

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
 Data File : BF099924.D
 Acq On : 28 Oct 2017 18:26
 Operator : SJ/JU
 Sample : I6141-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-A-COMP

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-BF102317.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	494	498	524	rBV	211259	382668	14.57%	1.714%
2	5.416	562	566	585	rBV	2104950	2310355	87.94%	10.346%
3	6.434	735	739	757	rBV	1887285	2346176	89.30%	10.507%
4	6.563	757	761	764	rBV	2552474	2351025	89.49%	10.528%
5	6.787	795	799	809	rBV	684456	604192	23.00%	2.706%
6	6.939	821	825	842	rBV	1974847	1868191	71.11%	8.366%
7	7.357	892	896	899	rBV	1470236	1411494	53.73%	6.321%
8	8.069	1013	1017	1032	rBV	892780	832035	31.67%	3.726%
9	9.145	1194	1200	1203	rBV	2694462	2627203	100.00%	11.765%
10	9.539	1263	1267	1273	rVB	426768	336702	12.82%	1.508%
11	9.822	1311	1315	1319	rBV2	1025272	878757	33.45%	3.935%
12	10.239	1383	1386	1389	rVB	47985	36155	1.38%	0.162%
13	10.616	1446	1450	1458	rBV	1255263	1191723	45.36%	5.337%
14	10.710	1463	1466	1471	rBV	61628	60241	2.29%	0.270%
15	11.316	1565	1569	1572	rBV	760722	736764	28.04%	3.299%
16	11.827	1652	1656	1664	rBV3	59441	90731	3.45%	0.406%
17	12.533	1772	1776	1779	rBV	69068	68040	2.59%	0.305%
18	12.610	1784	1789	1793	rBV6	20013	30397	1.16%	0.136%
19	12.763	1809	1815	1821	rBV	73458	90830	3.46%	0.407%
20	12.898	1834	1838	1841	rBV	1749632	1621339	61.71%	7.261%
21	13.774	1982	1987	1994	rBV3	129036	165576	6.30%	0.741%
22	13.963	2014	2019	2022	rBV	592281	577720	21.99%	2.587%
23	13.986	2022	2023	2030	rVB	38494	37261	1.42%	0.167%
24	14.410	2089	2095	2099	rBV6	47494	89178	3.39%	0.399%
25	14.468	2102	2105	2113	rVB3	57328	82354	3.13%	0.369%
26	14.692	2138	2143	2147	rBV7	18029	28866	1.10%	0.129%
