

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
 Data File : BF096791.D
 Acq On : 15 Jul 2017 00:23
 Operator : SJ/JU
 Sample : I4187-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CI-SB1-0-2

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-BF071317.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	4.798	474	478	486	rVB	158736	215394	9.19%	0.993%
2	5.234	547	552	555	rBV	2260637	2228678	95.07%	10.275%
3	6.269	723	728	731	rBV	2152808	2208851	94.23%	10.183%
4	6.392	745	749	753	rBV	2407048	2282905	97.39%	10.525%
5	6.622	784	788	792	rBV	762862	633550	27.03%	2.921%
6	6.781	811	815	818	rBV	1766936	1479690	63.12%	6.822%
7	7.186	879	884	887	rBV	1369777	1234678	52.67%	5.692%
8	7.904	1002	1006	1010	rBV	1050584	877825	37.45%	4.047%
9	8.986	1184	1190	1193	rBV	2409835	2344143	100.00%	10.807%
10	9.374	1253	1256	1259	rBV	238786	181048	7.72%	0.835%
11	9.657	1299	1304	1307	rBV	1139432	1026396	43.79%	4.732%
12	10.104	1377	1380	1383	rVB	37664	29118	1.24%	0.134%
13	10.439	1433	1437	1441	rBV	1364091	1261640	53.82%	5.816%
14	10.574	1457	1460	1467	rBV	45010	51071	2.18%	0.235%
15	10.974	1525	1528	1532	rBV2	60827	50590	2.16%	0.233%
16	11.021	1532	1536	1539	rVB3	30937	28228	1.20%	0.130%
17	11.133	1551	1555	1557	rBV	1005943	908694	38.76%	4.189%
