

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083118\
 Data File : BF108730.D
 Acq On : 1 Sep 2018 10:33
 Operator : JU/SJ
 Sample : J4729-16
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 082918-TIPC-E-D-S

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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	5.684	560	569	572	rBV4	27998	84476	3.42%	0.647%
2	6.660	730	735	740	rBV	47922	99180	4.02%	0.759%
3	6.772	751	754	790	rVB	375683	960424	38.89%	7.353%
4	7.007	790	794	815	rVB	129737	379384	15.36%	2.905%
5	7.154	815	819	844	rBV	1210065	1764455	71.44%	13.509%
6	7.566	886	889	912	rBV	441897	1214806	49.19%	9.301%
7	8.284	1007	1011	1040	rBV	157354	462056	18.71%	3.538%
8	9.348	1189	1192	1227	rBV	1485023	2372531	96.07%	18.164%
9	9.748	1256	1260	1271	rBV	23730	39869	1.61%	0.305%
10	10.036	1306	1309	1334	rBV2	299580	457468	18.52%	3.502%
11	10.695	1418	1421	1428	rBV	59151	58875	2.38%	0.451%
12	10.836	1441	1445	1470	rBV	377768	809970	32.80%	6.201%
13	11.542	1559	1565	1577	rBV	266613	516643	20.92%	3.955%
14	12.454	1714	1720	1724	rBV	23050	24721	1.00%	0.189%
15	13.118	1829	1833	1857	rBV	2088301	2469686	100.00%	18.908%
16	14.101	1992	2000	2003	rBV6	20926	59327	2.40%	0.454%
17	14.195	2012	2016	2025	rBV	412710	590090	23.89%	4.518%
18	14.936	2139	2142	2145	rBV	37427	38283	1.55%	0.293%
19	15.018	2152	2156	2161	rBV	32919	37871	1.53%	0.290%
20	15.295	2199	2203	2210	rVB	35269	42415	1.72%	0.325%
21	15.707	2268	2273	2276	rBV	37271	52285	2.12%	0.400%
22	15.748	2276	2280	2297	rVB	194476	393559	15.94%	3.013%
23	16.177	2348	2353	2359	rVB	33024	51103	2.07%	0.391%
24	16.718	2440	2445	2452	rVB2	27606	46377	1.88%	0.355%
25	17.365	2549	2555	2563	rVB5	15314	35651	1.44%	0.273%

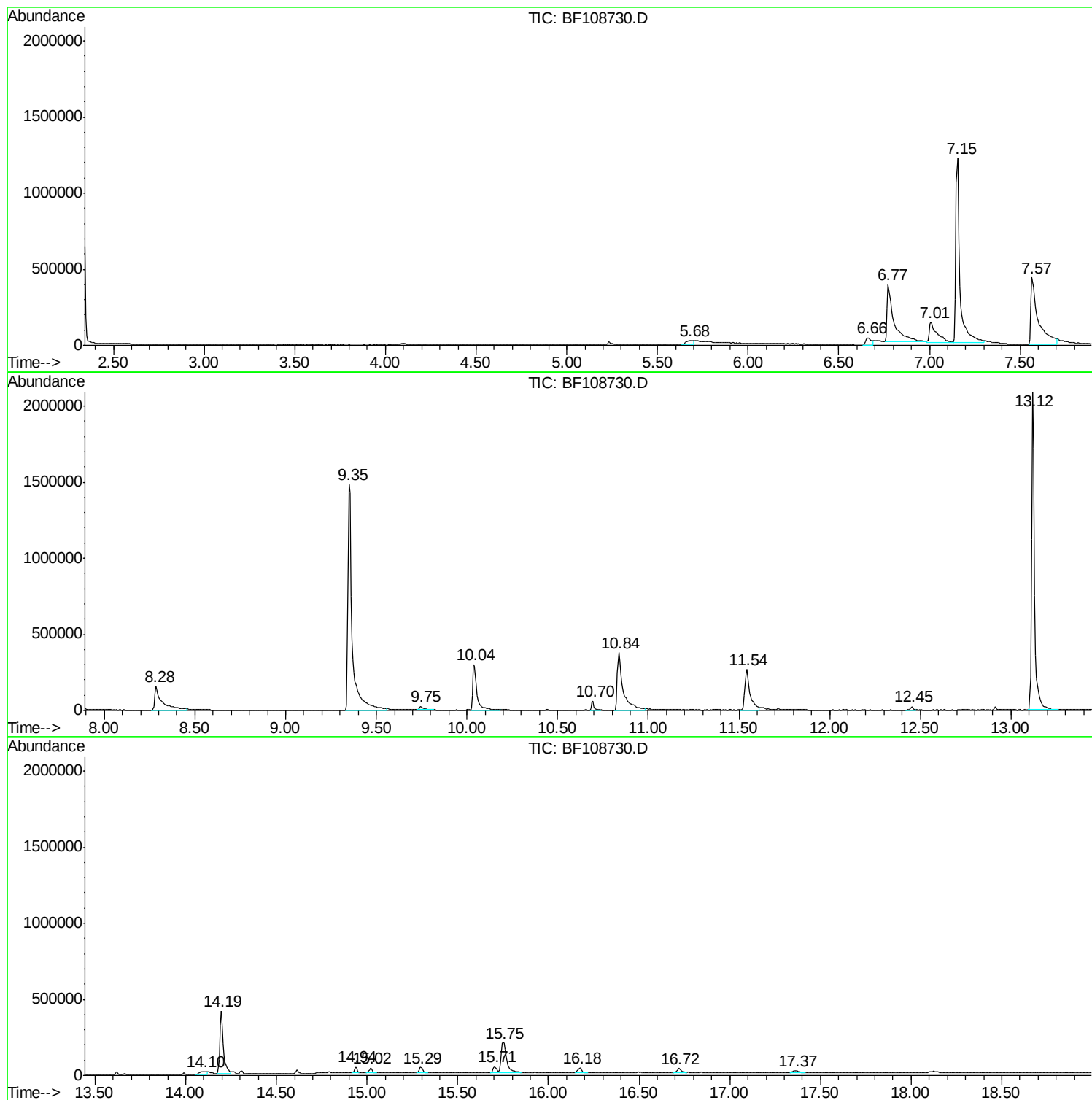