27	15.021	2193	2199	2203	rBV3	65904	144226	5.49%	0.646%
28	15.157	2219	2222	2226	rBV	60210	62541	2.38%	0.280%
29	15.245	2233	2237	2244	rVB2	114250	131323	5.00%	0.588%
30	15.304	2244	2247	2250	rBV2	28911	35186	1.34%	0.158%
31	15.368	2255	2258	2260	rVV	38751	49834	1.90%	0.223%
32	15.421	2263	2267	2278	rVB	489085	602482	22.93%	2.698%
33	15.804	2328	2332	2337	rVB2	51642	72618	2.76%	0.325%
34	15.857	2338	2341	2347	rVB8	16359	27570	1.05%	0.123%

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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 >
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35	16.292	2410	2415	2423	rVB9	29902	61312	2.33%	0.275%
36	16.733	2486	2490	2498	rVB	64378	119051	4.53%	0.533%
37	16.856	2506	2511	2516	rBV4	18849	33362	1.27%	0.149%
38	17.039	2538	2542	2550	rVB4	13882	28106	1.07%	0.126%
39	17.356	2591	2596	2604	rBV4	20614	42252	1.61%	0.189%
40	17.898	2683	2688	2696	rVB8	19051	38382	1.46%	0.172%
41	19.386	2937	2941	2950	rVB10	11860	26314	1.00%	0.118%

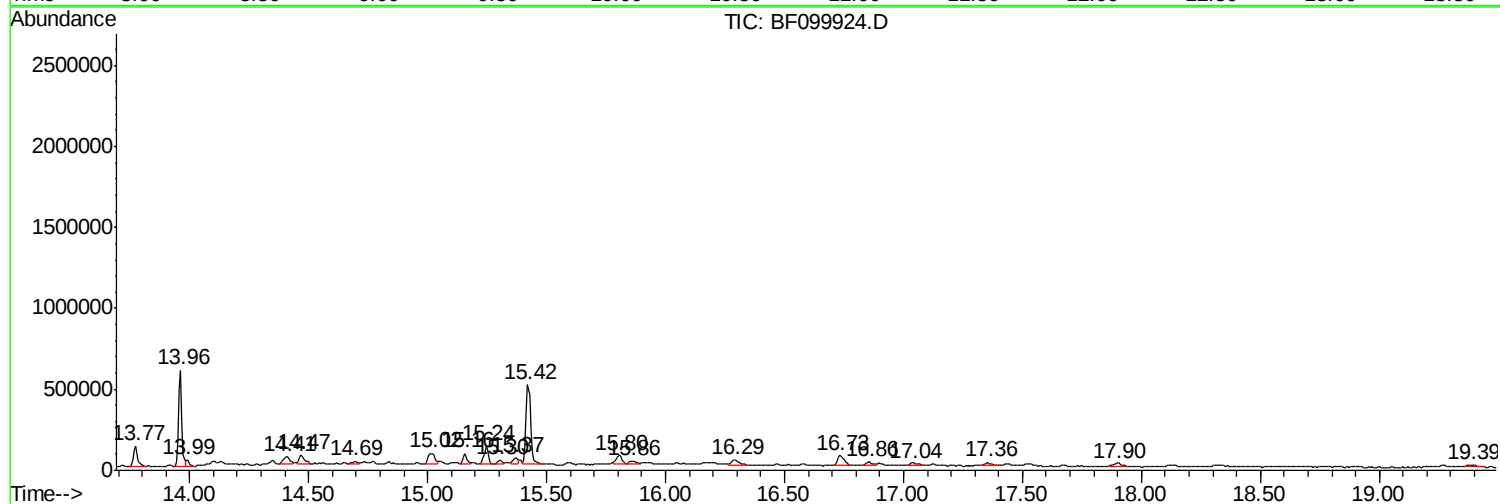
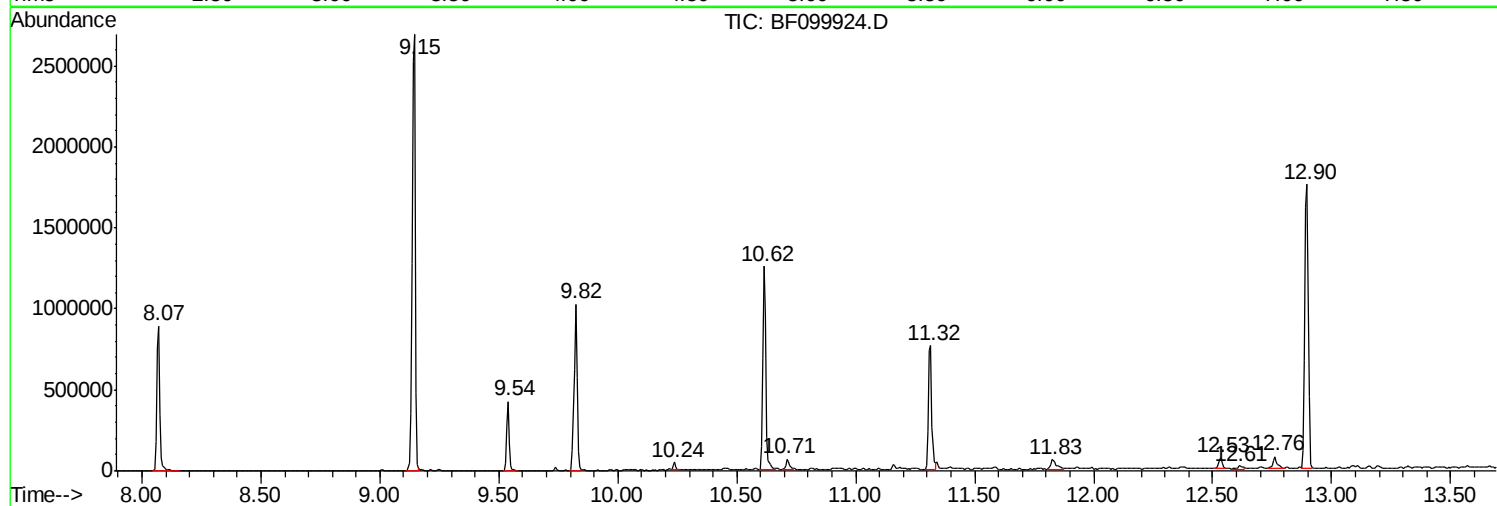
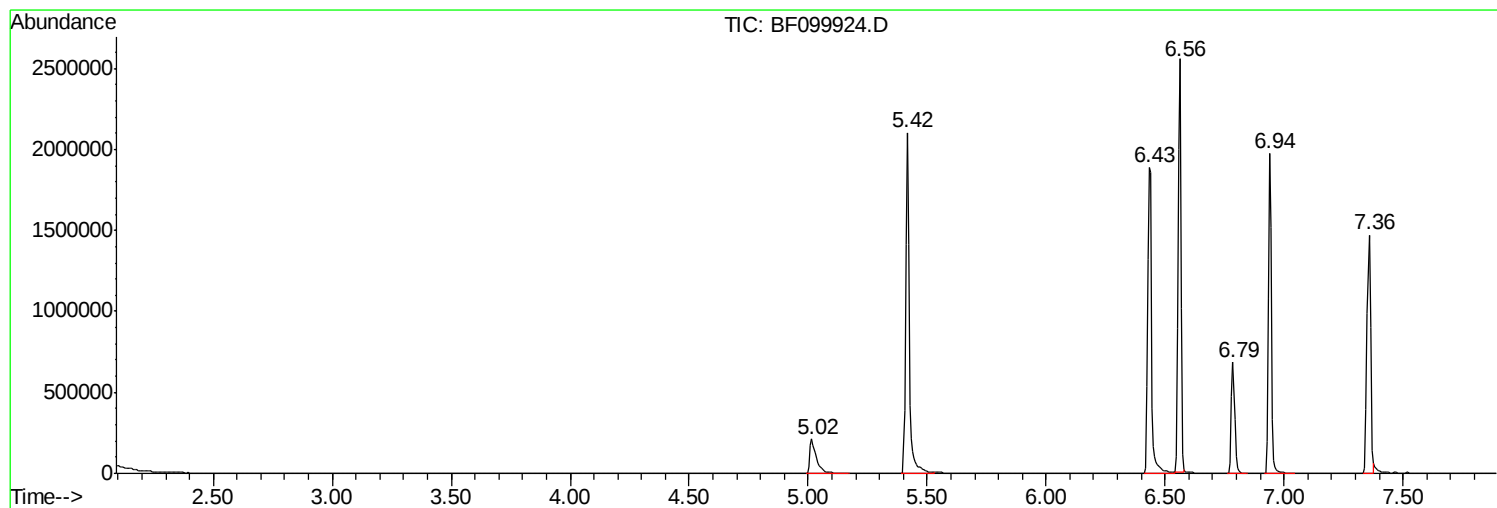
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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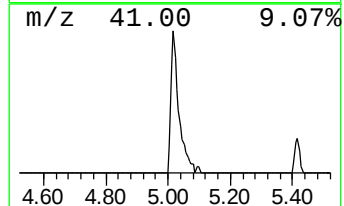
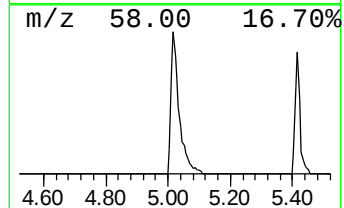
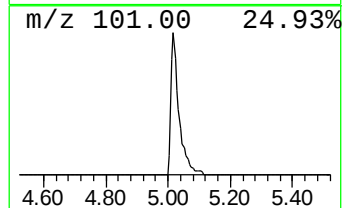
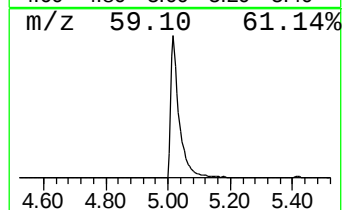
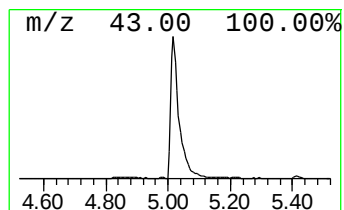
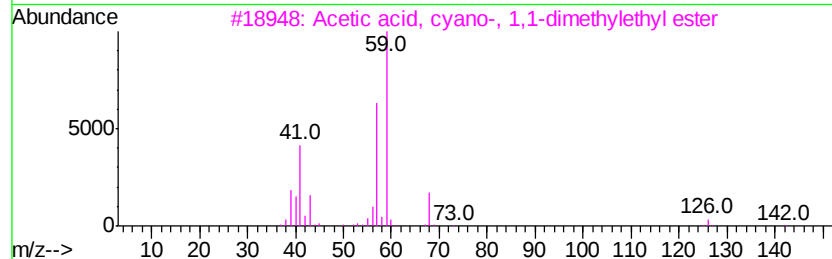
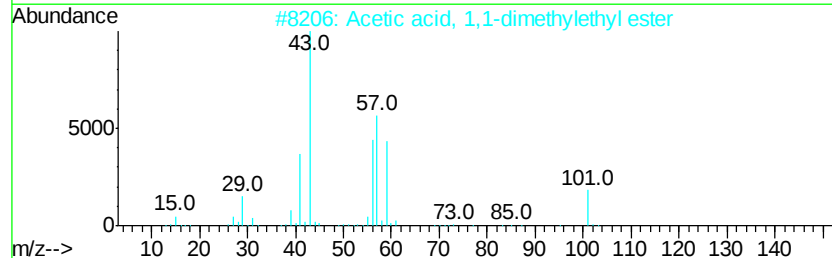
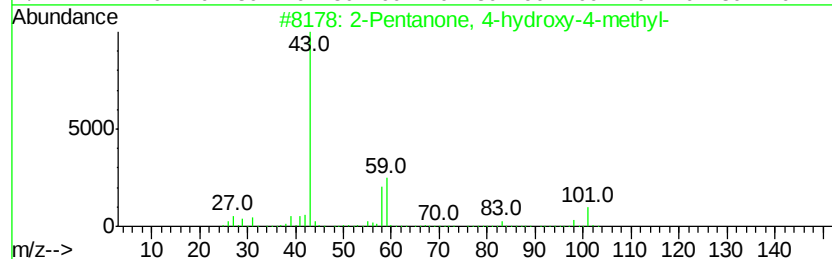
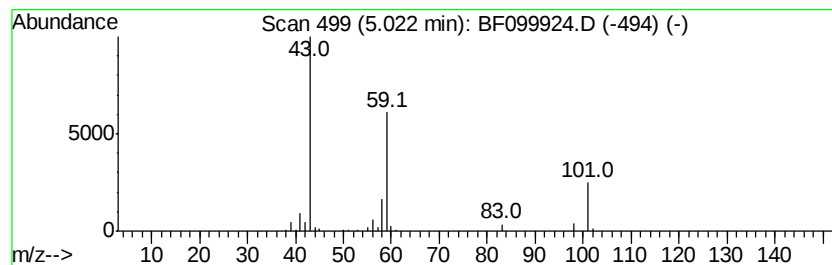
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.02	12.67 ng	382668	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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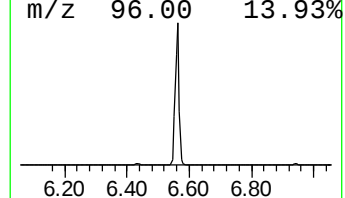
