

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052517\
 Data File : BF095434.D
 Acq On : 25 May 2017 20:55
 Operator : SJ/MA
 Sample : I3200-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 POST-EX-34-20170517

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-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	5.107	534	539	561	rBV	139226	370646	12.72%	1.598%
2	5.707	637	641	690	rBV	1077597	2573626	88.31%	11.093%
3	7.295	906	911	926	rBV	1250465	2256960	77.44%	9.728%
4	7.413	926	931	952	rVB	1724457	2813233	96.53%	12.125%
5	7.742	984	987	1002	rVB	468097	586077	20.11%	2.526%
6	7.984	1023	1028	1042	rBV	1630342	1977141	67.84%	8.522%
7	8.648	1136	1141	1159	rBV	854384	1461346	50.14%	6.299%
8	9.766	1327	1331	1350	rBV	405039	789516	27.09%	3.403%
9	11.536	1627	1632	1653	rBV	1873169	2914391	100.00%	12.561%
10	12.242	1747	1752	1761	rBV	230271	384006	13.18%	1.655%
11	12.601	1808	1813	1825	rBV2	548807	868286	29.79%	3.742%
12	13.430	1950	1954	1959	rVB	42000	46348	1.59%	0.200%
13	13.901	2029	2034	2052	rBV	776623	1381755	47.41%	5.955%
14	14.201	2081	2085	2088	rBV2	53473	72482	2.49%	0.312%
15	14.936	2206	2210	2214	rBV	31697	38631	1.33%	0.167%
16	15.007	2214	2222	2241	rVB	416527	731141	25.09%	3.151%
17	15.960	2376	2384	2393	rBV6	62276	124603	4.28%	0.537%
18	16.801	2521	2527	2532	rBV	32500	43873	1.51%	0.189%
19	17.048	2566	2569	2574	rBV2	18519	30590	1.05%	0.132%
20	17.101	2574	2578	2585	rVB	38934	55100	1.89%	0.237%
21	17.224	2596	2599	2606	rBV	29801	52251	1.79%	0.225%
22	17.324	2611	2616	2628	rBV	1578750	1900765	65.22%	8.192%
23	18.565	2822	2827	2833	rBV5	43608	91707	3.15%	0.395%
24	18.683	2842	2847	2859	rBV	367706	612599	21.02%	2.640%
25	19.353	2958	2961	2967	rBV2	49670	63703	2.19%	0.275%
26	20.077	3080	3084	3088	rBV	265529	287182	9.85%	1.238%
27	20.359	3128	3132	3141	rBV	291137	436083	14.96%	1.880%
28	20.806	3203	3208	3213	rBV	167287	237315	8.14%	1.023%