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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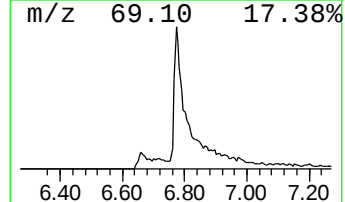
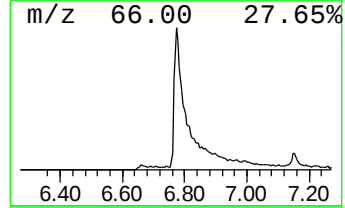
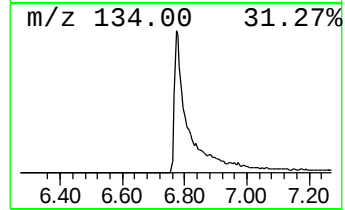
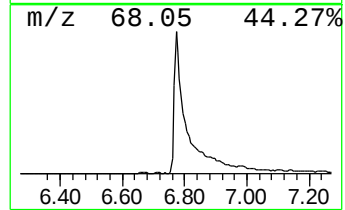
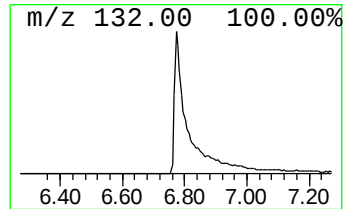
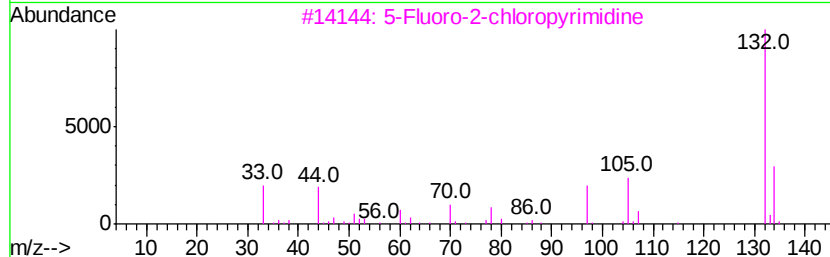
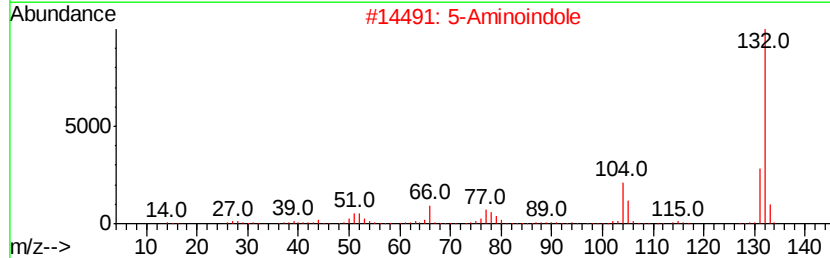
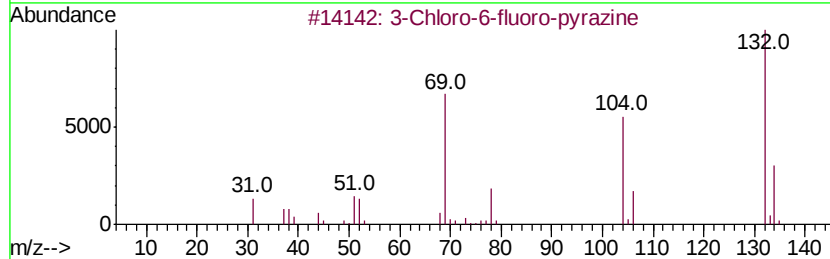
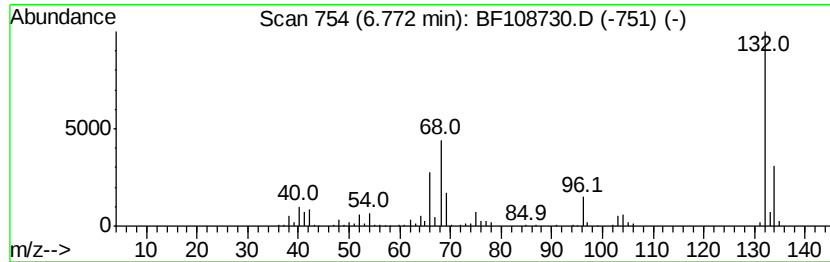
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	50.63 ng	960424	1,4-Dichlorobenzene-d4	7.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	22
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4			(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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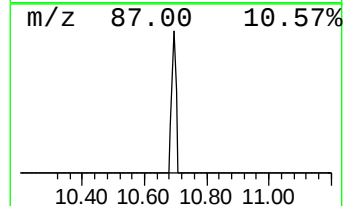
