

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
 Data File : BF104752.D
 Acq On : 24 Apr 2018 13:26
 Operator : JU/SJ
 Sample : J2493-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RS-RO-RT-27438

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-BF040618.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	5.016	493	498	506	rVB	73422	95758	3.27%	0.375%
2	5.434	564	569	579	rBV	1980325	1944948	66.46%	7.627%
3	6.451	737	742	760	rBV	1939143	2034024	69.51%	7.976%
4	6.581	760	764	767	rBV	2400048	2027904	69.30%	7.952%
5	6.804	799	802	806	rBV	746258	622592	21.28%	2.441%
6	6.963	825	829	832	rBV	1668052	1362946	46.58%	5.345%
7	7.375	894	899	902	rBV	1305581	1229310	42.01%	4.821%
8	8.092	1017	1021	1024	rBV	964470	825578	28.21%	3.237%
9	8.516	1088	1093	1097	rVB7	13493	29341	1.00%	0.115%
10	9.163	1199	1203	1207	rBV	1769815	1612067	55.09%	6.321%
11	9.239	1213	1216	1219	rVB	48614	43660	1.49%	0.171%
12	9.392	1238	1242	1243	rBV3	23262	29817	1.02%	0.117%
13	9.557	1266	1270	1273	rBV	228988	251478	8.59%	0.986%
14	9.710	1293	1296	1298	rBV3	37313	37368	1.28%	0.147%
15	9.751	1300	1303	1304	rVV2	51068	40906	1.40%	0.160%
16	9.769	1304	1306	1308	rVB	65814	45494	1.55%	0.178%
17	9.851	1316	1320	1323	rVB	956025	901703	30.81%	3.536%