18	11.151	1557	1558	1562	rVB	131857	92741	3.96%	0.428%
19	11.204	1565	1567	1571	rVB	39120	30517	1.30%	0.141%
20	11.680	1645	1648	1651	rVB	56734	49887	2.13%	0.230%
21	12.333	1756	1759	1763	rBV	179632	171276	7.31%	0.790%
22	12.563	1794	1798	1804	rVB	133850	129391	5.52%	0.597%
23	12.715	1820	1824	1827	rBV	1748466	1615099	68.90%	7.446%
24	12.892	1851	1854	1859	rVB3	21031	28168	1.20%	0.130%
25	13.627	1973	1979	1982	rBV2	113154	152645	6.51%	0.704%
26	13.757	1996	2001	2012	rVB	750326	794725	33.90%	3.664%
27	14.257	2083	2086	2090	rBV	70272	79215	3.38%	0.365%
28	14.609	2143	2146	2149	rBV3	31970	31364	1.34%	0.145%
29	14.674	2154	2157	2161	rVV2	46303	39696	1.69%	0.183%
30	14.757	2167	2171	2173	rBV2	63709	80092	3.42%	0.369%
31	14.851	2184	2187	2189	rBV	75896	81748	3.49%	0.377%
32	14.874	2189	2191	2196	rVB2	62884	71398	3.05%	0.329%
33	15.027	2214	2217	2221	rVB	42677	49536	2.11%	0.228%
34	15.080	2223	2226	2231	rVB	50308	49957	2.13%	0.230%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.139	2231	2236	2240	rBV	466004	544094	23.21%	2.508%
36	15.368	2271	2275	2280	rVB5	35415	47821	2.04%	0.220%
37	15.580	2306	2311	2315	rBV	64992	98711	4.21%	0.455%
38	15.627	2316	2319	2325	rVB7	31755	51546	2.20%	0.238%
39	16.274	2424	2429	2435	rBV8	38187	91178	3.89%	0.420%
