

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
 Data File : BF097105.D
 Acq On : 27 Jul 2017 5:05
 Operator : SJ/JU
 Sample : I4397-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-2A-14.5-15.0-072117

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-BF072517.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	4.634	464	467	479	rBV	127969	187891	8.86%	1.128%
2	5.093	541	545	561	rBV	1971506	2119588	100.00%	12.720%
3	6.157	721	726	741	rBV	1850468	1914790	90.34%	11.491%
4	6.269	741	745	755	rVB	1993149	1728734	81.56%	10.374%
5	6.498	780	784	794	rBV	640747	575046	27.13%	3.451%
6	6.651	806	810	819	rBV	1462541	1302485	61.45%	7.816%
7	7.063	876	880	883	rBV	1251721	1038188	48.98%	6.230%
8	7.198	900	903	913	rVB	24682	30135	1.42%	0.181%
9	7.704	987	989	995	rBV	22742	27634	1.30%	0.166%
10	7.781	998	1002	1006	rBV	947001	745563	35.17%	4.474%
11	8.857	1181	1185	1188	rBV	1992339	1717266	81.02%	10.306%
12	9.257	1249	1253	1256	rBV	260989	199765	9.42%	1.199%
13	9.528	1295	1299	1302	rBV	644920	571471	26.96%	3.429%
14	10.310	1429	1432	1438	rBV	962043	851303	40.16%	5.109%
15	10.451	1453	1456	1463	rBV	36767	39950	1.88%	0.240%
16	10.998	1546	1549	1552	rBV	593389	509364	24.03%	3.057%
17	11.022	1552	1553	1557	rVB	56529	37410	1.76%	0.225%
18	11.251	1588	1592	1598	rBV3	32948	35616	1.68%	0.214%
19	11.557	1641	1644	1647	rBV	54767	50340	2.37%	0.302%
20	12.204	1751	1754	1758	rBV	87179	76365	3.60%	0.458%
21	12.339	1774	1777	1784	rVB3	31783	36630	1.73%	0.220%
22	12.427	1787	1792	1797	rVB	115886	114309	5.39%	0.686%
23	12.586	1814	1819	1822	rBV	1321112	1225092	57.80%	7.352%
24	13.133	1909	1912	1914	rBV	40416	35139	1.66%	0.211%
25	13.398	1950	1957	1960	rBV8	15759	31700	1.50%	0.190%
26	13.498	1968	1974	1980	rBV2	81001	115161	5.43%	0.691%
27	13.627	1991	1996	1999	rBV	599312	580034	27.37%	3.481%
28	13.733	2011	2014	2018	rBV6	25734	52087	2.46%	0.313%