18	10.092	1359	1361	1365	rBV4	53181	73246	2.50%	0.287%
19	10.257	1385	1389	1394	rBV	694946	917541	31.35%	3.598%
20	10.492	1426	1429	1434	rVB	116592	125905	4.30%	0.494%
21	10.645	1451	1455	1458	rBV	1448515	1346235	46.00%	5.279%
22	10.757	1470	1474	1477	rBV	310074	363165	12.41%	1.424%
23	11.222	1550	1553	1560	rVB	342159	365409	12.49%	1.433%
24	11.339	1570	1573	1579	rBV	1086679	1054102	36.02%	4.133%
25	11.575	1610	1613	1617	rBV	163901	165810	5.67%	0.650%
26	12.557	1777	1780	1784	rVB	140521	141644	4.84%	0.555%
27	12.786	1816	1819	1823	rBV	138692	134714	4.60%	0.528%
28	12.927	1838	1843	1847	rVB	2478591	2926332	100.00%	11.475%
29	13.398	1920	1923	1926	rVB	237382	205361	7.02%	0.805%
30	13.457	1930	1933	1935	rBV	155680	127052	4.34%	0.498%
31	13.816	1991	1994	1997	rVB	191801	182566	6.24%	0.716%
32	13.951	2014	2017	2020	rBV	272127	322011	11.00%	1.263%
33	13.992	2020	2024	2026	rVV2	1162547	1293073	44.19%	5.071%
34	14.016	2026	2028	2033	rVB	303062	252983	8.65%	0.992%

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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

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35	14.545	2115	2118	2121	rBV2	61016	71314	2.44%	0.280%
36	14.580	2121	2124	2128	rBV	142623	143571	4.91%	0.563%