40	16.439	2454	2457	2460	rBV2	26845	39142	1.67%	0.180%
41	16.545	2472	2475	2480	rBV4	27020	34010	1.45%	0.157%
42	16.815	2518	2521	2525	rBV	28791	43439	1.85%	0.200%
43	16.962	2541	2546	2554	rBV10	50587	127689	5.45%	0.589%
44	17.521	2639	2641	2645	rBV5	15278	23643	1.01%	0.109%

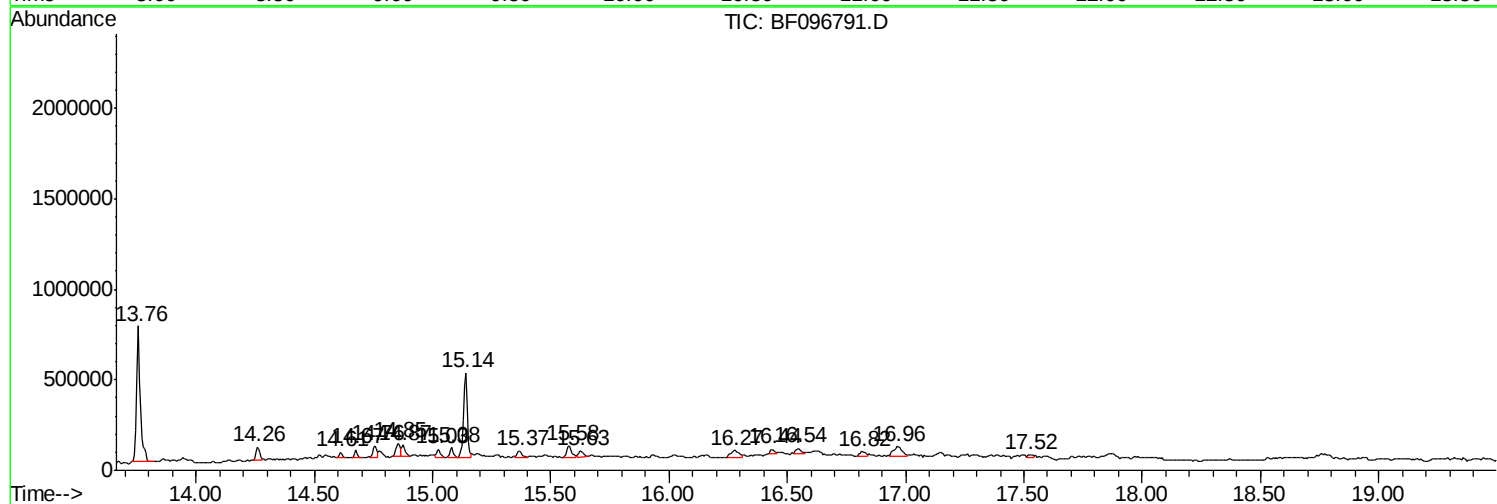
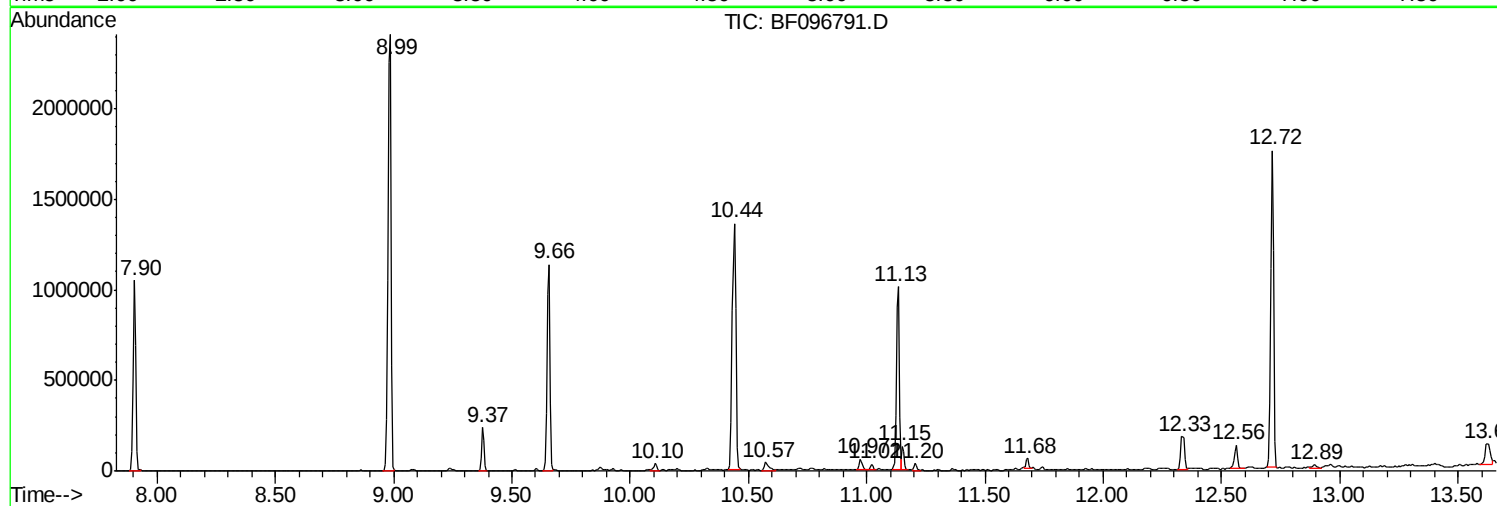
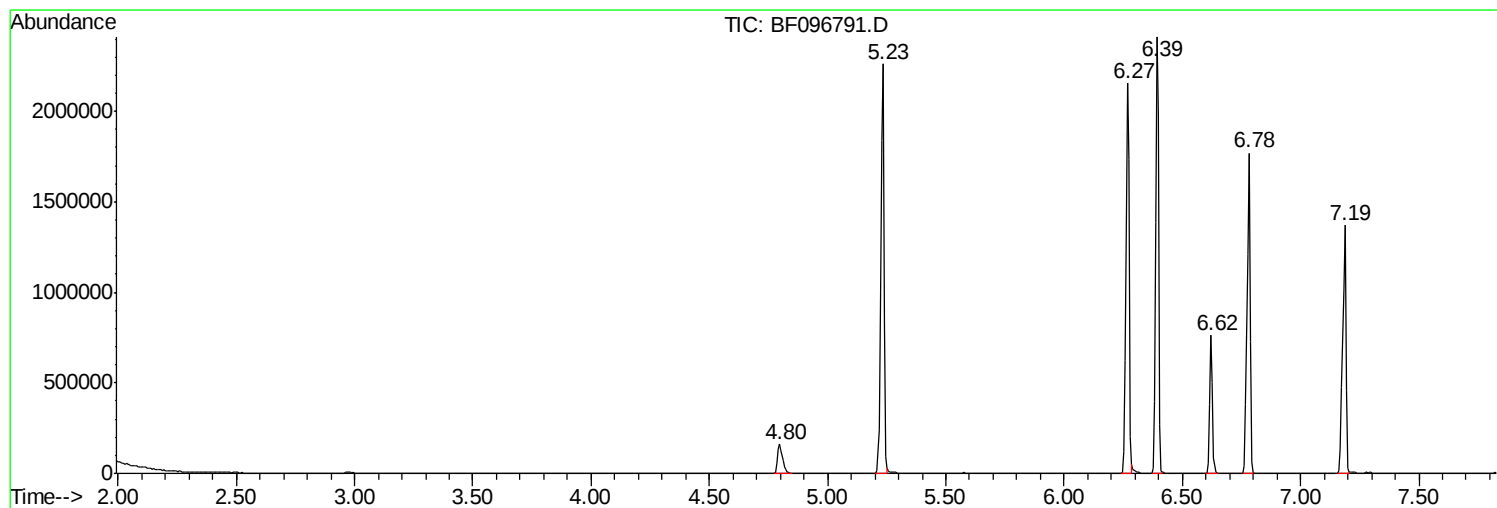
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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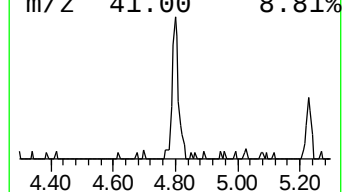
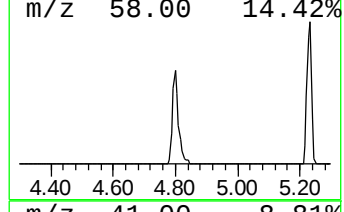
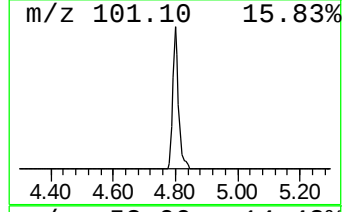
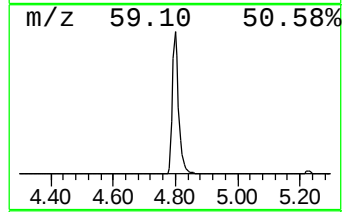
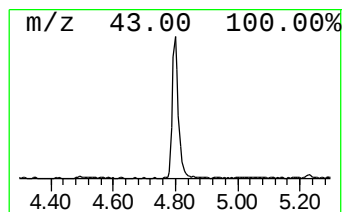
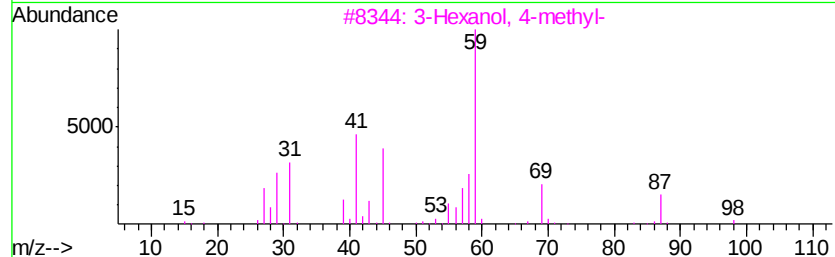
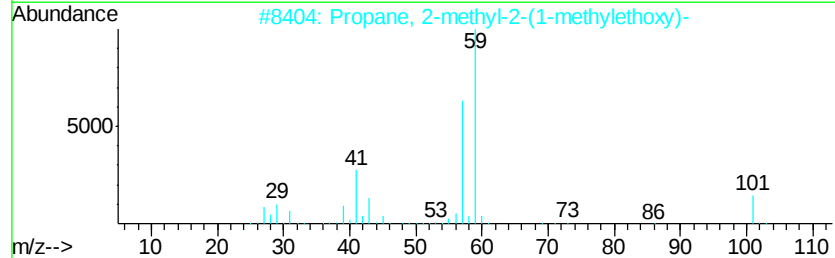
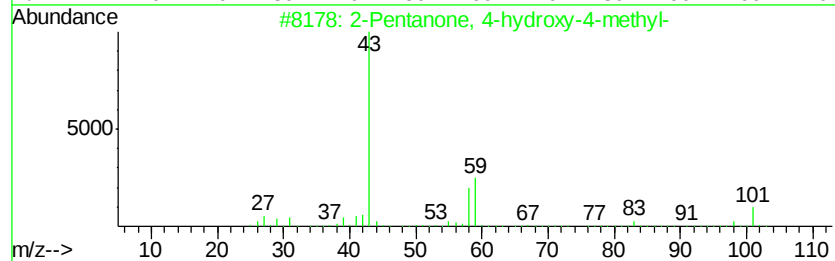
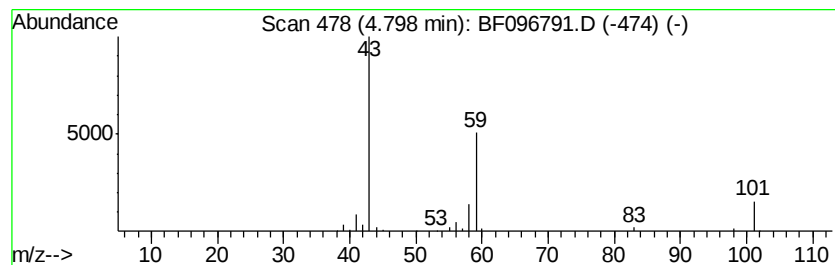
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.80	6.80 ng	215394	1,4-Dichlorobenzene-d4	6.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	25
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2		000115-22-0	9



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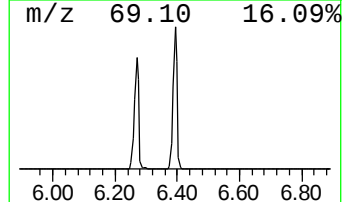
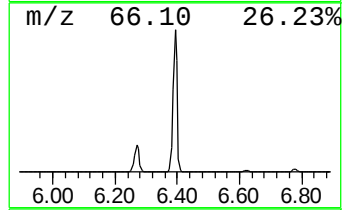