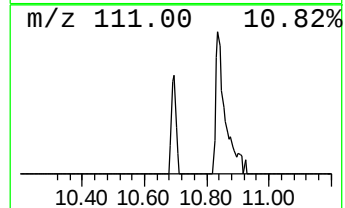
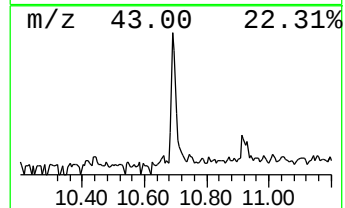
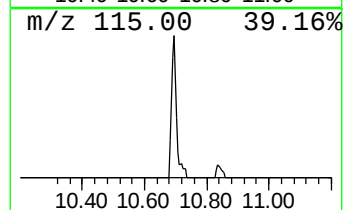
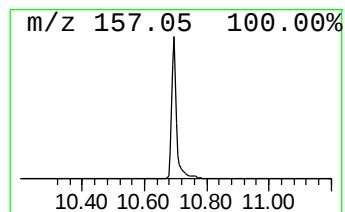
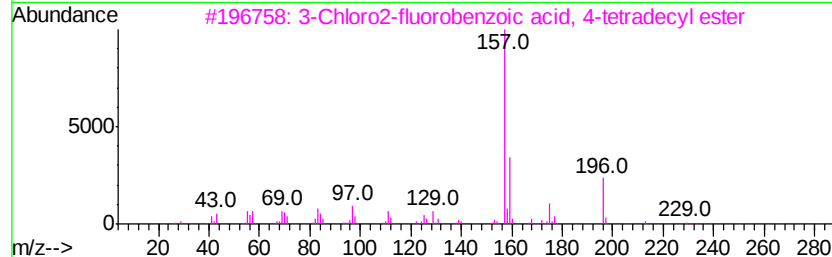
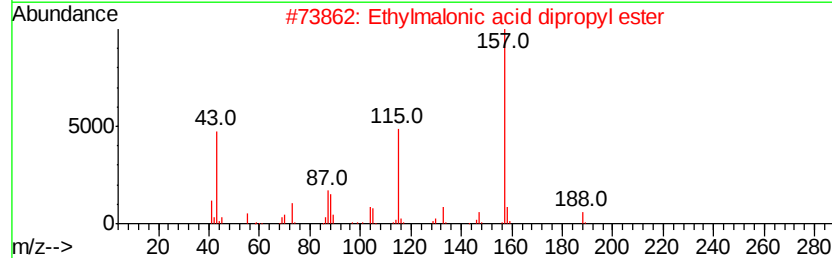
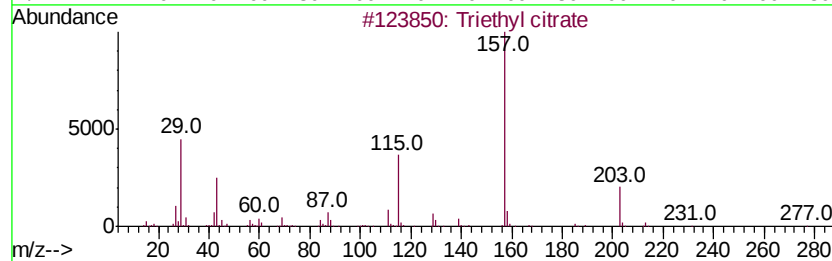
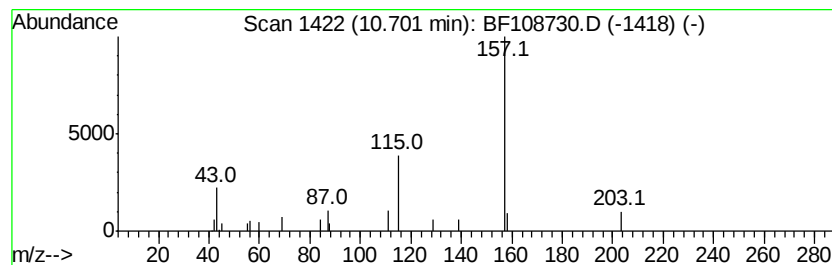
Instrument :
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ClientSampleId :
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Peak Number 3 Triethyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.70	2.57 ng	58875	Acenaphthene-d10		10.04
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	86
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	50
3	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClF02	1000338-64-7	36
4	3-Chloro2-fluorobenzoic acid, 6-...	342	C19H28ClF02	1000338-64-1	36
5	3-Chloro2-fluorobenzoic acid, 6-...	370	C21H32ClF02	1000338-64-9	36