37	14.886	2172	2176	2191	rVB10	110682	338245	11.56%	1.326%
38	15.033	2197	2201	2203	rBV	167035	195769	6.69%	0.768%
39	15.063	2203	2206	2208	rVV	123102	128949	4.41%	0.506%
40	15.092	2208	2211	2221	rVB2	105540	214431	7.33%	0.841%
41	15.398	2260	2263	2269	rVB	102206	119729	4.09%	0.469%
42	15.463	2269	2274	2282	rBV	696141	879751	30.06%	3.450%
43	16.151	2385	2391	2398	rBV5	126173	277862	9.50%	1.090%

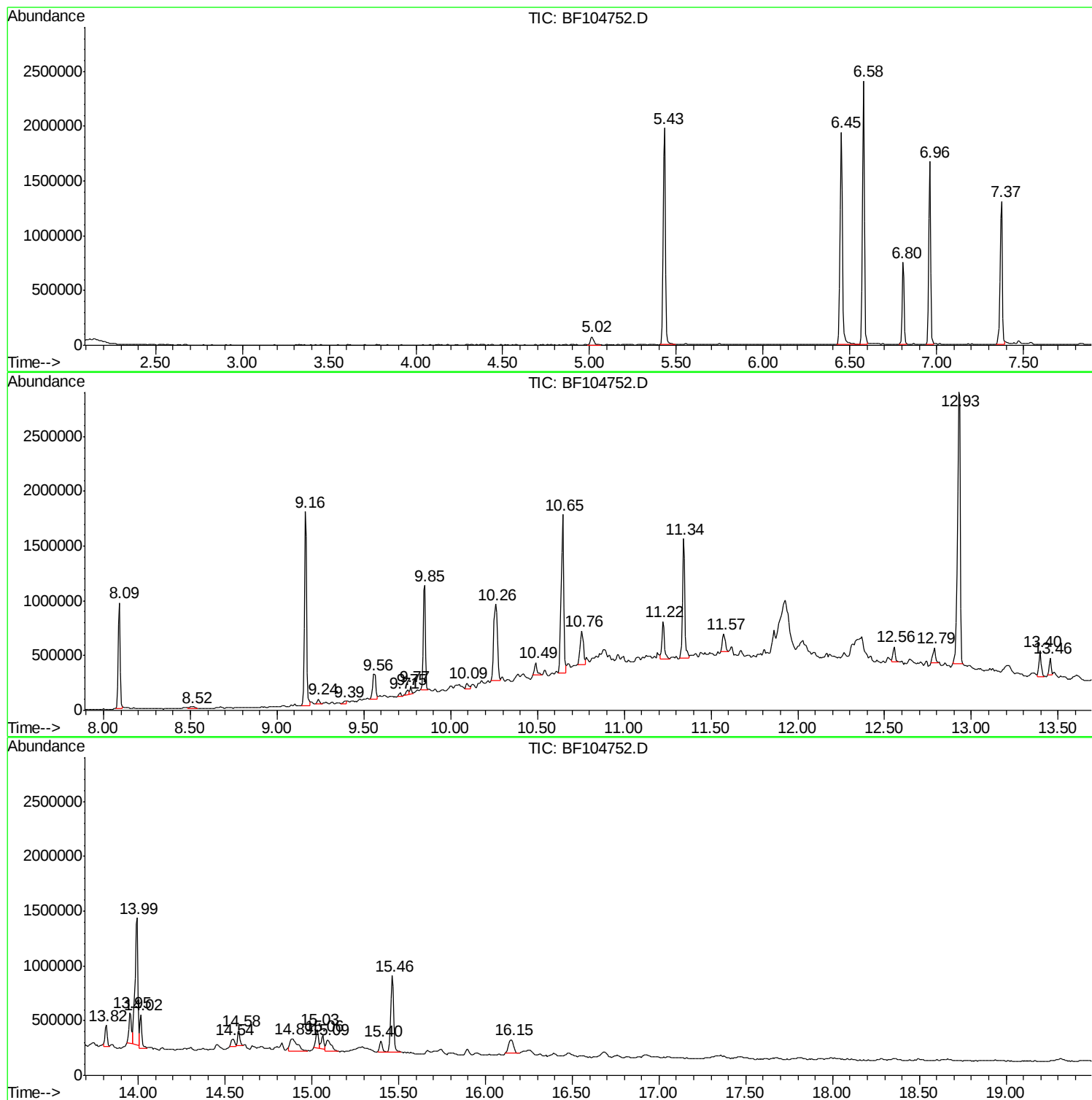
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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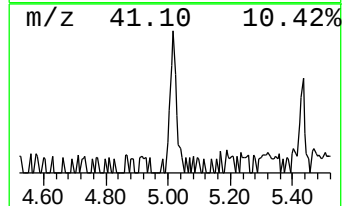
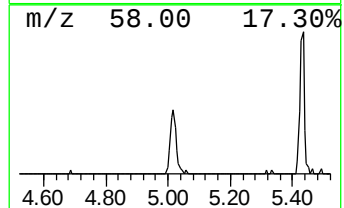
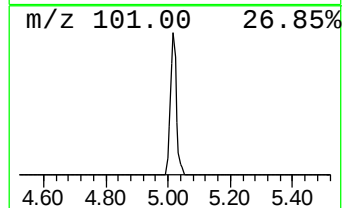
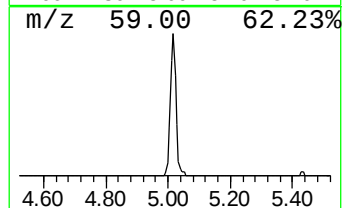
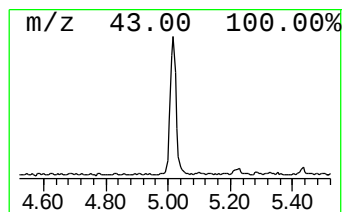
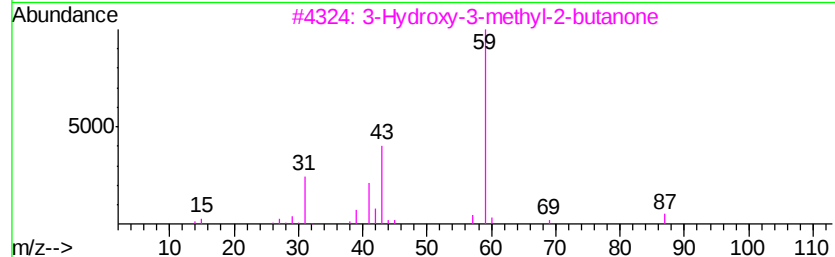
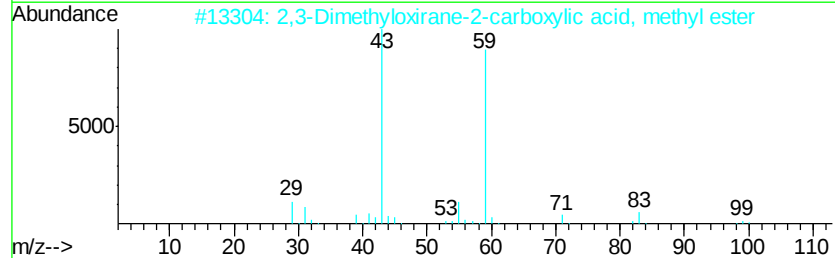
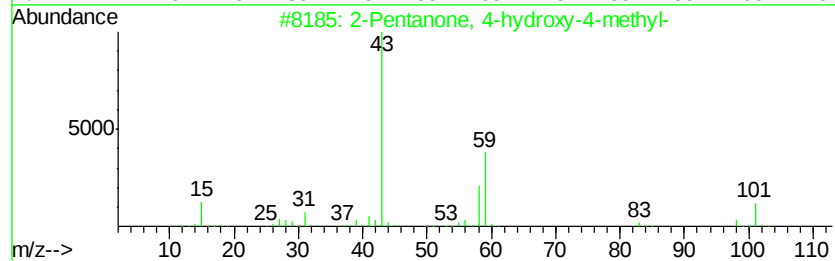
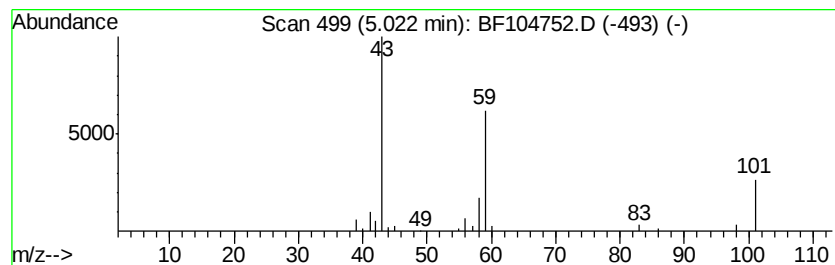
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.08 ng	95758	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	23
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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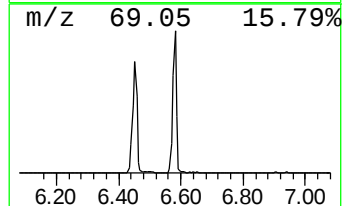