29	14.092	2068	2075	2076	rBV6	27332	53935	2.54%	0.324%
30	14.980	2222	2226	2231	rBV	322206	370299	17.47%	2.222%
31	16.198	2430	2433	2434	rBV3	26659	35439	1.67%	0.213%
32	16.745	2524	2526	2533	rBV6	30667	28793	1.36%	0.173%
33	17.780	2700	2702	2707	rBV6	20568	22633	1.07%	0.136%
34	18.051	2745	2748	2750	rBV3	33201	39687	1.87%	0.238%

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Misc :
ALS Vial : 26 Sample Multiplier: 1

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T-2A-14.5-15.0-072117

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	18.209	2773	2775	2779	rBV4	21962	24478	1.15%	0.147%
36	18.421	2809	2811	2816	rBV6	21260	29013	1.37%	0.174%
37	18.456	2816	2817	2821	rBV4	20941	31373	1.48%	0.188%
38	18.709	2858	2860	2864	rBV5	23608	36692	1.73%	0.220%
39	19.021	2910	2913	2915	rBV4	29471	42160	1.99%	0.253%

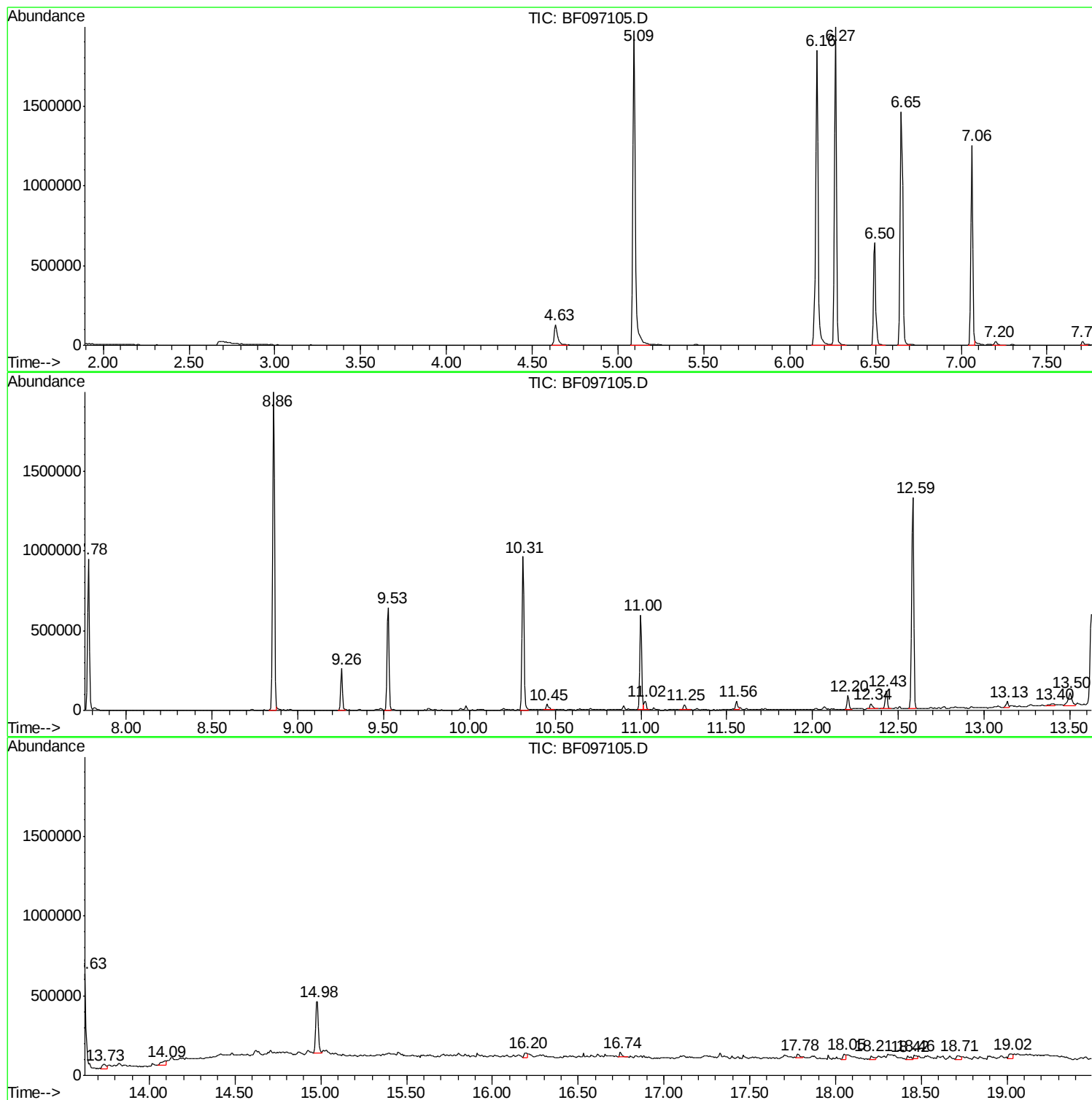
