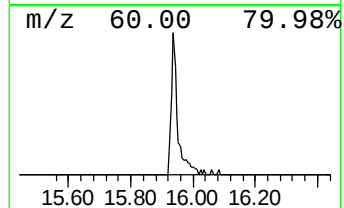
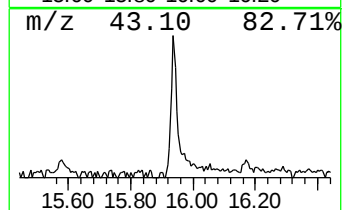
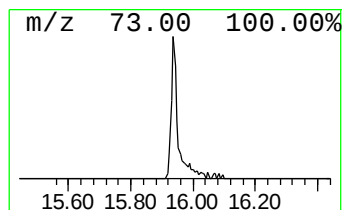
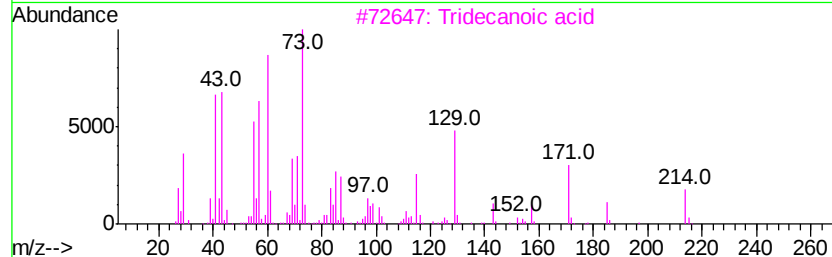
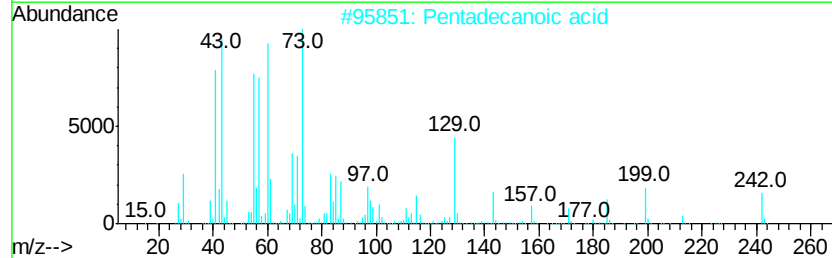
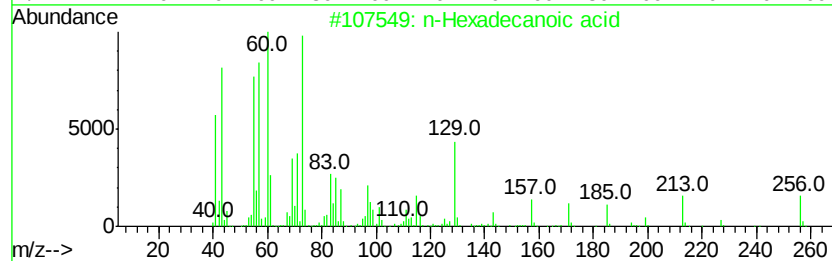
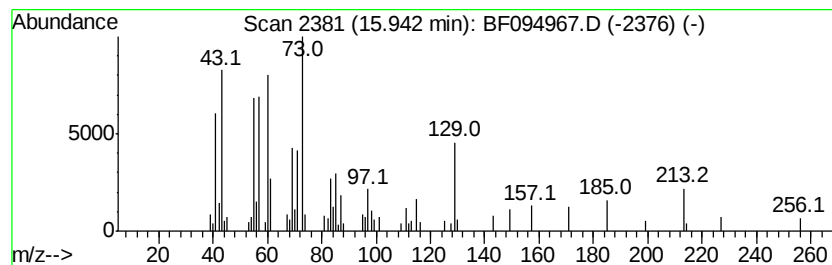
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	4.10 ng	152375	Phenanthrene-d10	14.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	86
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	18



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ALS Vial : 14 Sample Multiplier: 1

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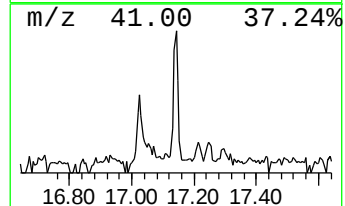
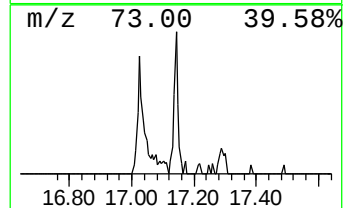
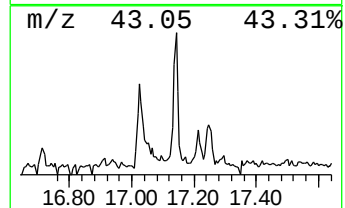
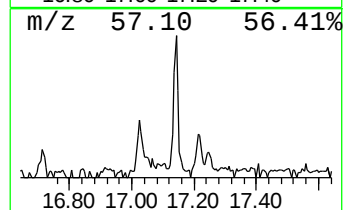
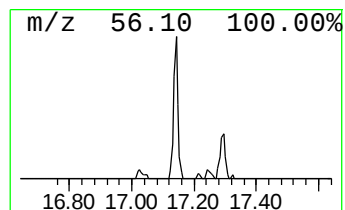
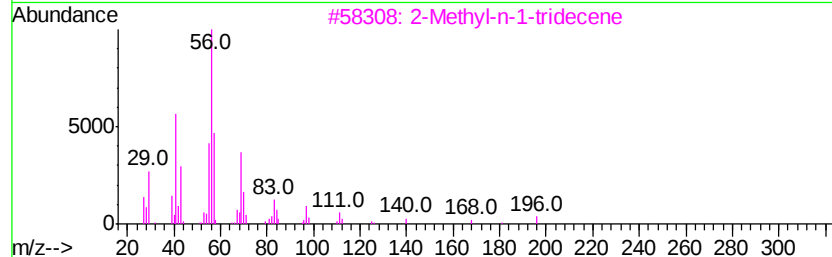