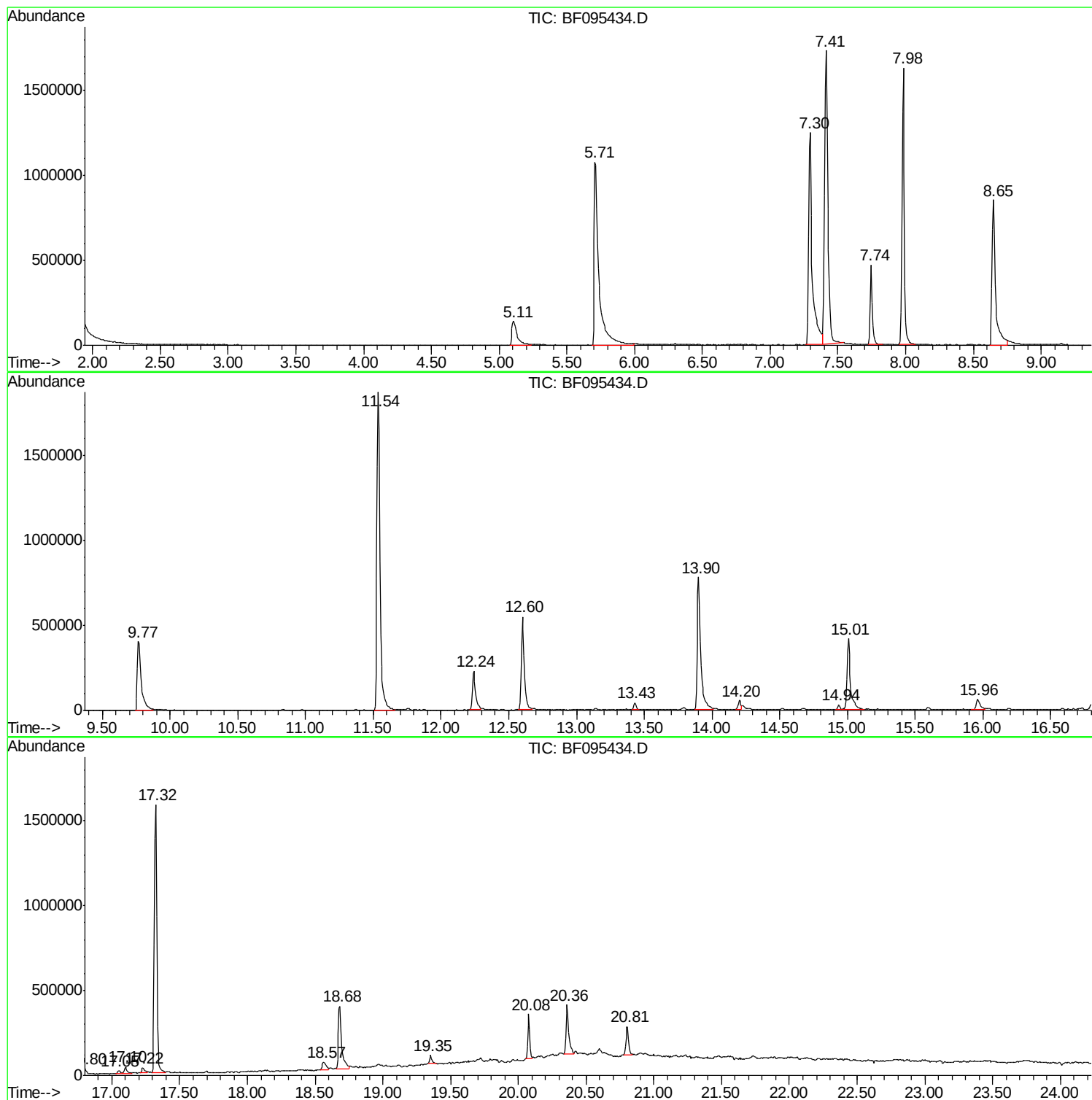
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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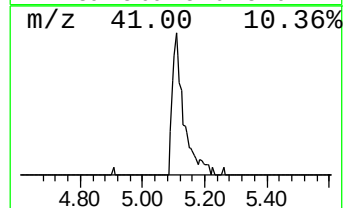
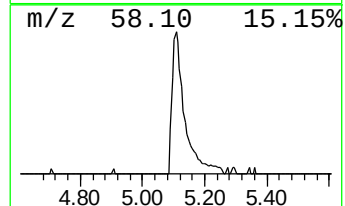
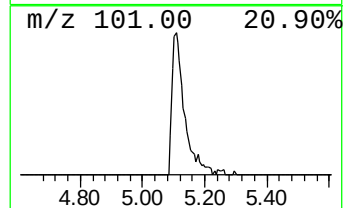
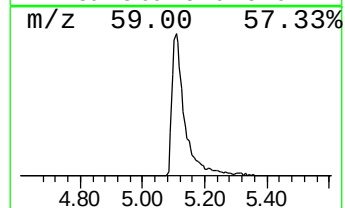
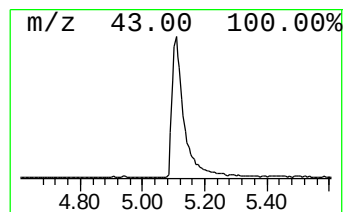
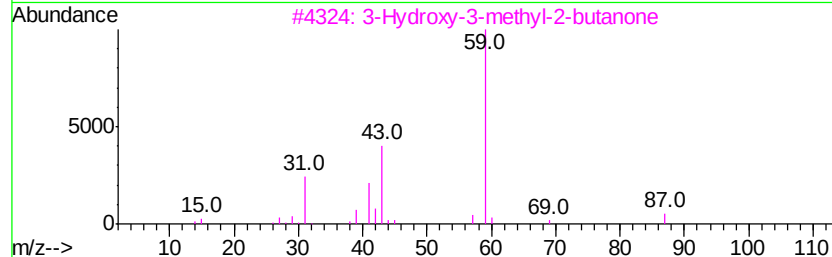
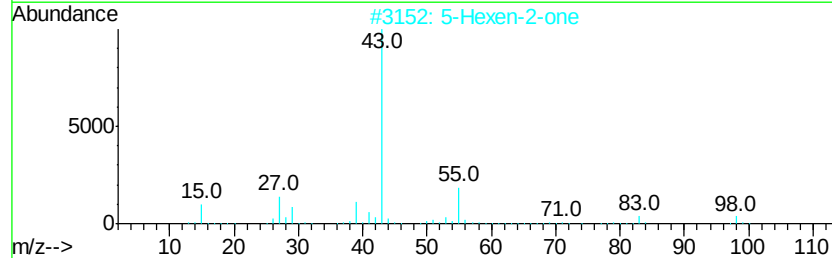
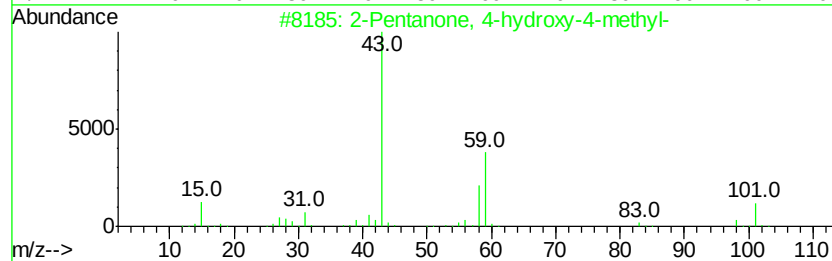
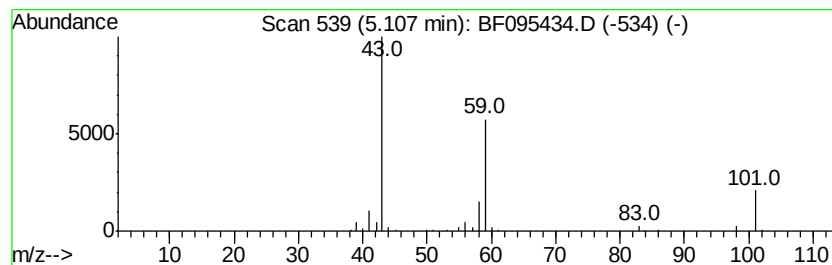
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	12.65 ng	370646	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9
5		1,2-Butanediol	90	C4H10O2	000584-03-2	9



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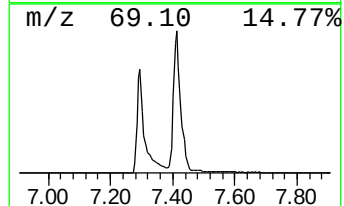
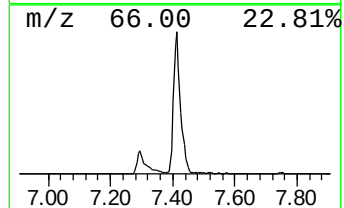
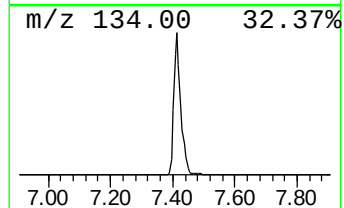
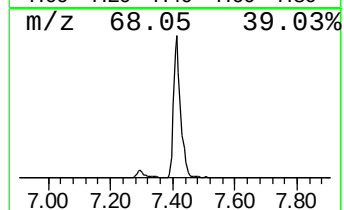
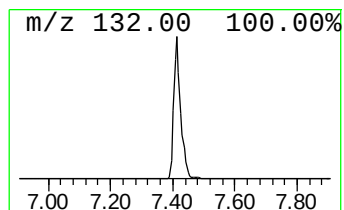