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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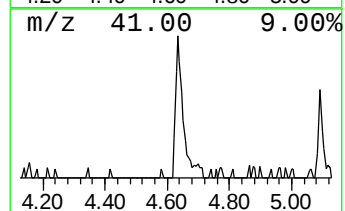
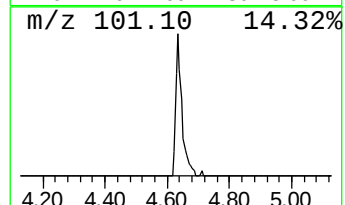
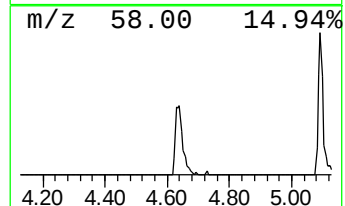
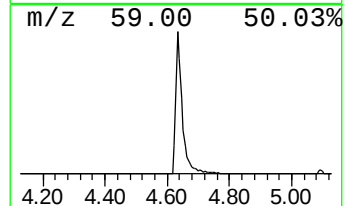
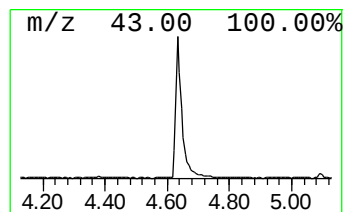
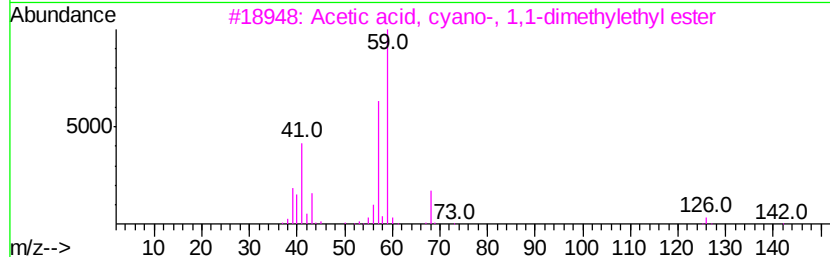
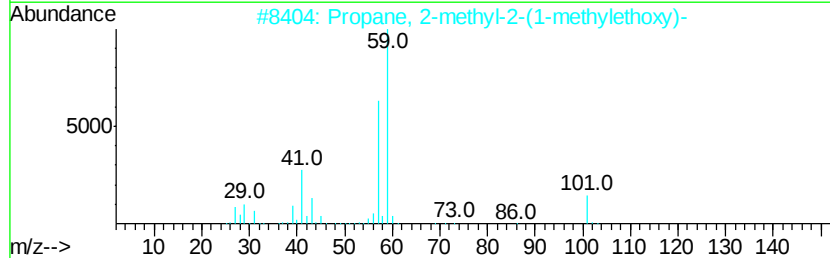
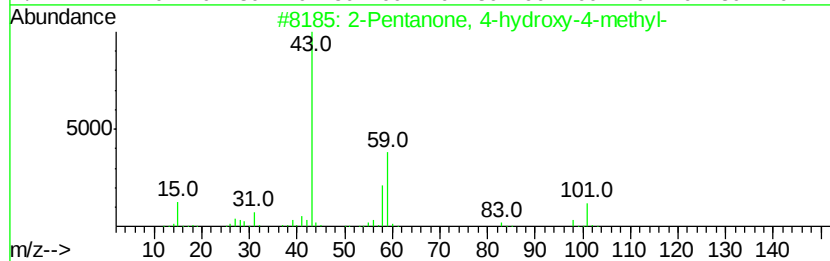
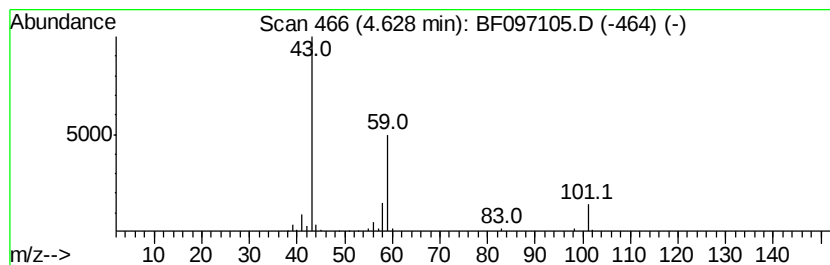
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.63	6.53 ng	187891	1,4-Dichlorobenzene-d4	6.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethv...	141	C7H11NO2	001116-98-9	25
4	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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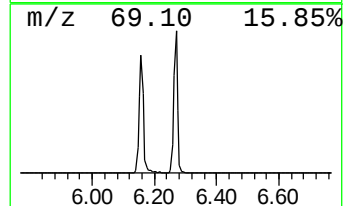
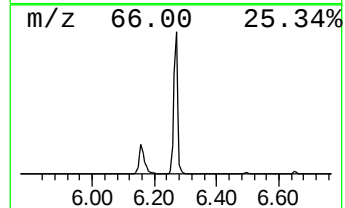
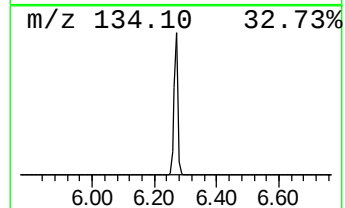
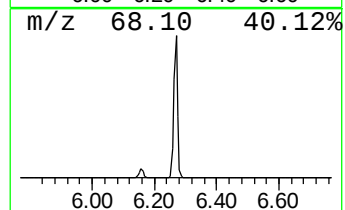
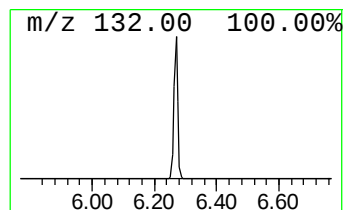