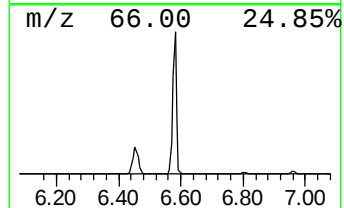
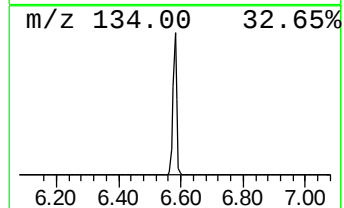
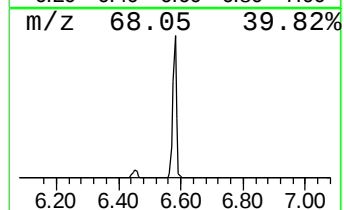
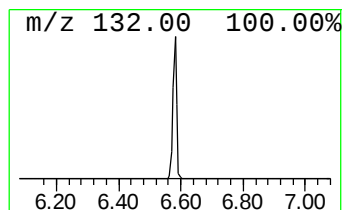
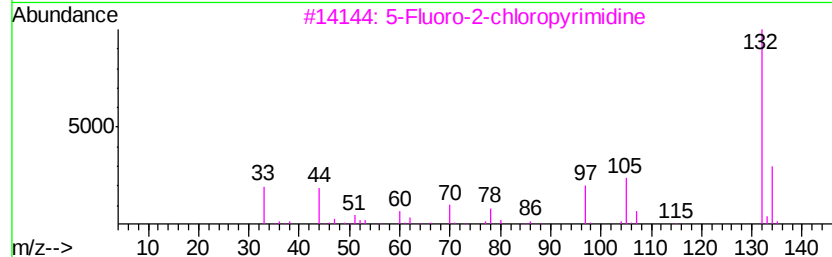
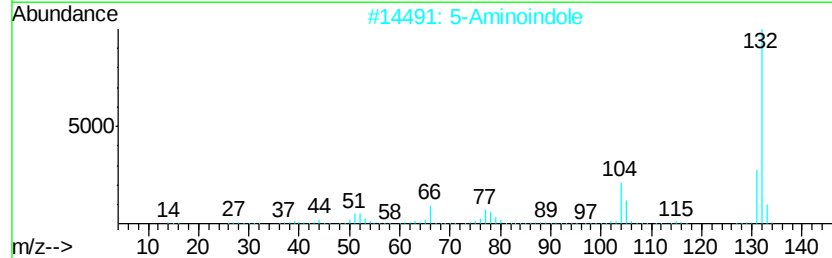
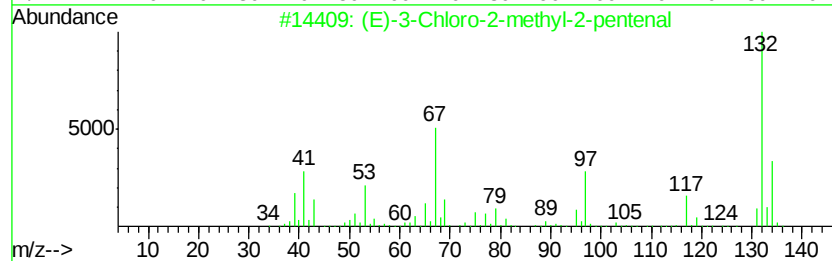
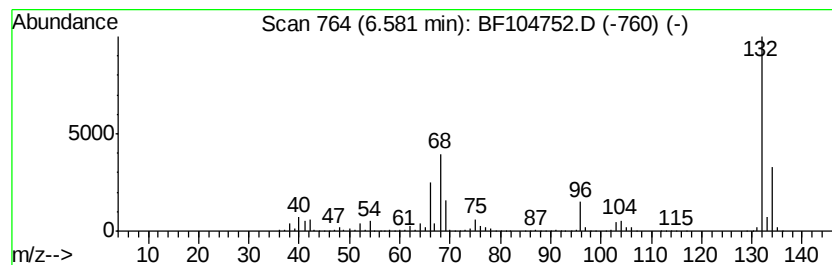
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	65.14 ng	2027900	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	16
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-6-fluoro-pyrimidine			132	C4H2ClFN2	051422-01-6	9
5	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	9



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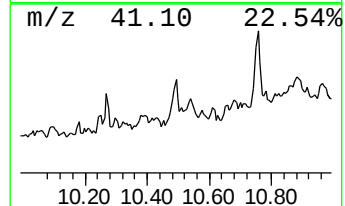
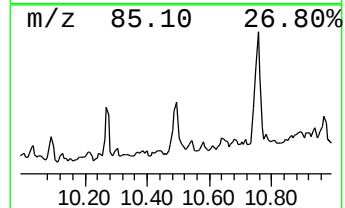
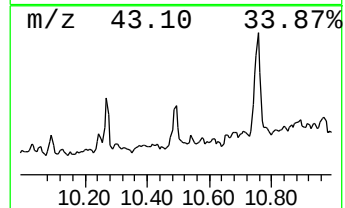
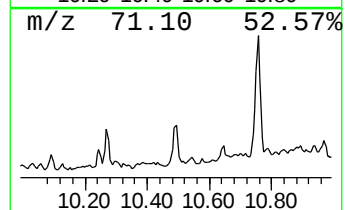
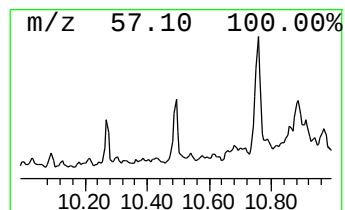
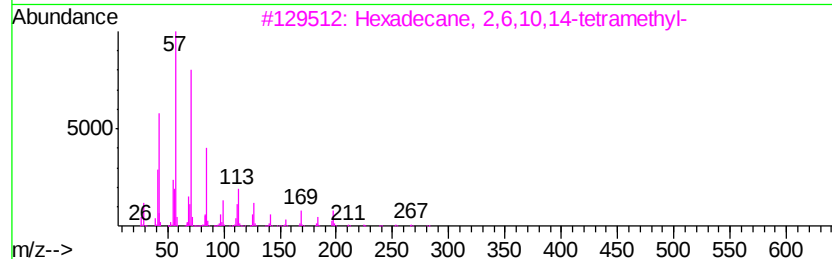
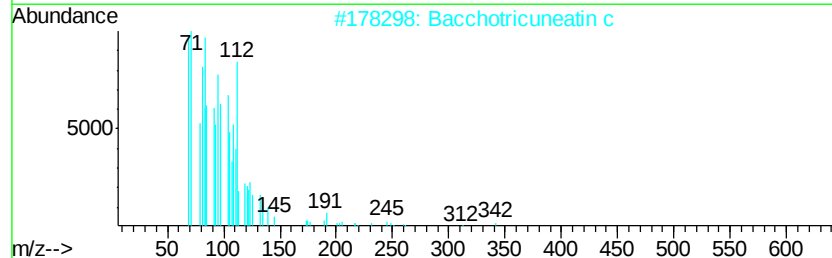
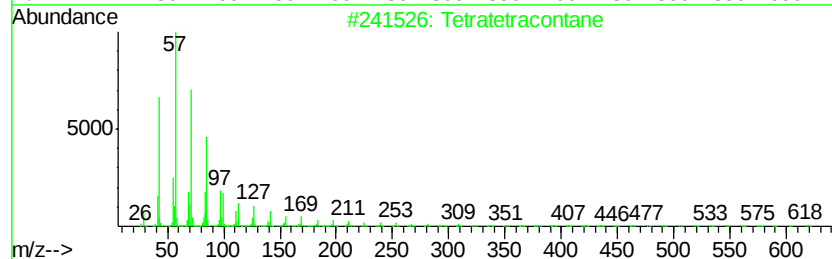
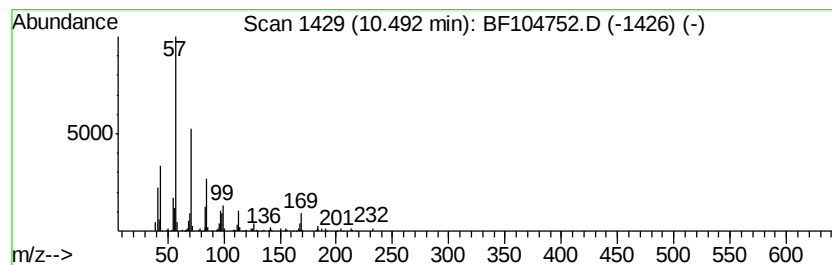
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.49	2.79 ng	125905	Acenaphthene-d10	9.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetratetracontane	619 C44H90	007098-22-8 59