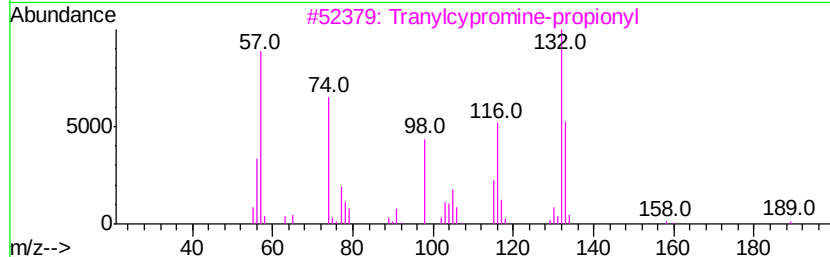
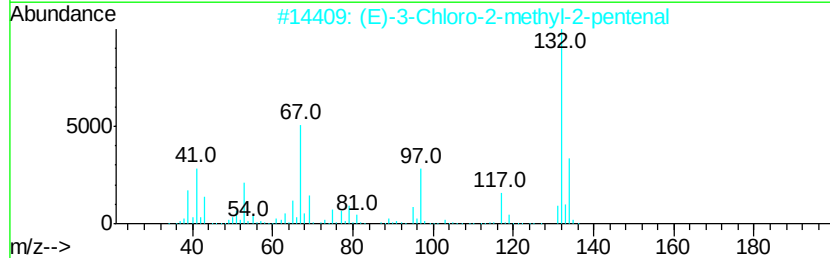
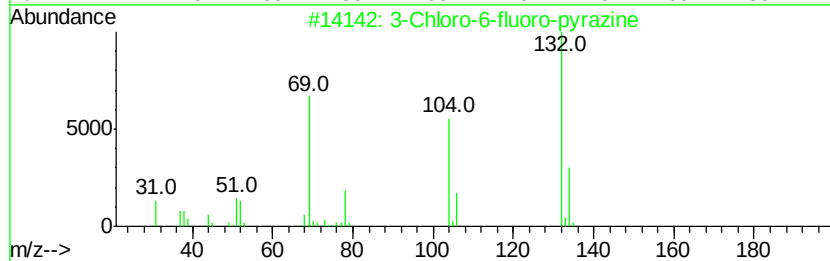
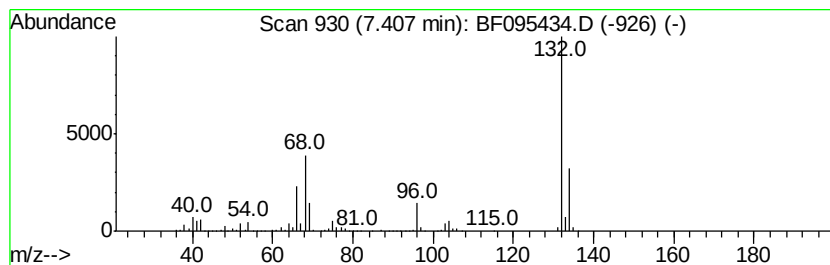
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Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	96.00 ng	2813230	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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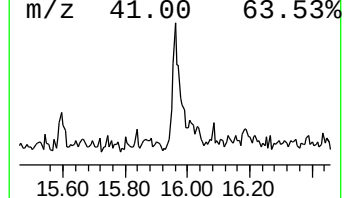
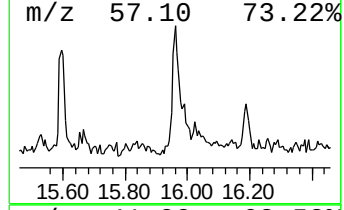
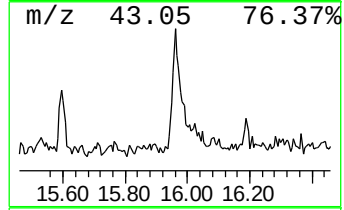
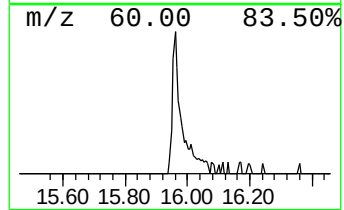
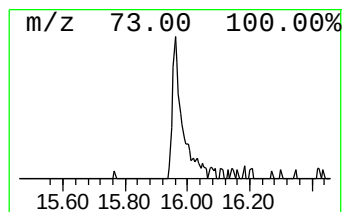
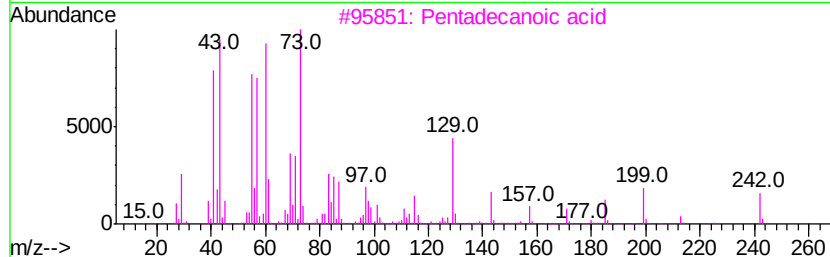
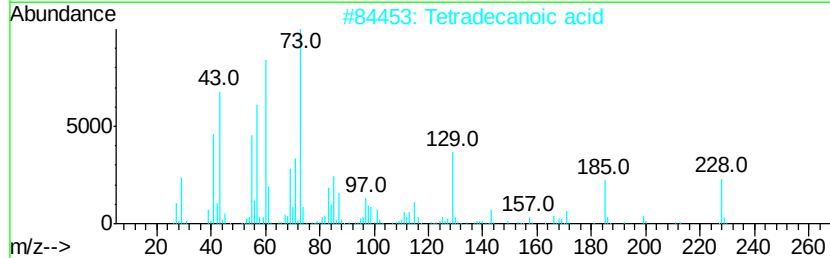
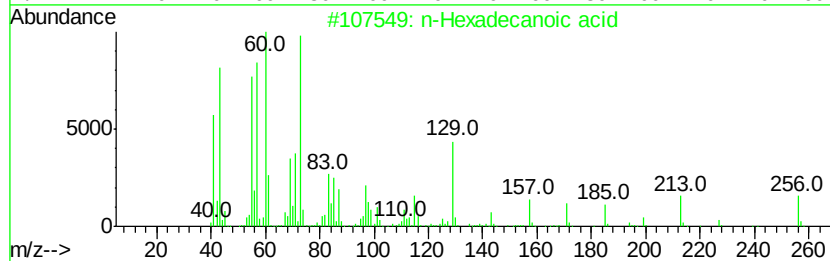
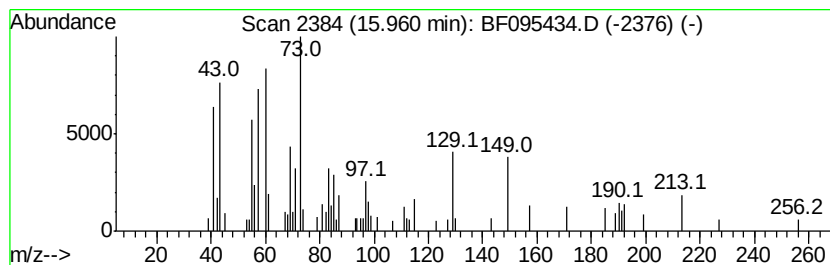
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.41 ng	124603	Phenanthrene-d10	15.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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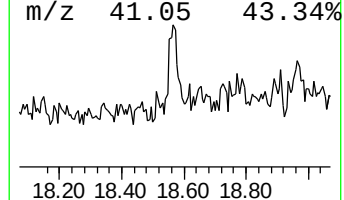