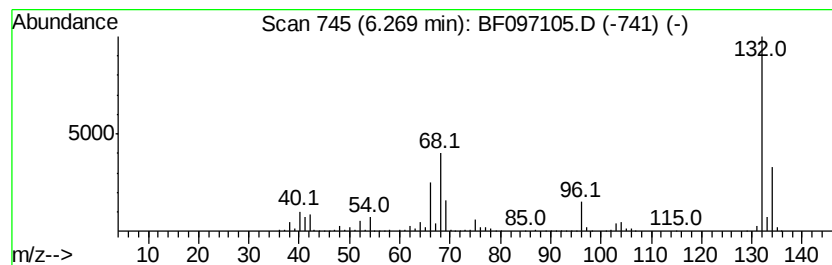
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	60.13 ng	1728730	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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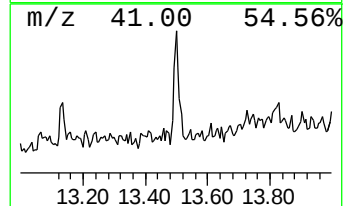
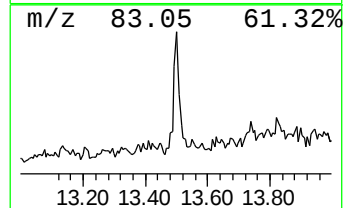
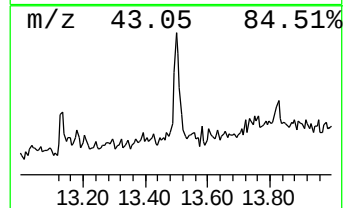
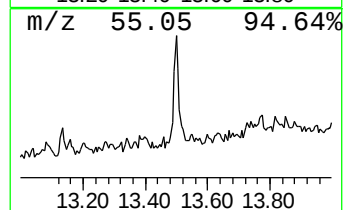
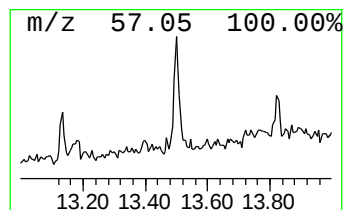
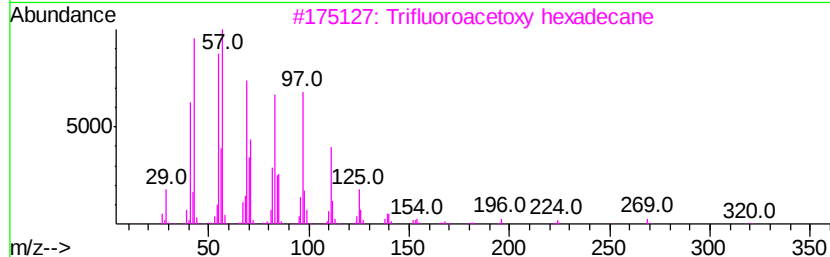
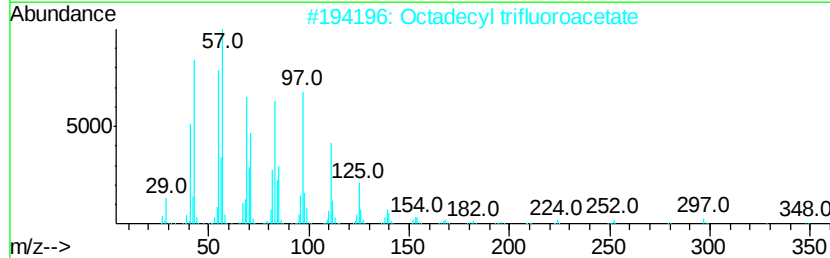
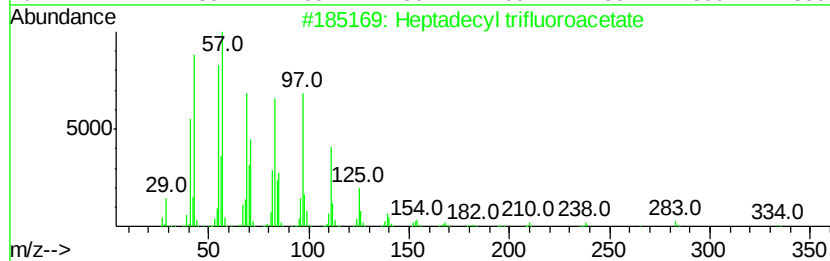
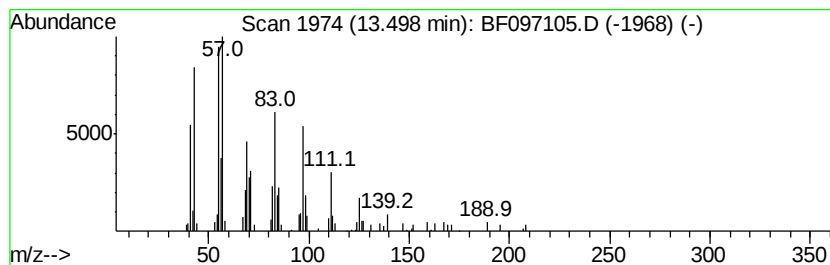
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	3.97 ng	115161	Chrysene-d12	13.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5		1-Hexadecanol	242	C16H34O	036653-82-4	90



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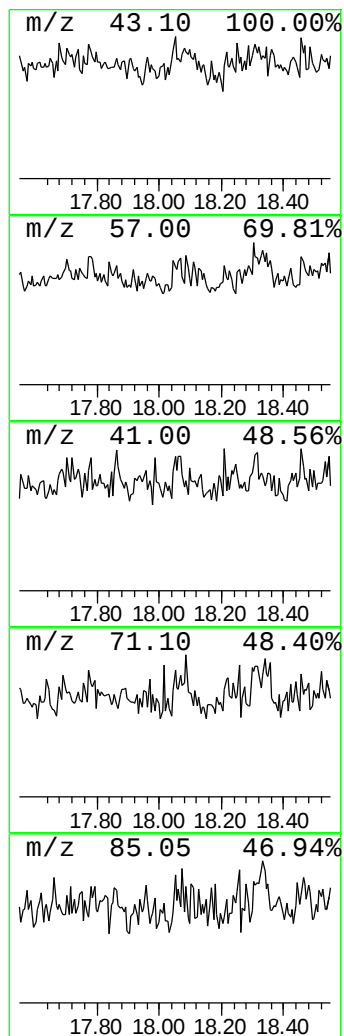
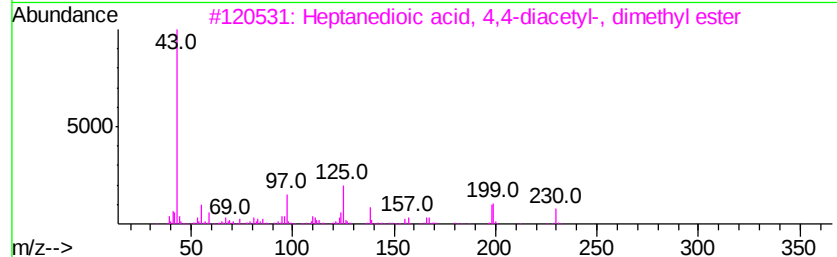