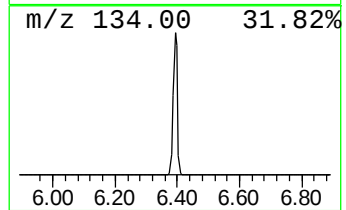
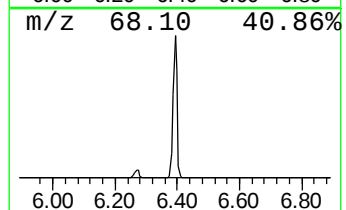
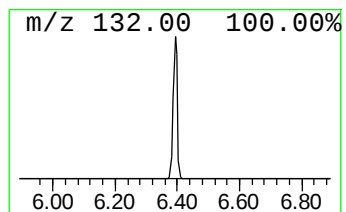
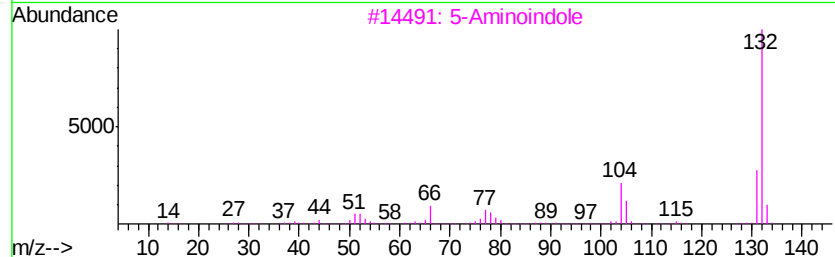
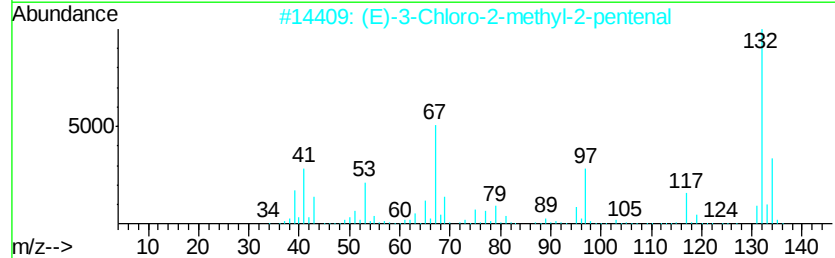
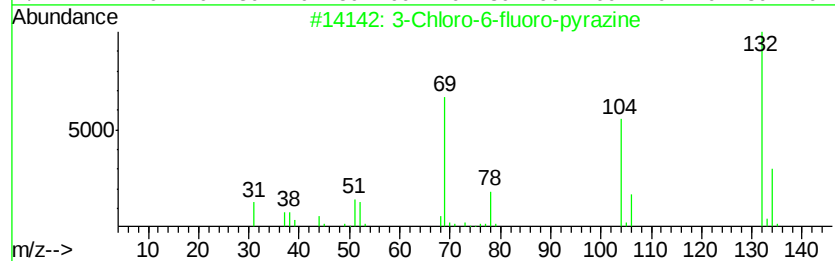
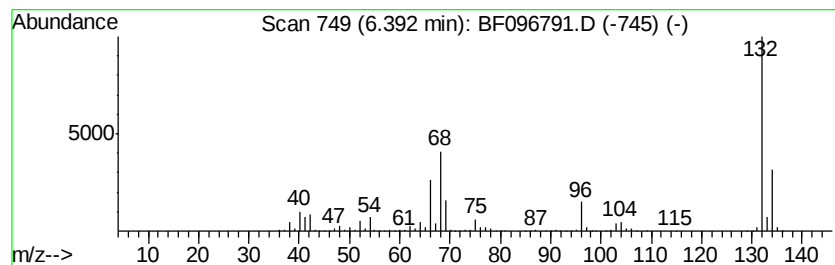
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	72.07 ng	2282910	1,4-Dichlorobenzene-d4	6.62

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	16
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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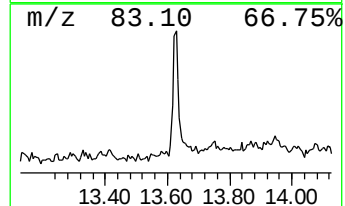
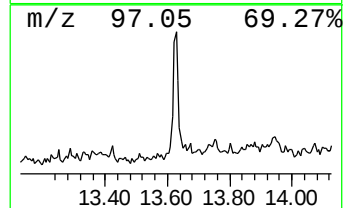
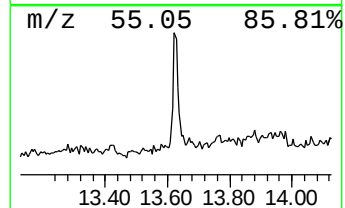
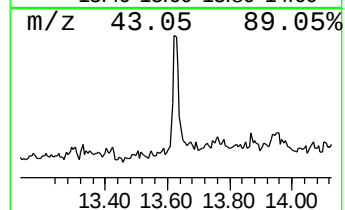
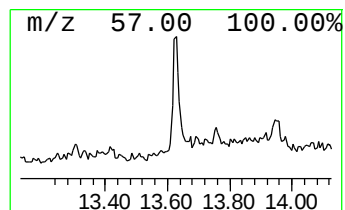
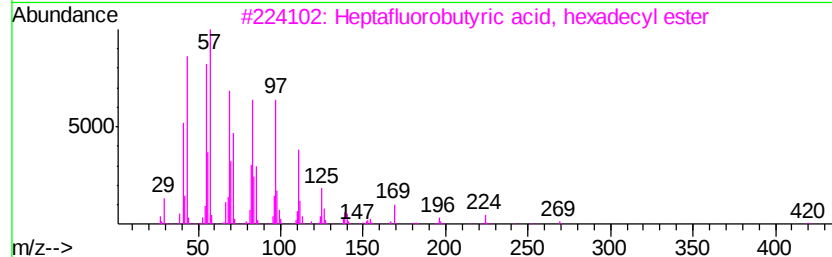
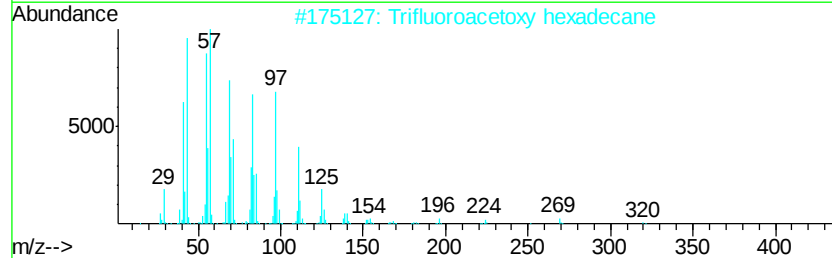
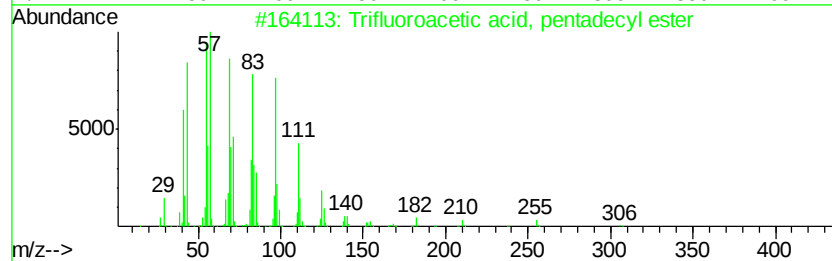
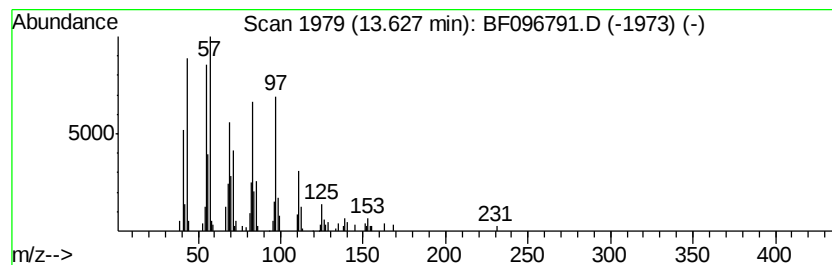
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	3.84 ng	152645	Chrysene-d12	13.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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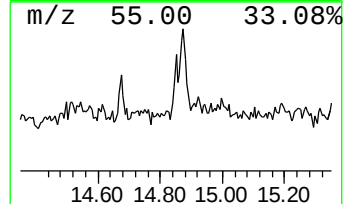
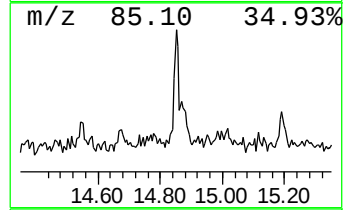
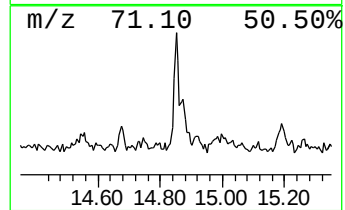
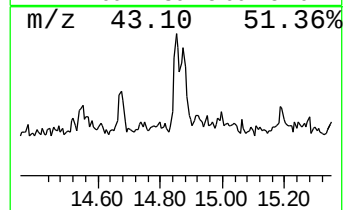