2		Bacchotricuneatin c	342 C20H22O5	066563-30-2 58
3		Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42	000638-36-8 53
4		Undecane	156 C11H24	001120-21-4 50
5		Tritetracontane	605 C43H88	007098-21-7 50



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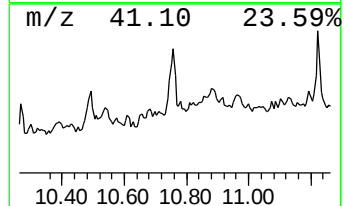
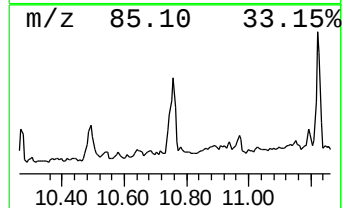
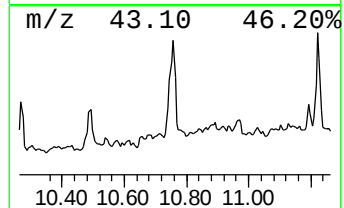
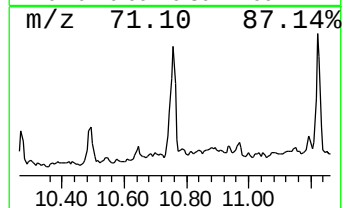
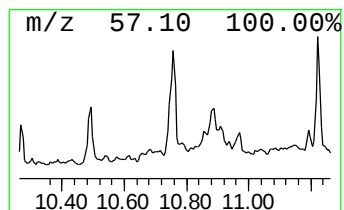
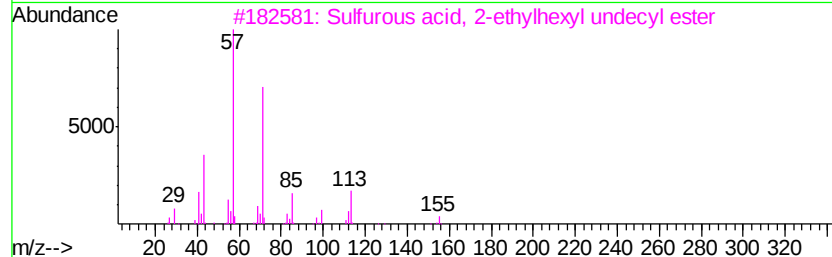
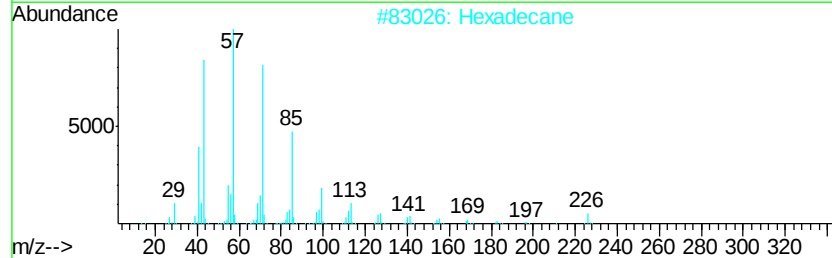
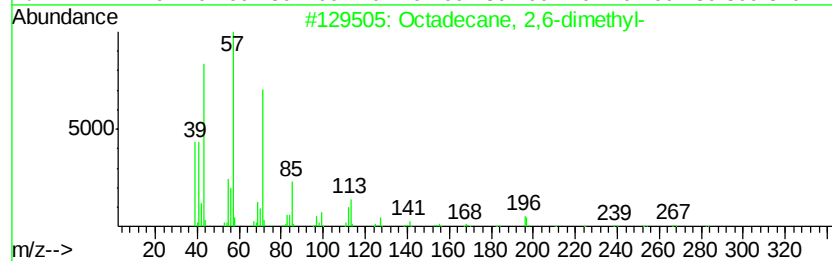
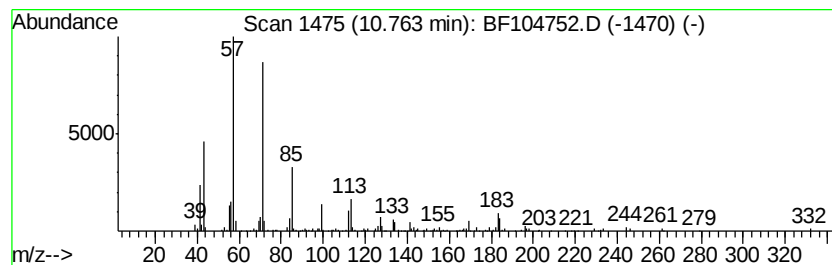
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecane, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.76	6.89 ng	363165	Phenanthrene-d10		11.34
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	80
2	Hexadecane	226	C16H34	000544-76-3	80
3	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	74
4	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	72
5	Tridecane, 7-methyl-	198	C14H30	026730-14-3	70



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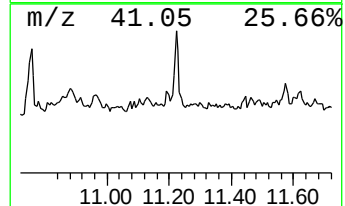
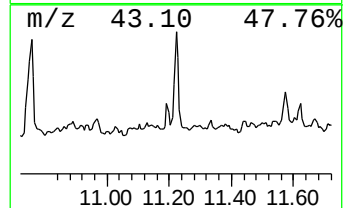
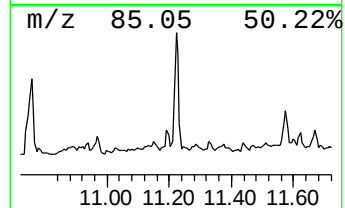