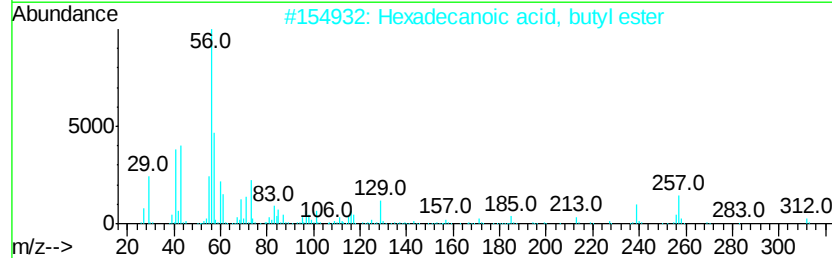
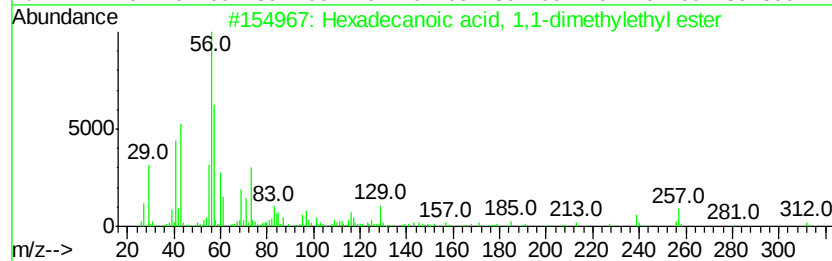
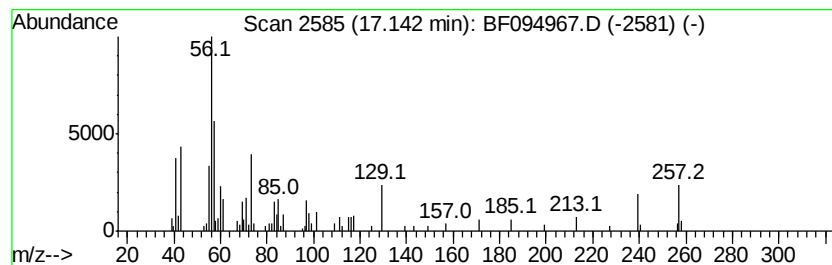
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	2.32 ng	85262	Chrysene-d12	18.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	45
3		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
4		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32



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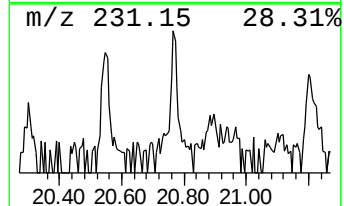
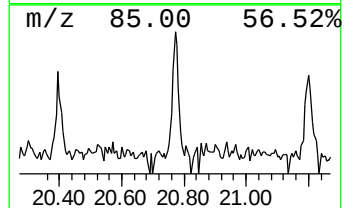
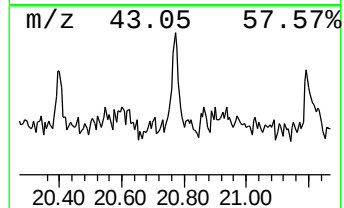
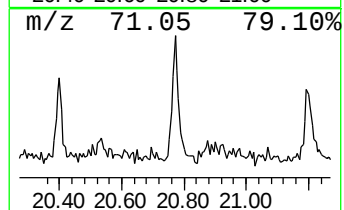
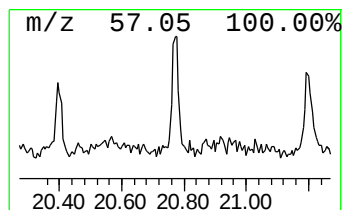
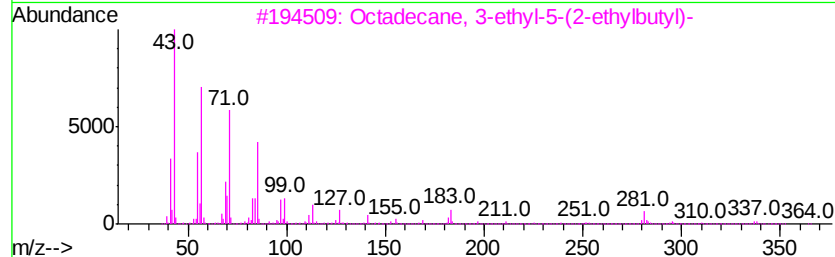
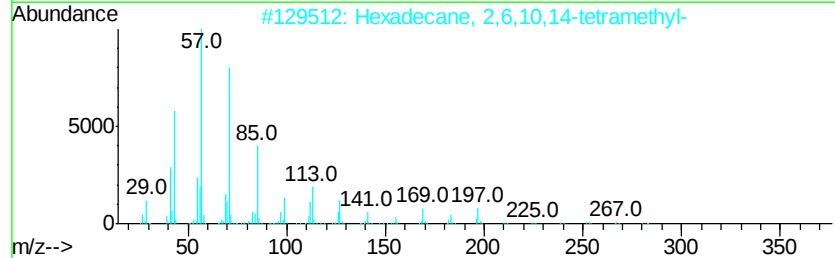
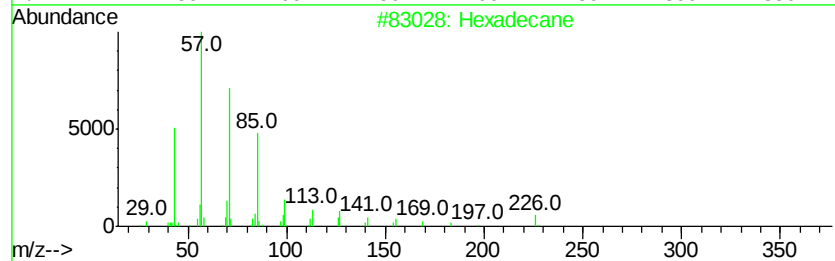
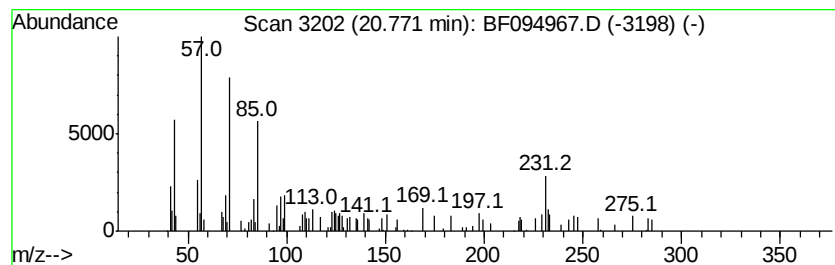
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.77	2.94 ng	88675	Perylene-d12	20.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	64