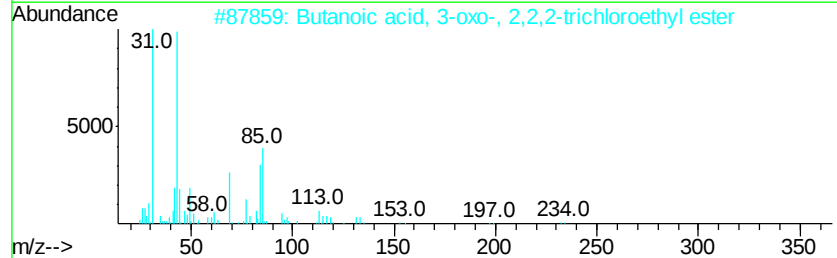
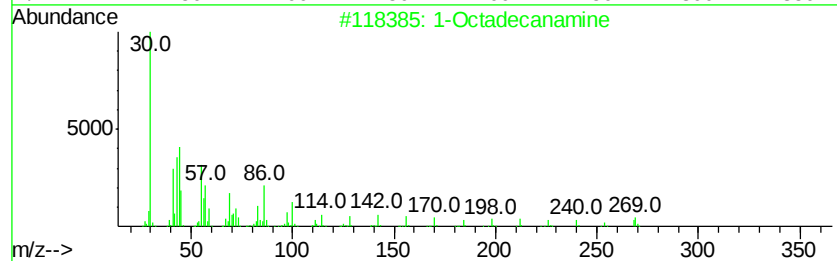
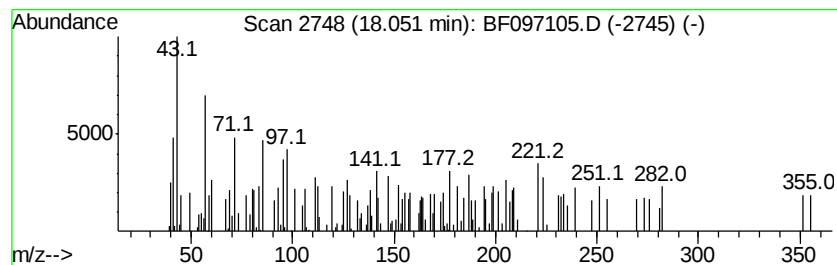
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown18.05 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	2.14 ng	39687	Perylene-d12	14.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecanamine	269	C18H39N	000124-30-1	25
2		Butanoic acid, 3-oxo-, 2,2,2-tri...	232	C6H7Cl3O3	058547-15-2	12
3		Heptanedioic acid, 4,4-diacetyl-...	272	C13H20O6	013984-59-3	10
4		Eicosane	282	C20H42	000112-95-8	9
5		Cyclooct-4-en-1-ol, 8-iodo-, ace...	294	C10H15IO2	344302-49-4	9



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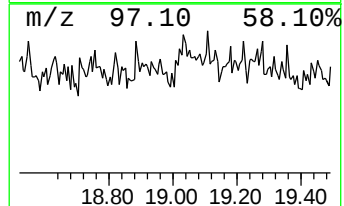
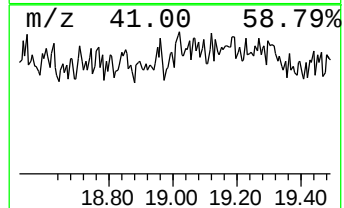
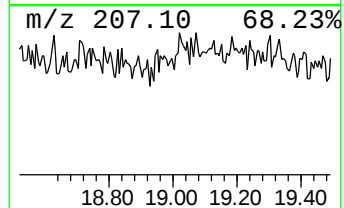
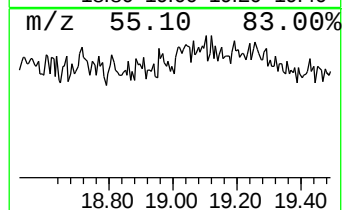
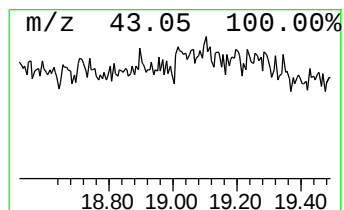
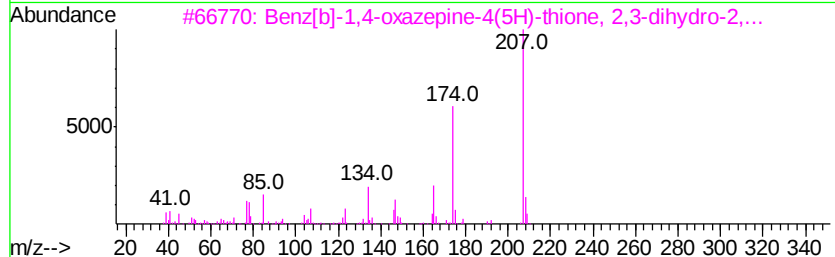
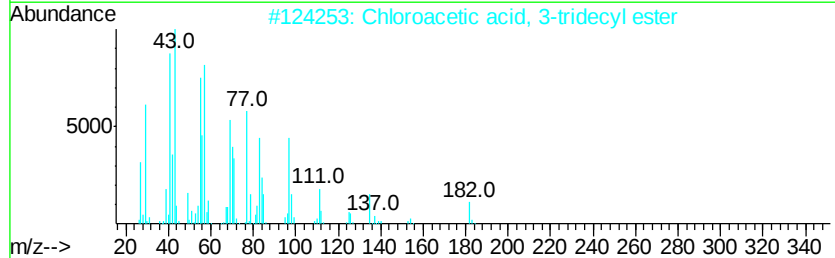