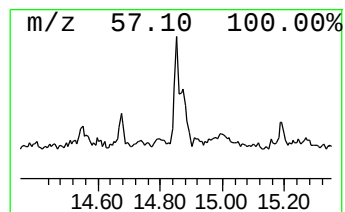
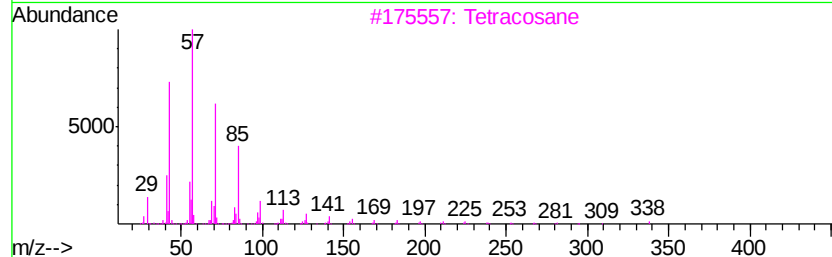
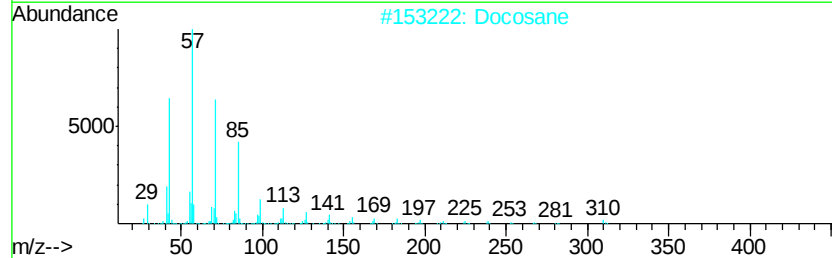
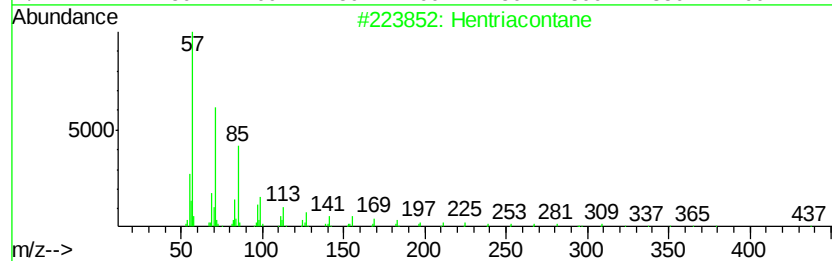
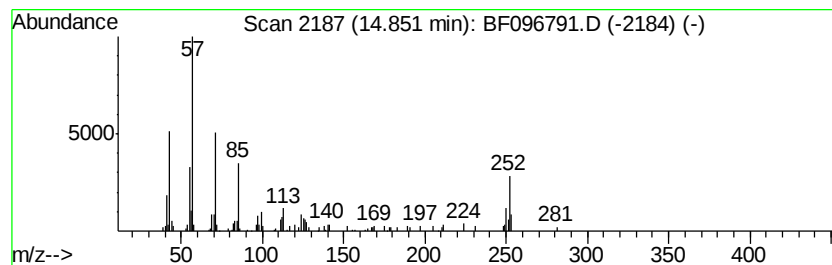
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	3.00 ng	81748	Perylene-d12	15.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	58
2	Docosane		310	C22H46	000629-97-0	58
3	Tetracosane		338	C24H50	000646-31-1	58
4	Octadecane		254	C18H38	000593-45-3	58
5	Tetratetracontane		619	C44H90	007098-22-8	52



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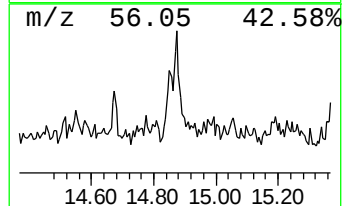
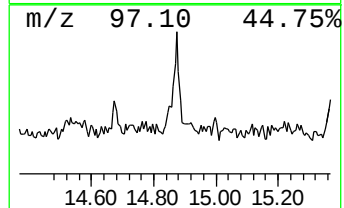
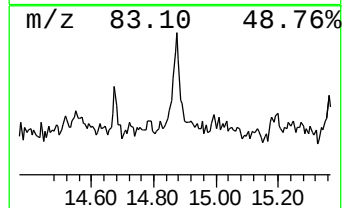
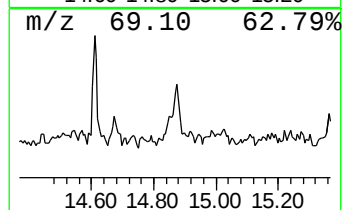
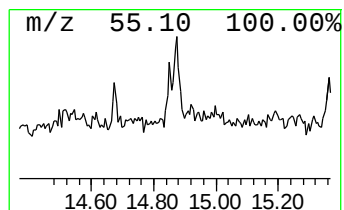
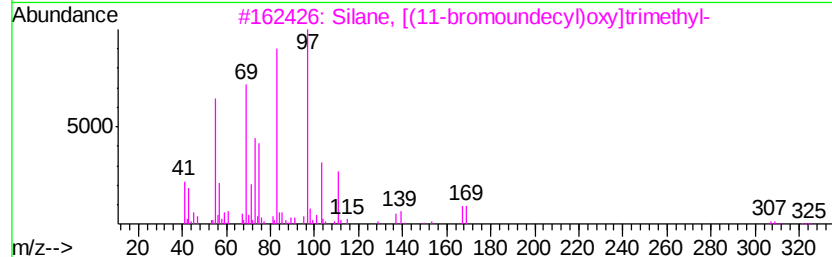
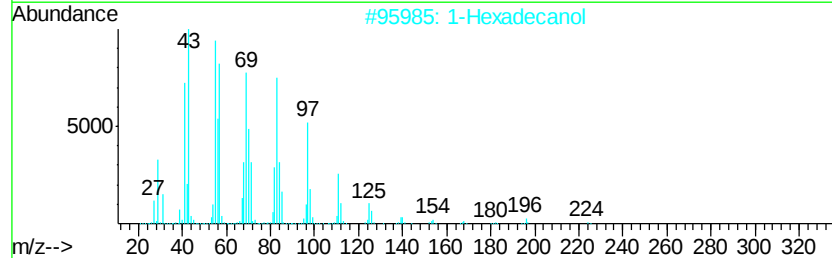
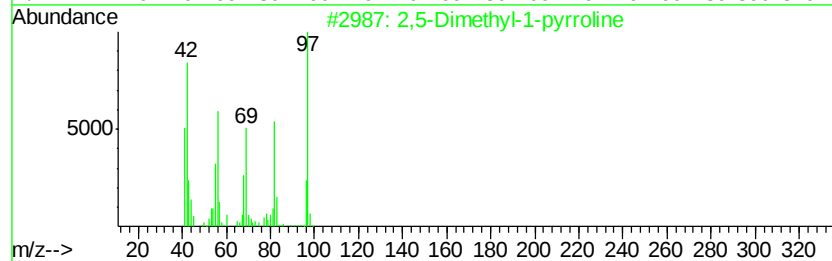
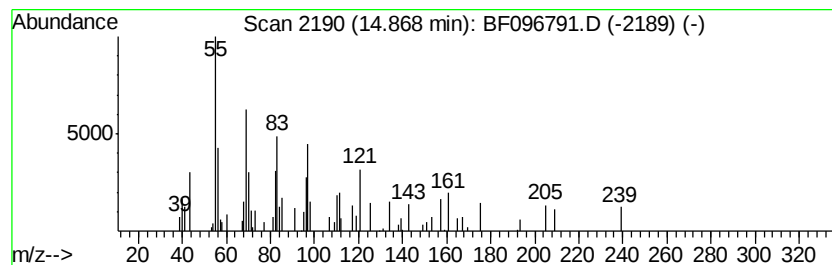
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.87 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.62 ng	71398	Perylene-d12	15.14

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Dimethyl-1-pyrroline			97	C6H11N	000822-64-0	49
2	1-Hexadecanol			242	C16H34O	036653-82-4	47
3	Silane, [(11-bromoundecyl)oxy]tr...			322	C14H31BrOSi	026305-83-9	38