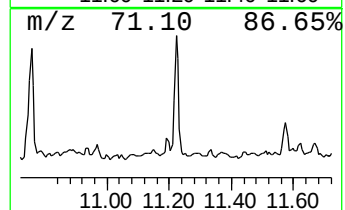
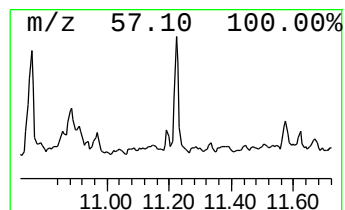
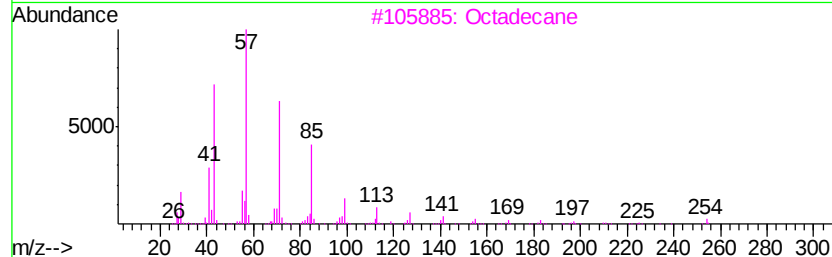
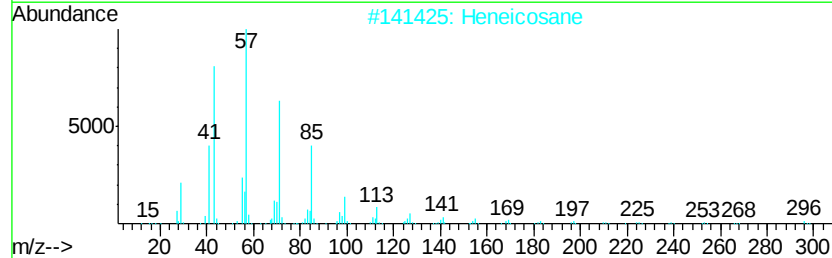
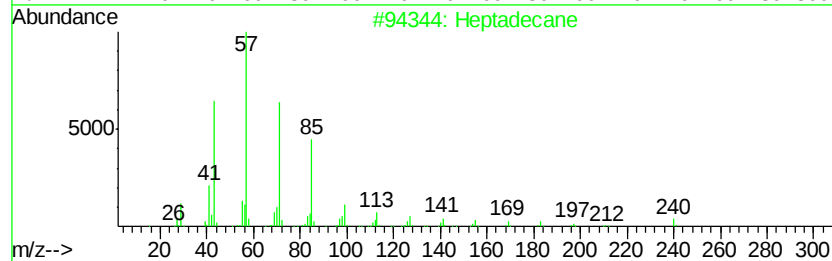
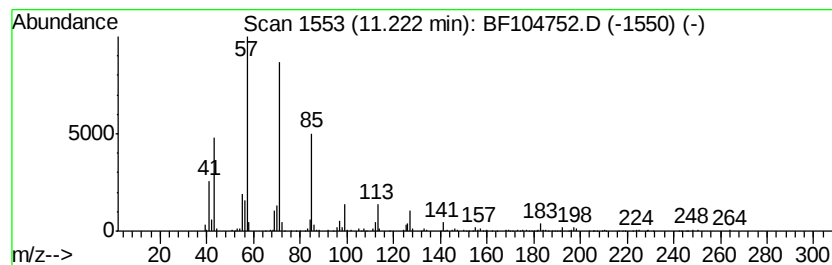
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.22	6.93 ng	365409	Phenanthrene-d10	11.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042418\
Data File : BF104752.D
Acq On : 24 Apr 2018 13:26
Operator : JU/SJ
Sample : J2493-01
Misc :
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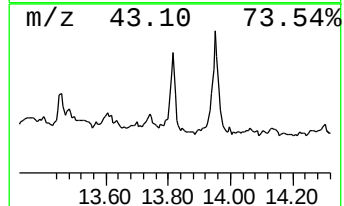
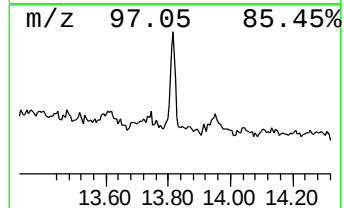
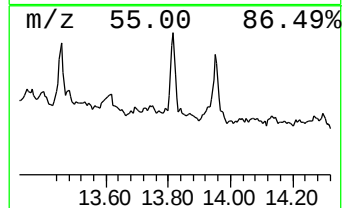
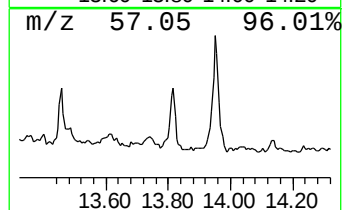
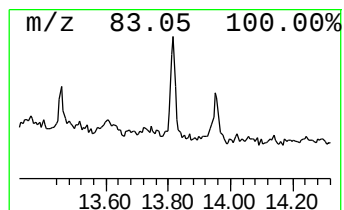
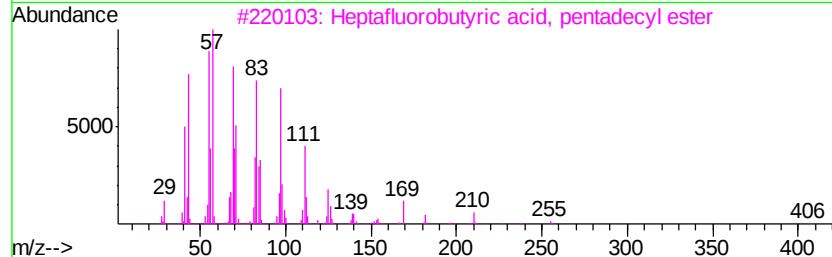
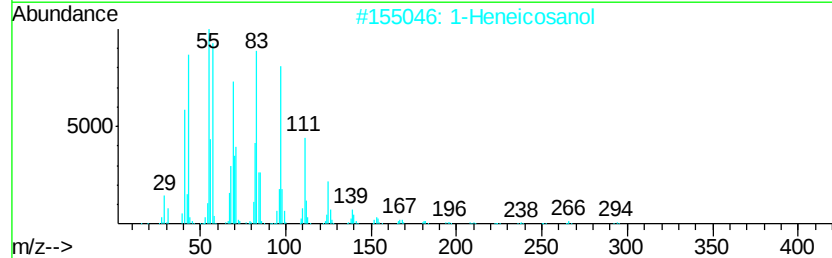
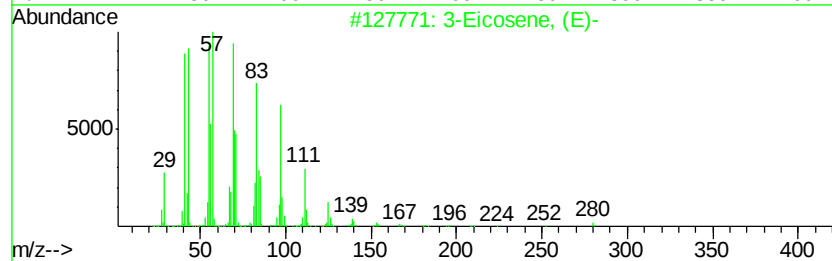
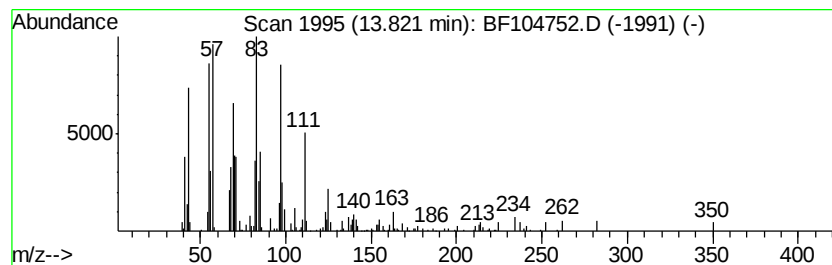
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ClientSampleId :
RS-RO-RT-27438

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.82	2.82 ng	182566	Chrysene-d12		13.99		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Heptafluorobutyric acid, pentadecanoic acid	424	C19H31F7O2	959261-23-5	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Behenic alcohol	326	C22H46O	000661-19-8	90