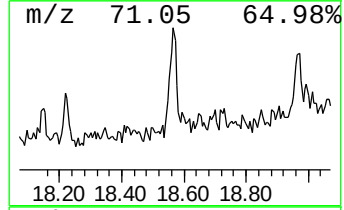
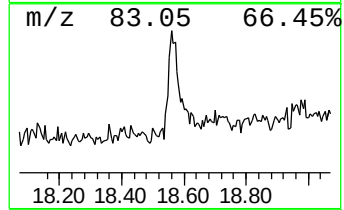
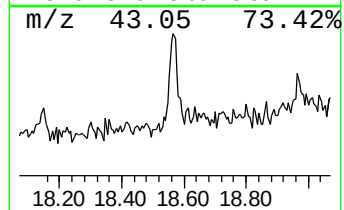
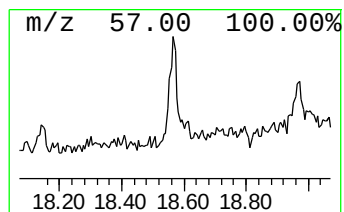
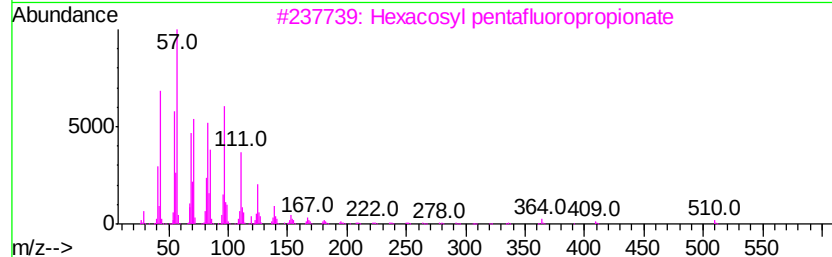
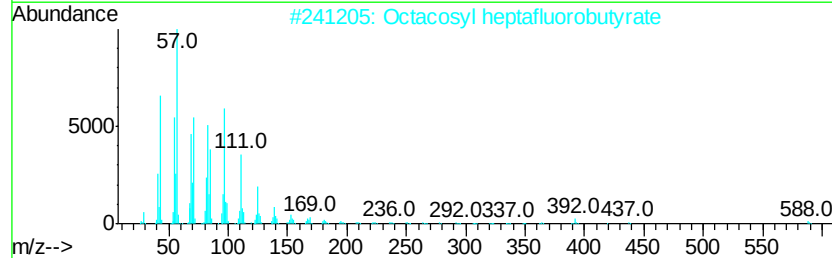
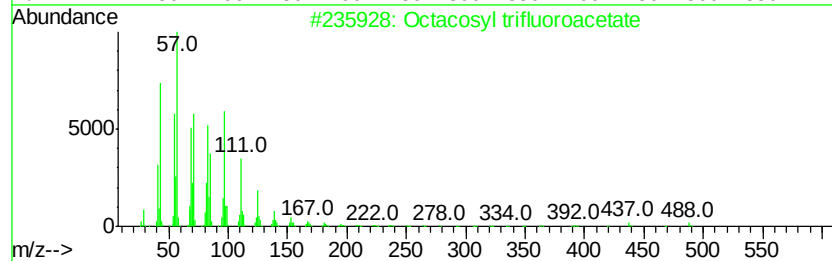
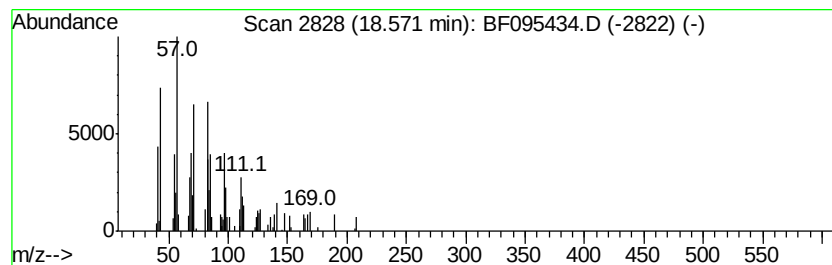
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Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	2.99 ng	91707	Chrysene-d12	18.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl		trifluoroacetate	506	C30H57F3O2	1000351-74-9	68
2	Octacosyl		heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	64
3	Hexacosyl		pentafluoropropionate	528	C29H53F5O2	1000351-81-2	58
4	Hexacosyl		trifluoroacetate	478	C28H53F3O2	1000351-75-0	58
5	Hexacosyl		heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	58



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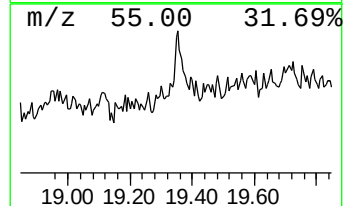