4	n-Tridecan-1-ol			200	C13H28O	000112-70-9	38
5	1-Dodecanol			186	C12H26O	000112-53-8	38



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096791.D
Acq On : 15 Jul 2017 00:23
Operator : SJ/JU
Sample : I4187-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CI-SB1-0-2

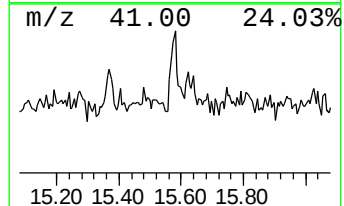
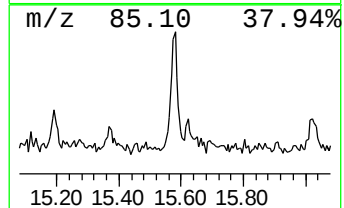
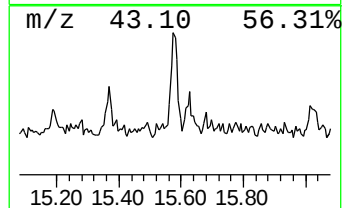
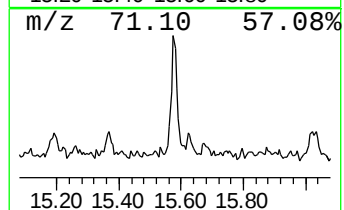
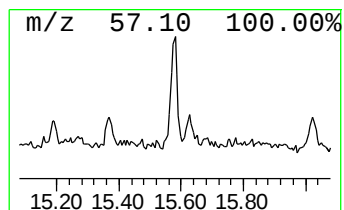
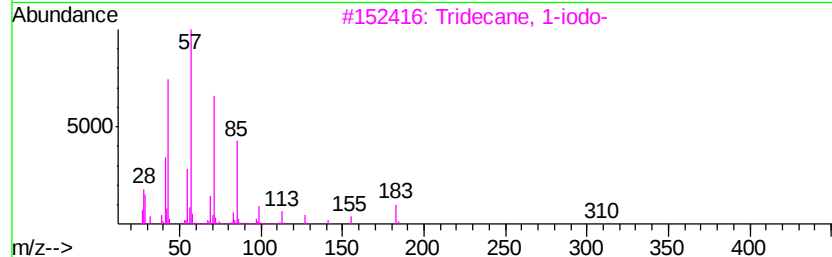
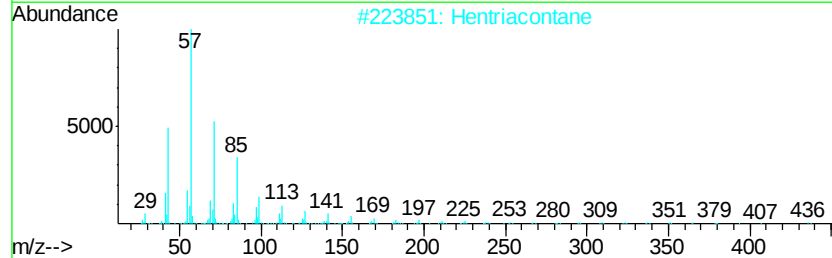
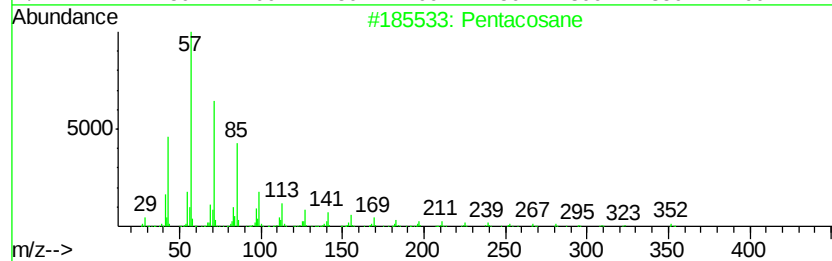
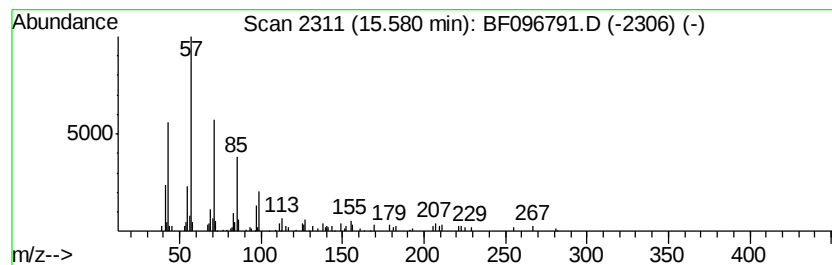
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	3.63 ng	98711	Perylene-d12	15.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	72
2	Hentriacontane		437	C31H64	000630-04-6	64
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	58
4	Tetrapentacontane		759	C54H110	005856-66-6	53
5	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	53



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096791.D
Acq On : 15 Jul 2017 00:23
Operator : SJ/JU
Sample : I4187-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CI-SB1-0-2

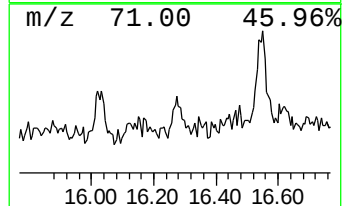