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Operator : JU/SJ
Sample : J2493-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RS-RO-RT-27438

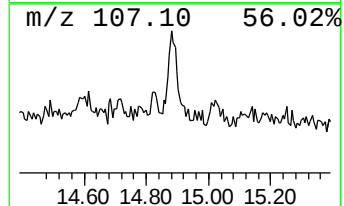
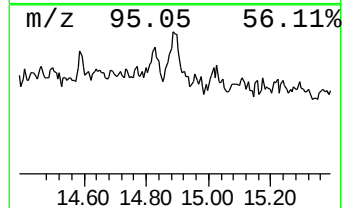
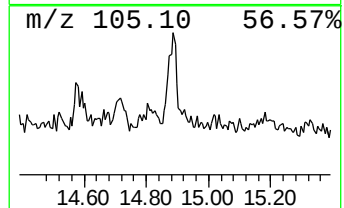
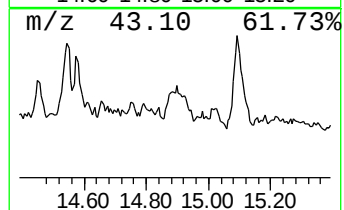
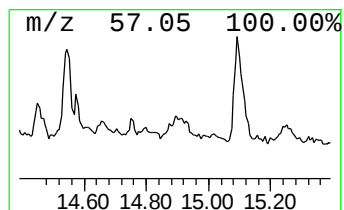
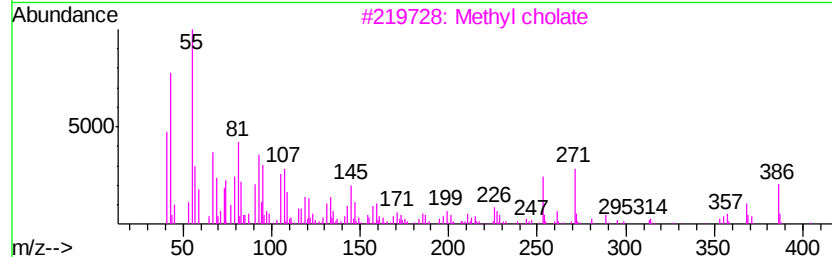
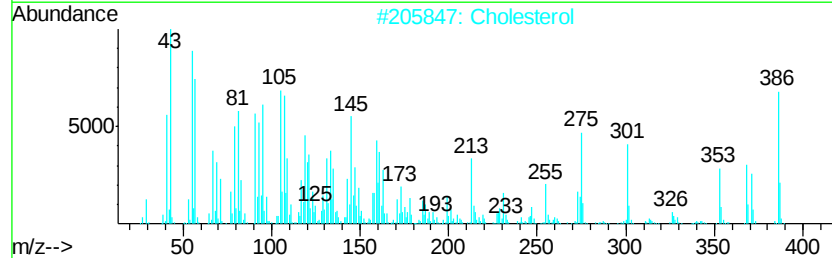
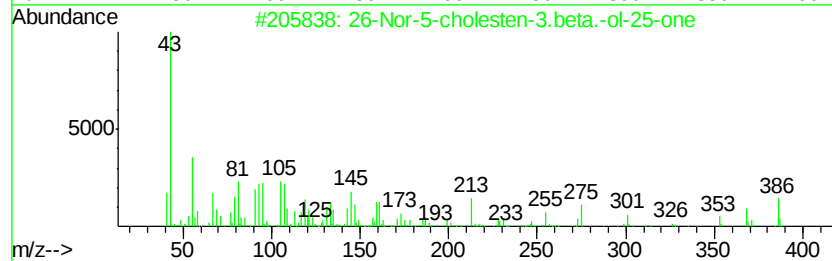
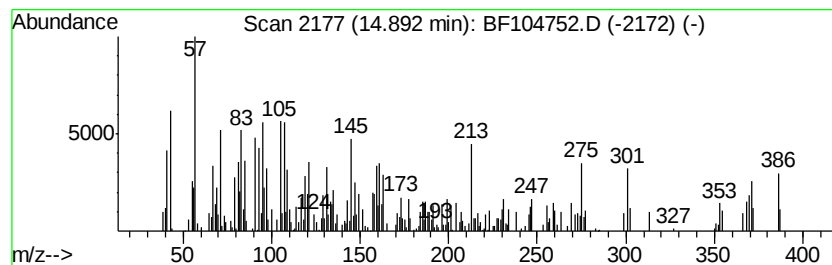
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 26-Nor-5-cholesten-3.beta.-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	7.69 ng	338245	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	95
2		Cholesterol	386	C27H46O	000057-88-5	93
3		Methyl cholate	422	C25H42O5	001448-36-8	40
4		Cholestane, 4,5-epoxy-, (4.alpha...	386	C27H46O	006079-19-2	38
5		Cholest-5-en-3-ol (3.beta.)-, pr...	442	C30H50O2	000633-31-8	22



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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RS-RO-RT-27438

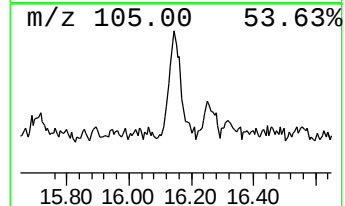
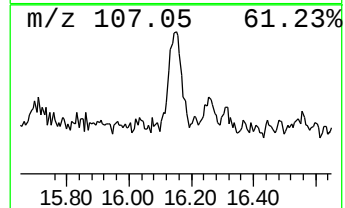