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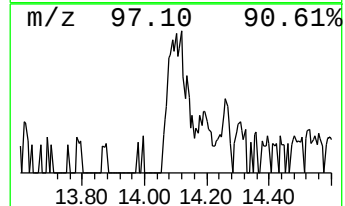
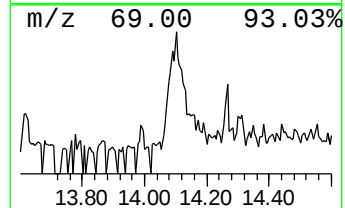
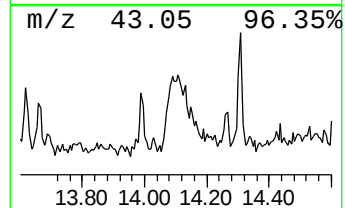
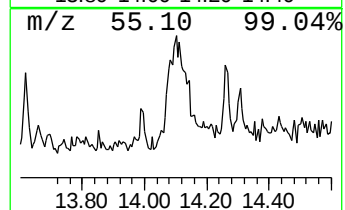
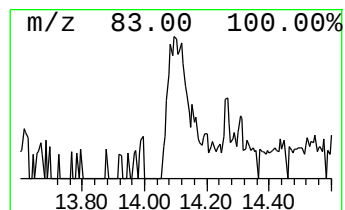
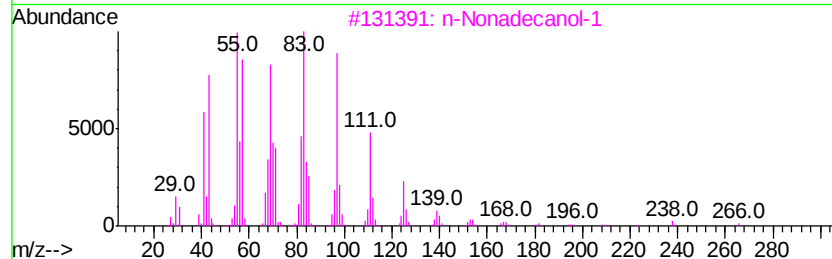
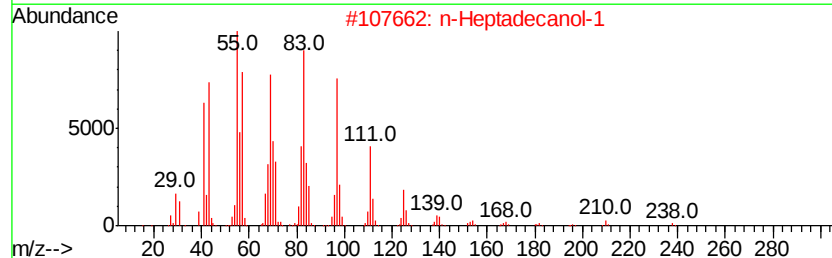
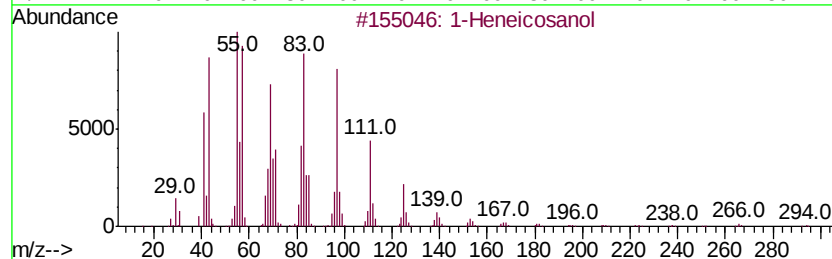
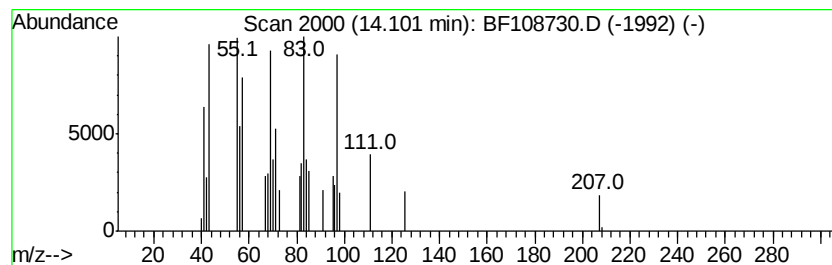
Instrument :
BNA_F
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	2.01 ng	59327	Chrysene-d12	14.19
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol	312 C21H44O	015594-90-8	90
2	n-Heptadecanol-1	256 C17H36O	001454-85-9	90
3	n-Nonadecanol-1	284 C19H40O	001454-84-8	87
4	11-Tricosene	322 C23H46	052078-56-5	87
5	3-Eicosene, (E)-	280 C20H40	074685-33-9	86