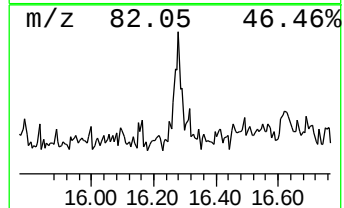
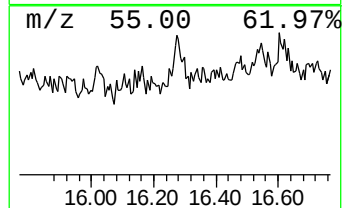
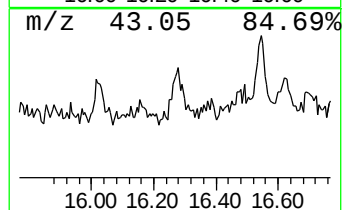
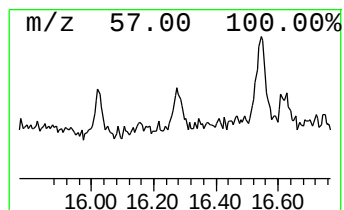
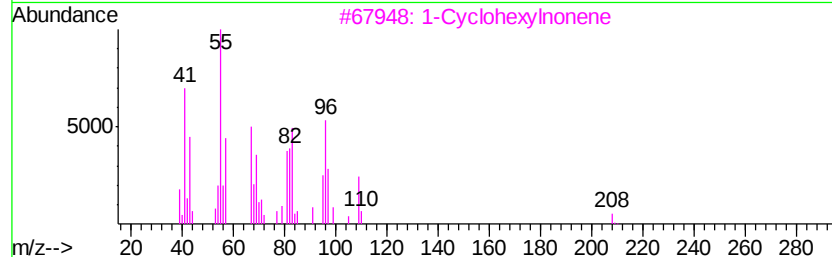
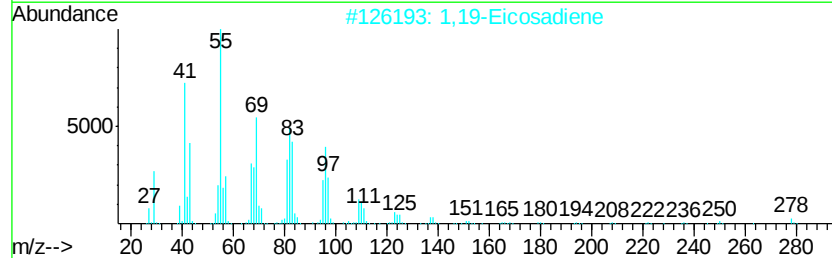
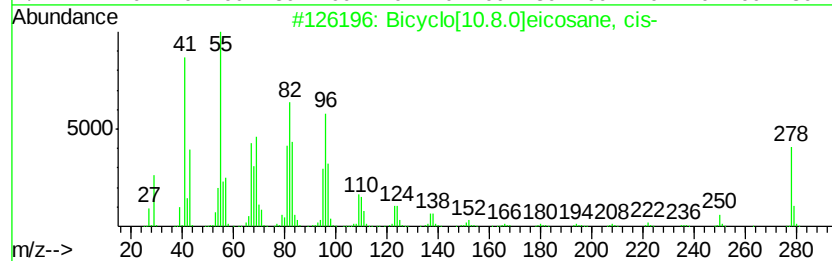
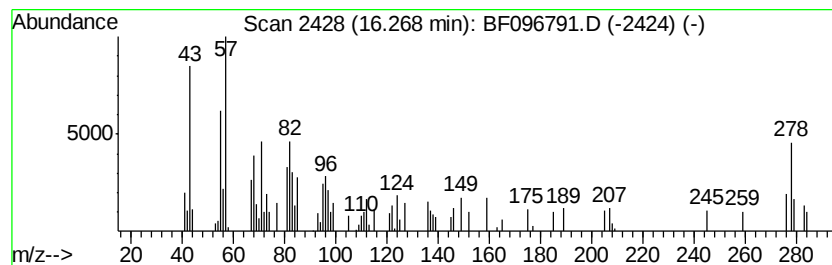
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Bicyclo[10.8.0]eicosane, cis- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.27	3.35 ng	91178	Perylene-d12	15.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	62
2		1,19-Eicosadiene	278	C20H38	014811-95-1	46
3		1-Cyclohexylnonene	208	C15H28	114614-84-5	43
4		Z-13-Octadecen-1-yl acetate	310	C20H38O2	060037-58-3	25
5		Phosphonic acid, [(methylsulfonyl...]	230	C6H15O5PS	040137-11-9	25



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096791.D
Acq On : 15 Jul 2017 00:23
Operator : SJ/JU
Sample : I4187-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

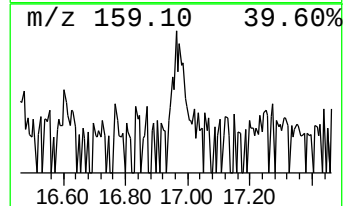
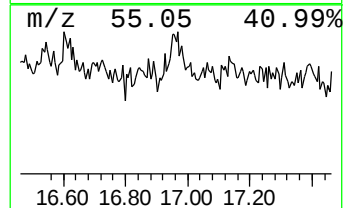
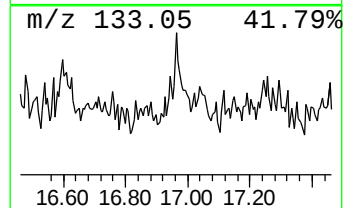
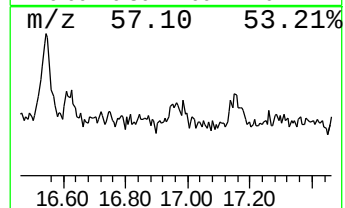
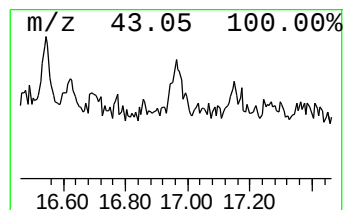
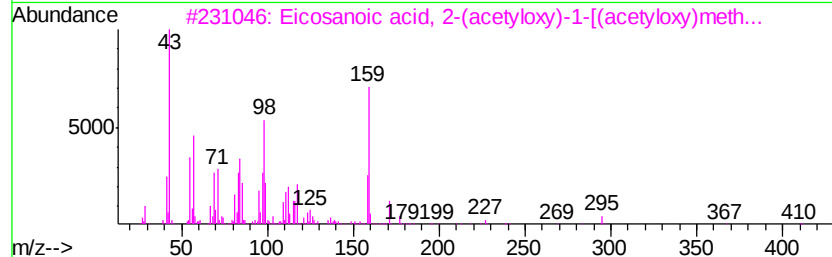
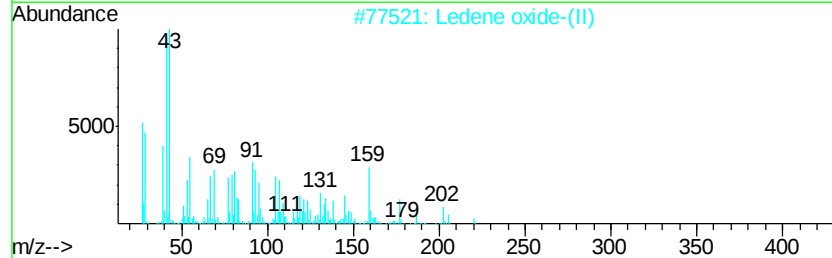