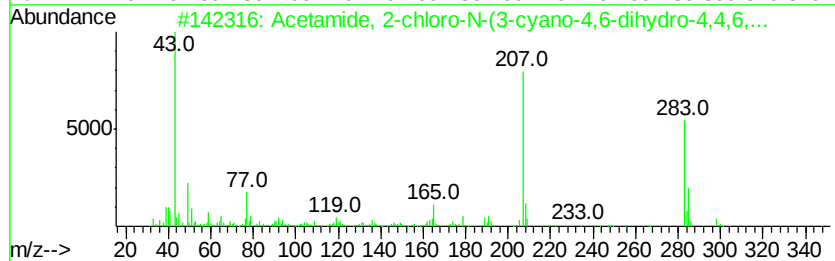
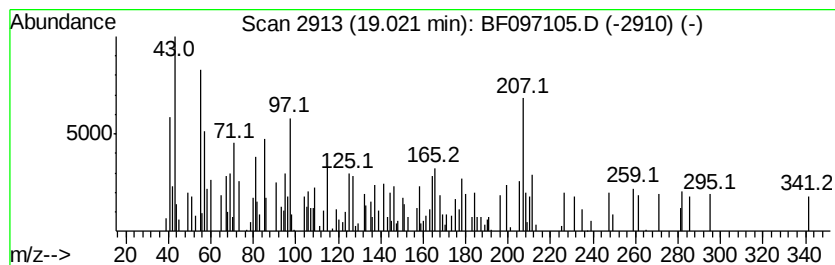
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown19.02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	2.28 ng	42160	Perylene-d12	14.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetamide, 2-chloro-N-(3-cyano-4...	298	C13H15ClN2O2S	1000350-39-4	27
2		Chloroacetic acid, 3-tridecyl ester	276	C15H29ClO2	1000280-08-2	16
3		Benz[b]1,4-oxazepine-4(5H)-thio...	207	C11H13NOS	1000258-63-4	11
4		4H-Pyran-4-one, 3,5-diacetyl-2,6...	208	C11H12O4	019396-77-1	10
5		Pyrido[2,3-d]pyrimidine, 4-phenyl-	207	C13H9N3	028732-75-4	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	6.5	ng	187891	1	6.50	575046	20.0
unknown6.27	6.27	60.1	ng	1728730	1	6.50	575046	20.0
Heptadecyl triflu...	13.50	4.0	ng	115161	5	13.63	580034	20.0
unknown18.05	18.05	2.1	ng	39687	6	14.98	370299	20.0
unknown19.02	19.02	2.3	ng	42160	6	14.98	370299	20.0