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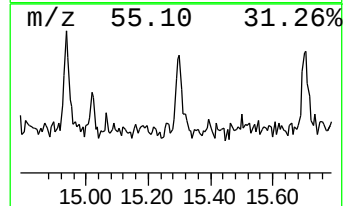
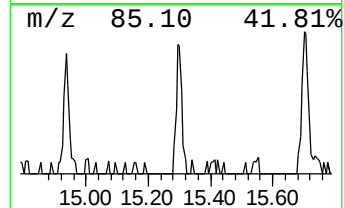
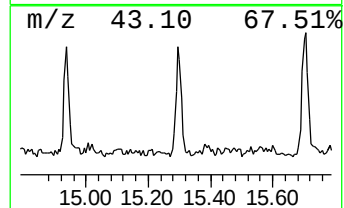
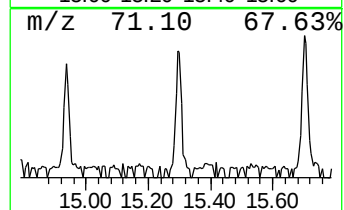
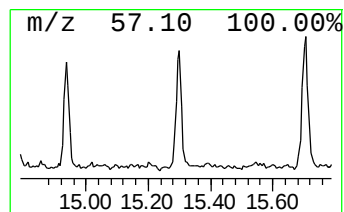
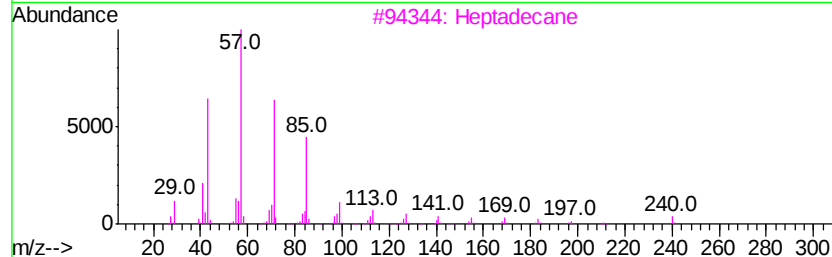
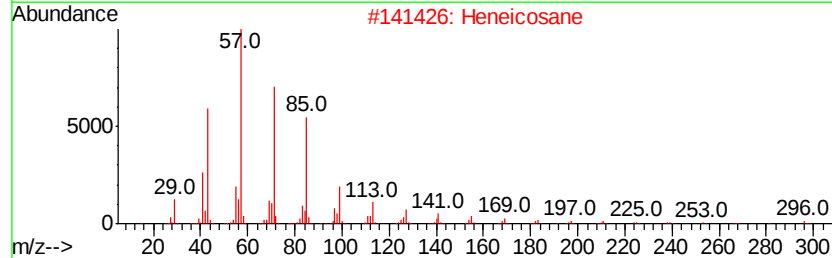
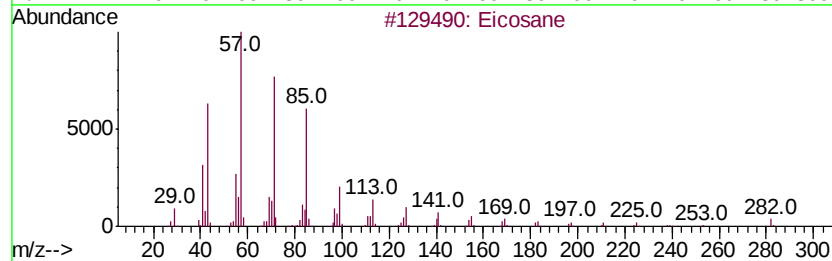
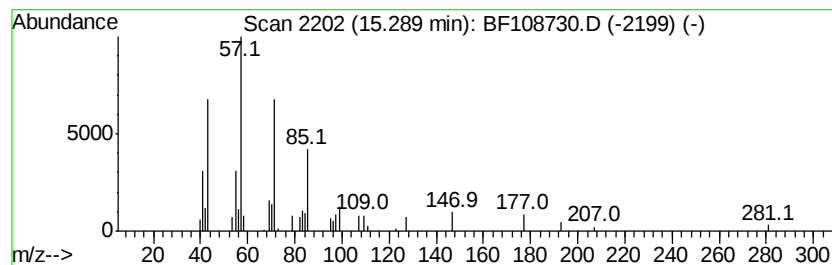
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.16 ng	42415	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	87
2	Heneicosane		296	C21H44	000629-94-7	83
3	Heptadecane		240	C17H36	000629-78-7	80
4	Hexadecane		226	C16H34	000544-76-3	80
5	Octadecane		254	C18H38	000593-45-3	80



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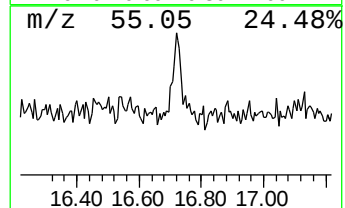
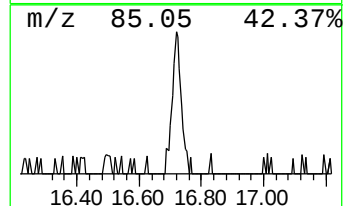
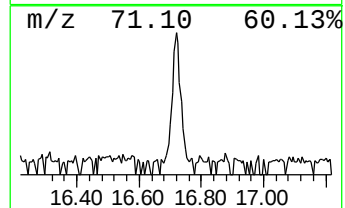