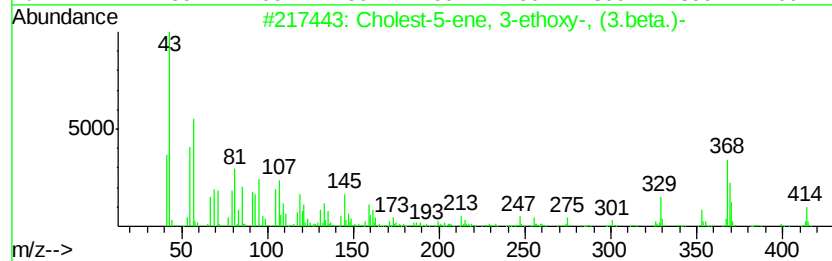
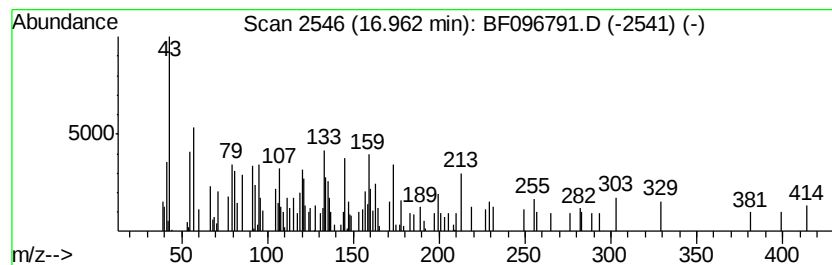
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.96 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	4.69 ng	127689	Perylene-d12	15.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cholest-5-ene, 3-ethoxy-, (3.bet...	414 C29H50O	000986-19-6 11
2		Ledene oxide-(II)	220 C15H24O	1000159-36-7 10
3		Eicosanoic acid, 2-(acetyloxy)-1...	470 C27H50O6	055429-68-0 10
4		Benzofuran, 7-(2,4-dinitrophenox...	388 C19H20N2O7	062059-48-7 10
5		5-Isoxazolidinemethanol, 2-acety...	201 C9H15NO4	064018-47-9 9



Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
Data File : BF096791.D
Acq On : 15 Jul 2017 00:23
Operator : SJ/JU
Sample : I4187-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CI-SB1-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	4.80	6.8 ng		215394	1	6.62	633550	20.0
unknown6.39	6.39	72.1 ng		2282910	1	6.62	633550	20.0
Trifluoroacetic a...	13.63	3.8 ng		152645	5	13.76	794725	20.0
Hentriacontane	14.85	3.0 ng		81748	6	15.14	544094	20.0
unknown14.87	14.87	2.6 ng		71398	6	15.14	544094	20.0
Pentacosane	15.58	3.6 ng		98711	6	15.14	544094	20.0
Bicyclo[10.8.0]ei...	16.27	3.4 ng		91178	6	15.14	544094	20.0
unknown16.96	16.96	4.7 ng		127689	6	15.14	544094	20.0