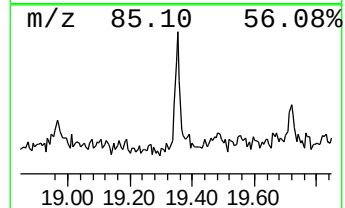
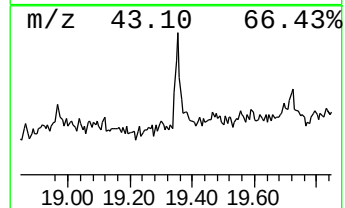
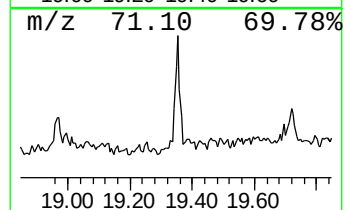
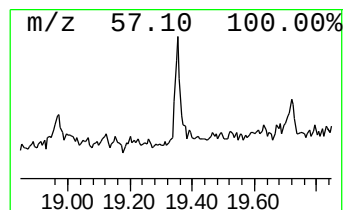
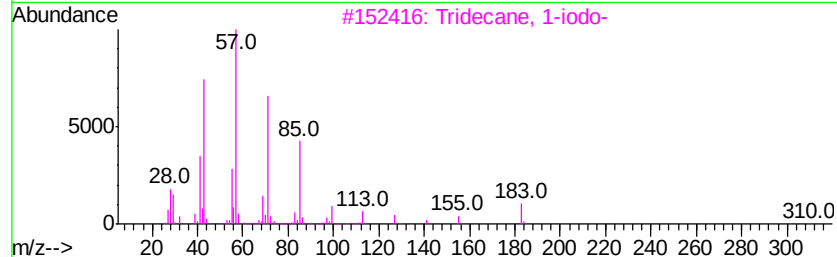
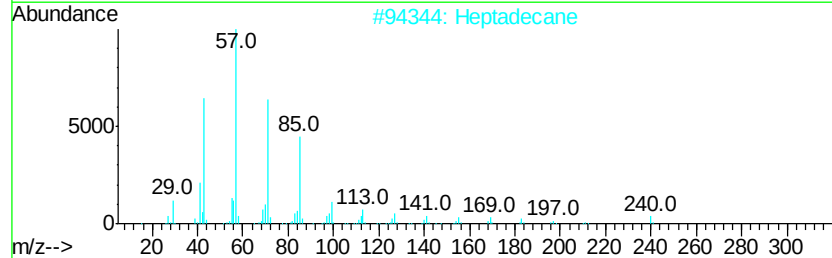
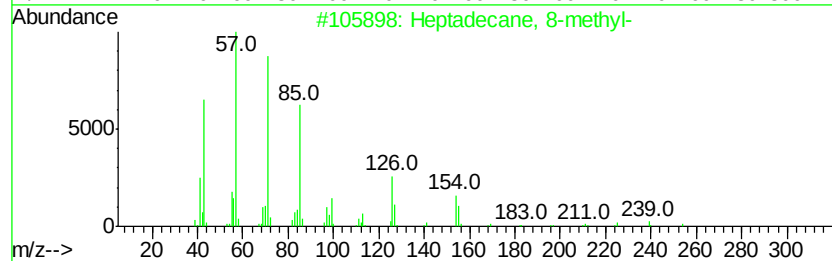
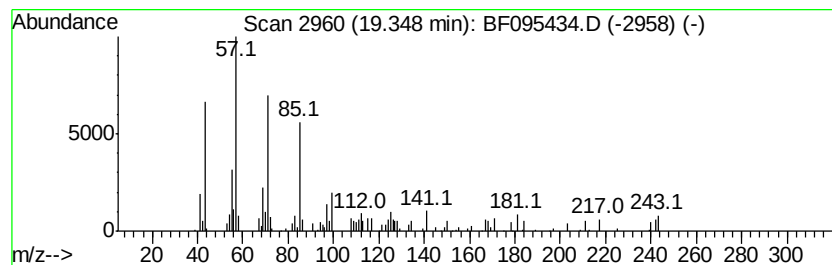
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptadecane, 8-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	2.08 ng	63703	Chrysene-d12	18.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86
2		Heptadecane	240	C17H36	000629-78-7	83
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
4		Octacosane	394	C28H58	000630-02-4	74
5		10-Methylnonadecane	282	C20H42	056862-62-5	72



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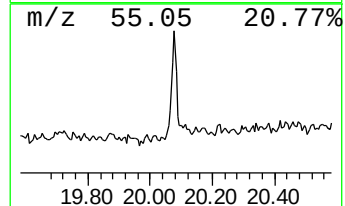
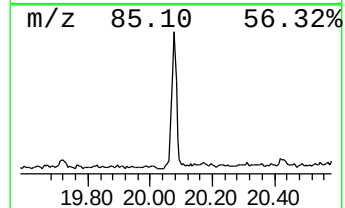
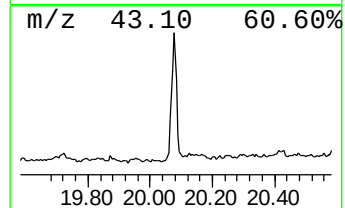