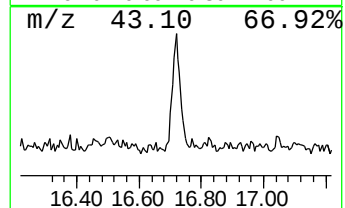
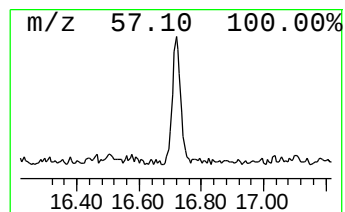
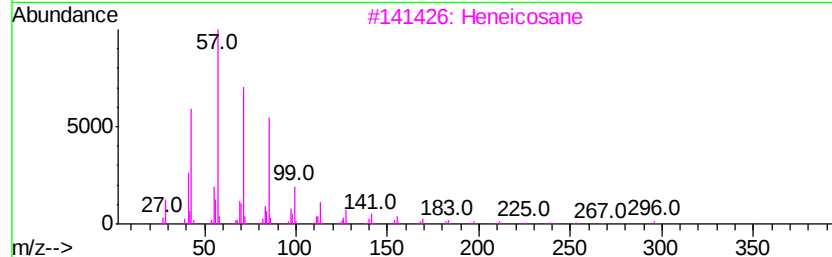
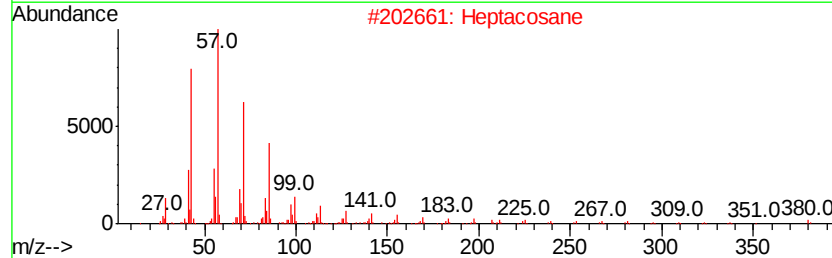
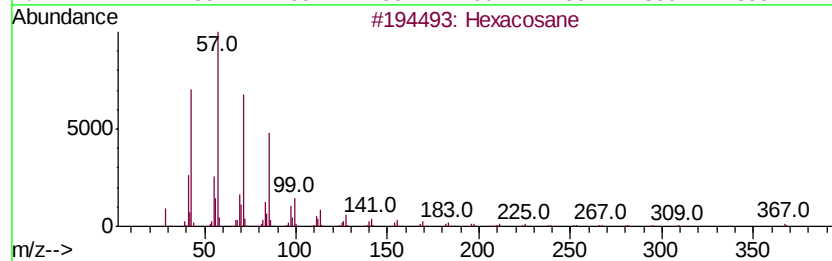
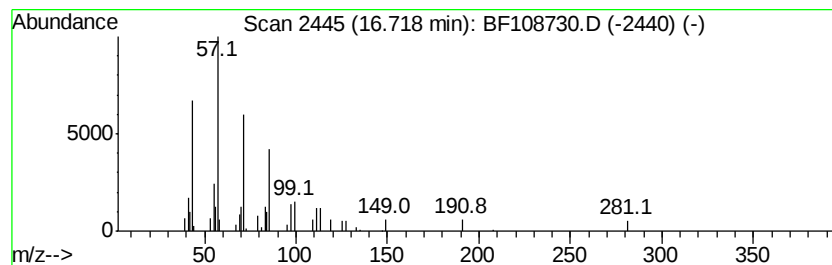
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.36 ng	46377	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	86
2	Heptacosane		380	C27H56	000593-49-7	86
3	Heneicosane		296	C21H44	000629-94-7	80
4	Heptacosane, 1-chloro-		414	C27H55Cl	062016-79-9	78
5	Sulfurous acid, 2-propyl tridecy...		306	C16H34O3S	1000309-12-4	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.77	6.77	50.6	ng	960424	1	7.01	379384	20.0
Triethyl citrate	10.70	2.6	ng	58875	3	10.04	457468	20.0
1-Heneicosanol	14.10	2.0	ng	59327	5	14.19	590090	20.0
Eicosane	15.29	2.2	ng	42415	6	15.75	393559	20.0
Hexacosane	16.72	2.4	ng	46377	6	15.75	393559	20.0