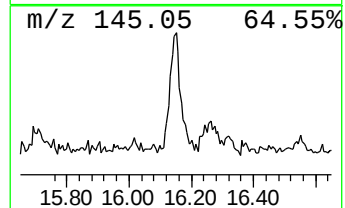
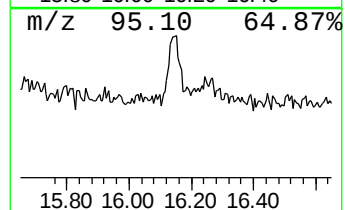
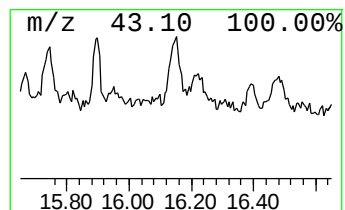
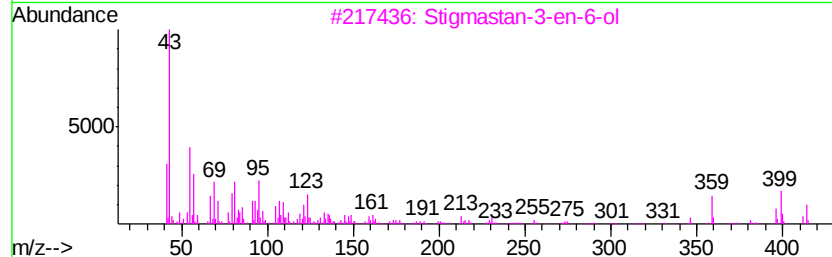
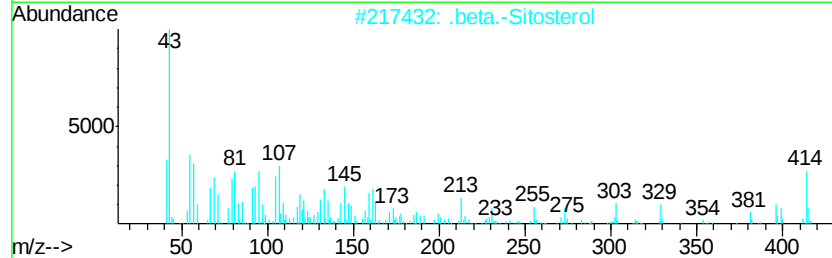
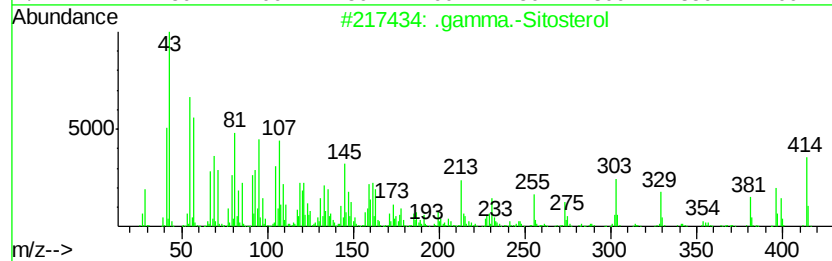
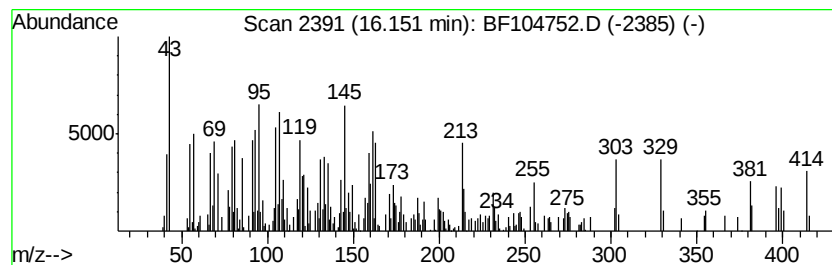
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	6.32 ng	277862	Perylene-d12	15.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	91
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	86
3		Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	10
4		5.alpha.-Stigmast-9(11)-en-3.bet...	414	C29H50O	077794-81-1	10
5		2,20-Cyclo-8,9-secoaspidospermid...	396	C24H32N2O3	056145-37-0	10



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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.02	3.1 ng		95758	1	6.80	622592	20.0
unknown6.58	6.58	65.1 ng		2027900	1	6.80	622592	20.0
Tetratetracontane	10.49	2.8 ng		125905	3	9.85	901703	20.0
Octadecane, 2,6-d...	10.76	6.9 ng		363165	4	11.34	1054100	20.0
Heptadecane	11.22	6.9 ng		365409	4	11.34	1054100	20.0
3-Eicosene, (E)-	13.82	2.8 ng		182566	5	13.99	1293070	20.0
26-Nor-5-choleste...	14.89	7.7 ng		338245	6	15.46	879751	20.0
.gamma.-Sitosterol	16.15	6.3 ng		277862	6	15.46	879751	20.0