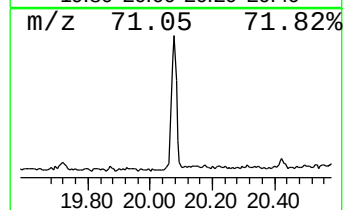
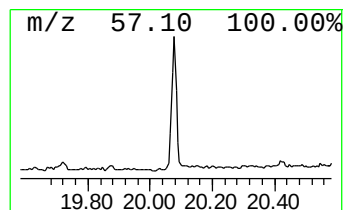
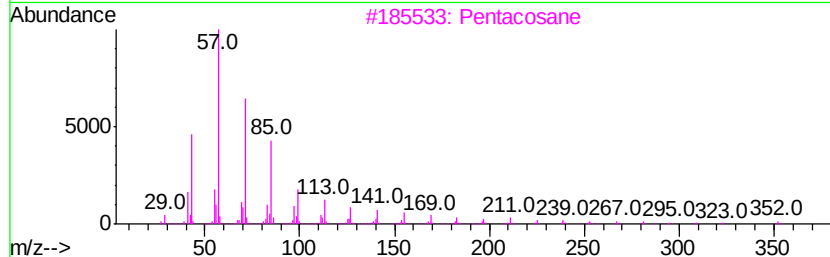
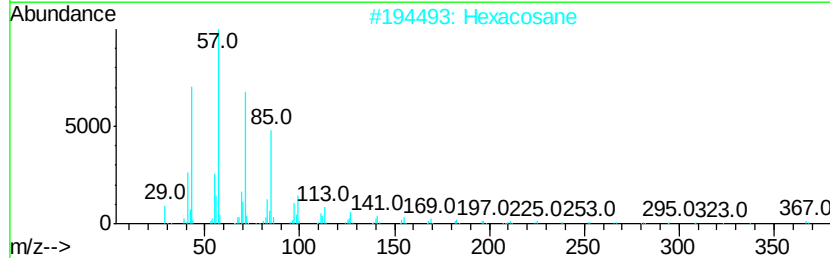
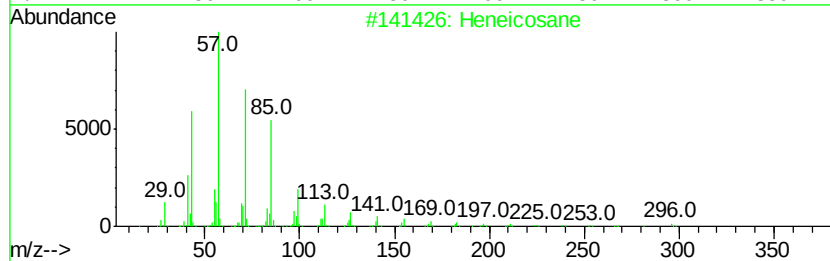
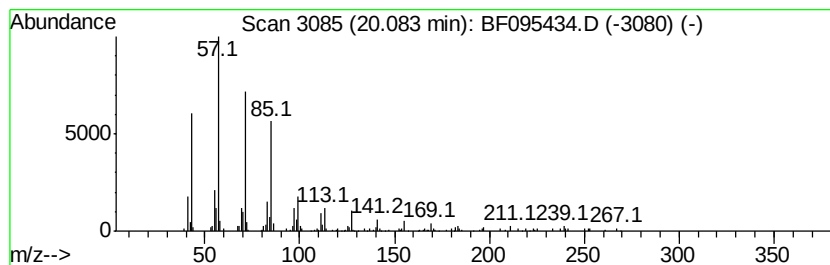
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.08	13.17 ng	287182	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Pentacosane	352	C25H52	000629-99-2	90
4		triacontane	422	C30H62	000638-68-6	90
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052517\
Data File : BF095434.D
Acq On : 25 May 2017 20:55
Operator : SJ/MA
Sample : I3200-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POST-EX-34-20170517

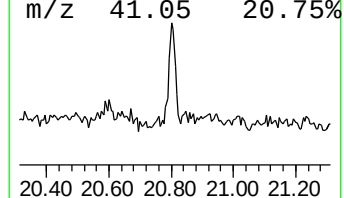
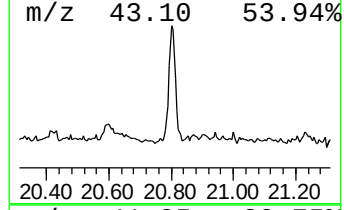
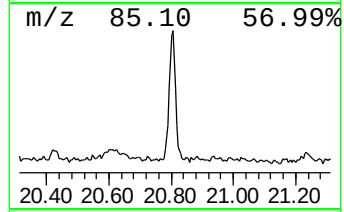
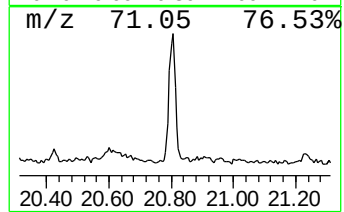
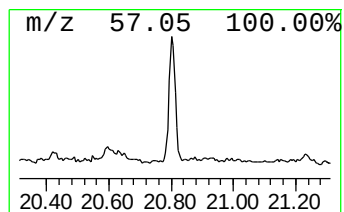
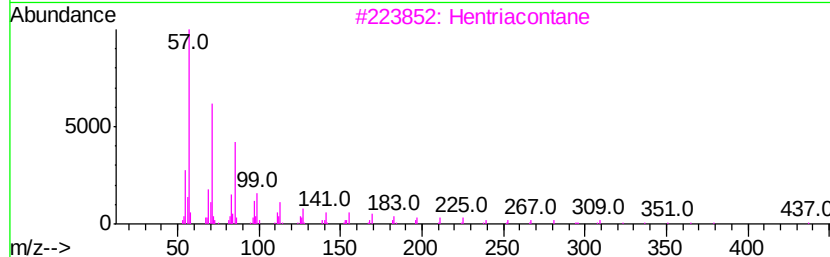
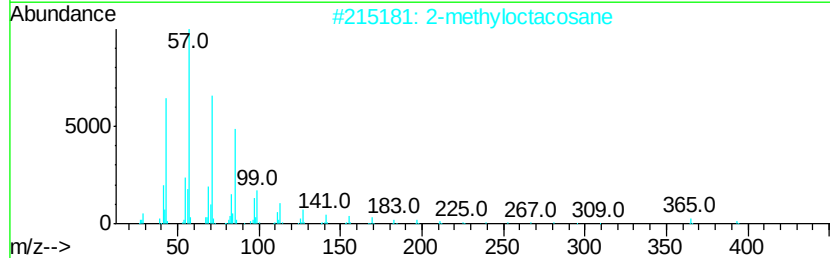