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	58
3	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	52
4	Hexatriacontane	507	C36H74	000630-06-8	52
5	Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	50



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Sample : I2947-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-0-2.0

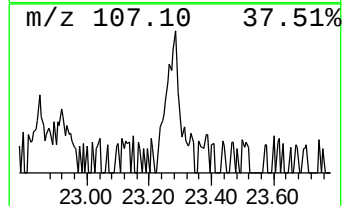
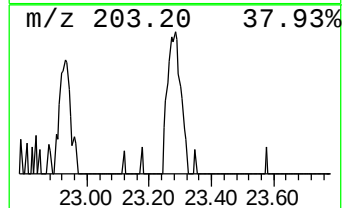
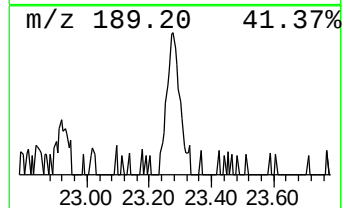
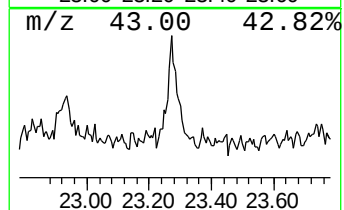
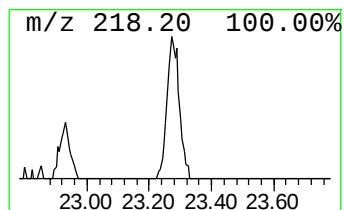
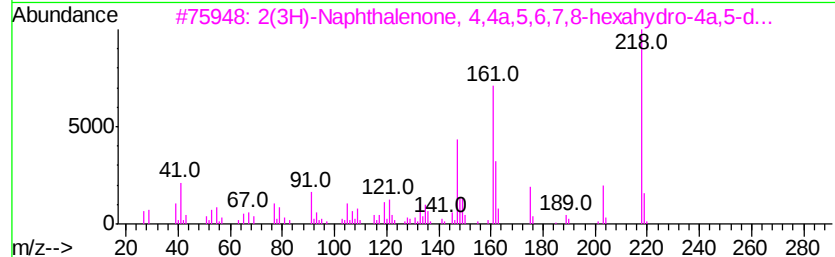
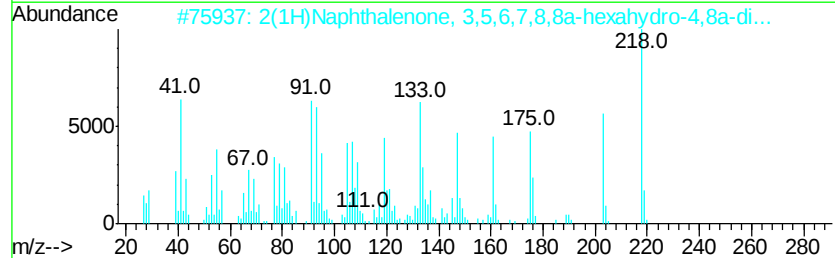
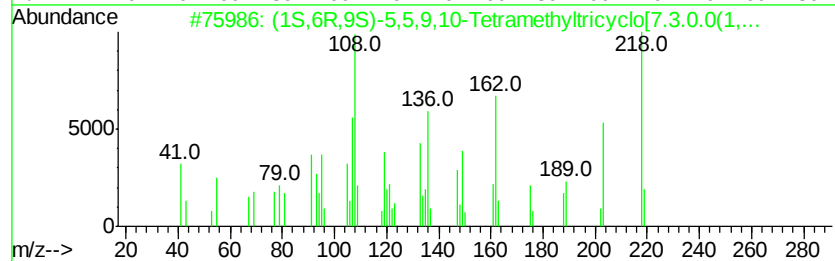
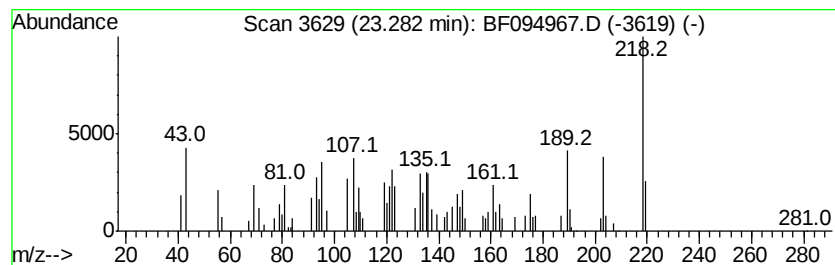
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 (1S,6R,9S)-5,5,9,10-Tetrame... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	5.21 ng	157490	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	53
2		2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	50
3		2(3H)-Naphthalenone, 4,4a,5,6,7,...	218	C15H22O	019598-45-9	43
4		Cyclopenta[c]pyran-7-carboxaldeh...	218	C12H10O4	018234-46-3	38
5		1-Pyrrolin-2-amine, N-(1-adamant...	218	C14H22N2	300695-00-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094967.D
Acq On : 8 May 2017 4:06
Operator : SJ/MA
Sample : I2947-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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
2-Pentanone, 4-hy...	5.04	8.9	ng	256465	1	7.72	577695	20.0
unknown7.38	7.38	89.7	ng	2591680	1	7.72	577695	20.0
n-Hexadecanoic acid	15.94	4.1	ng	152375	4	14.97	743265	20.0
Hexadecanoic acid...	17.14	2.3	ng	85262	5	18.64	734365	20.0
Hexadecane	20.77	2.9	ng	88675	6	20.30	604177	20.0
(1S,6R,9S)-5,5,9,...	23.28	5.2	ng	157490	6	20.30	604177	20.0