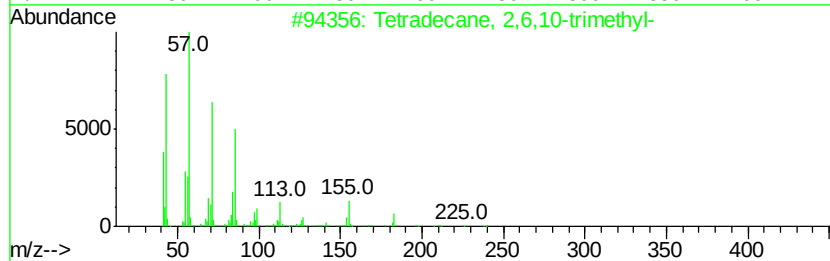
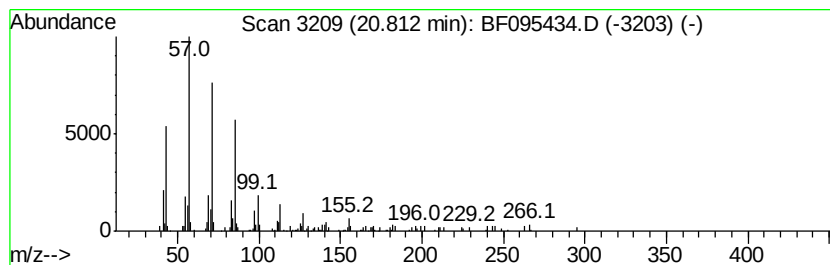
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecane, 2,6,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	10.88 ng	237315	Perylene-d12	20.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	94
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052517\
Data File : BF095434.D
Acq On : 25 May 2017 20:55
Operator : SJ/MA
Sample : I3200-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POST-EX-34-20170517

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...	5.11	12.7	ng	370646	1	7.74	586077	20.0
unknown7.41	7.41	96.0	ng	2813230	1	7.74	586077	20.0
n-Hexadecanoic acid	15.96	3.4	ng	124603	4	15.01	731141	20.0
Octacosyl trifluo...	18.57	3.0	ng	91707	5	18.68	612599	20.0
Heptadecane, 8-me...	19.35	2.1	ng	63703	5	18.68	612599	20.0
Heneicosane	20.08	13.2	ng	287182	6	20.36	436083	20.0
Tetradecane, 2,6,...	20.81	10.9	ng	237315	6	20.36	436083	20.0