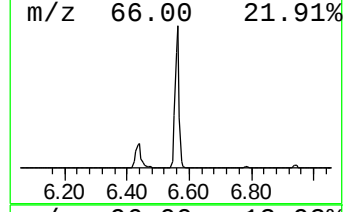
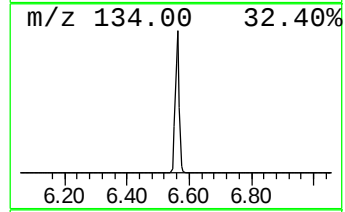
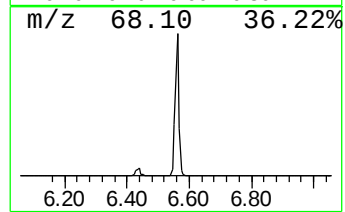
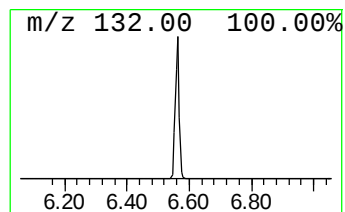
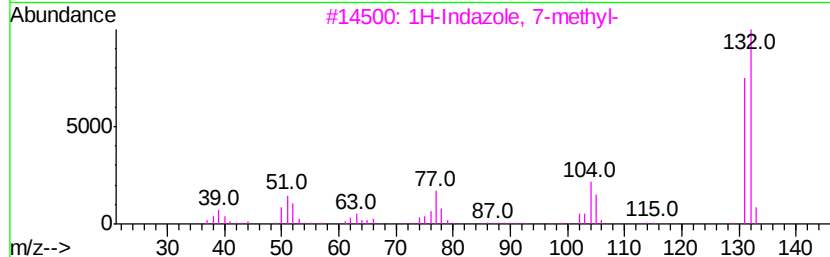
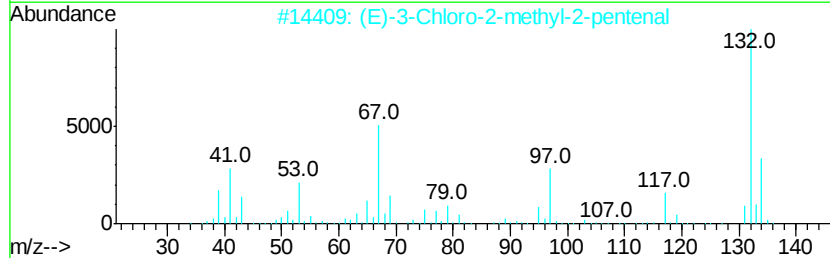
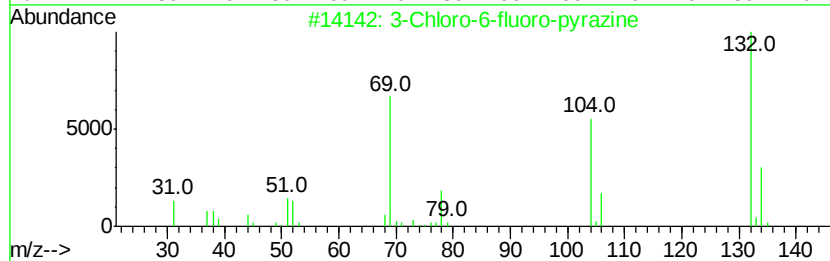
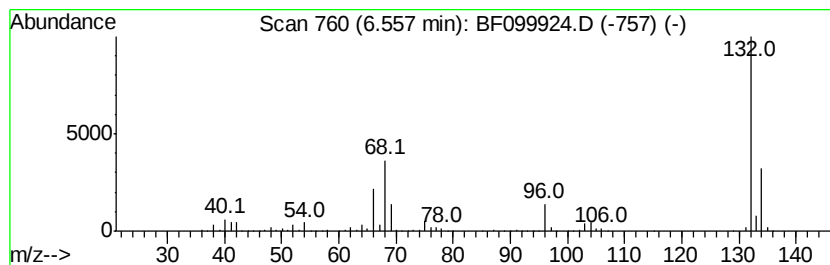
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	77.82 ng	2351030	1,4-Dichlorobenzene-d4	6.79

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	12
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		Xenon	132	Xe	007440-63-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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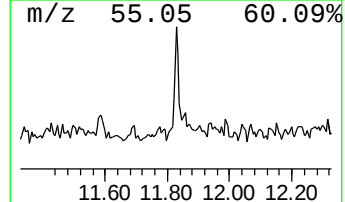
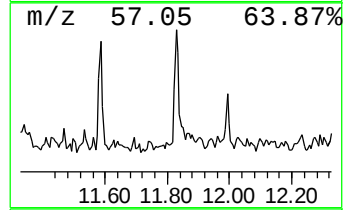
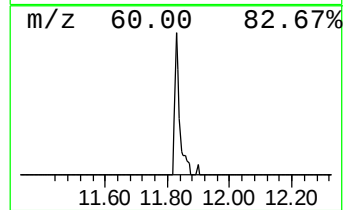
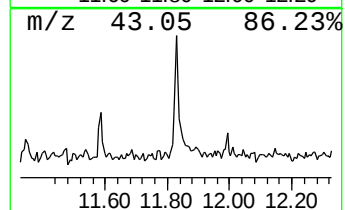
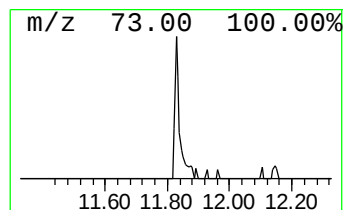
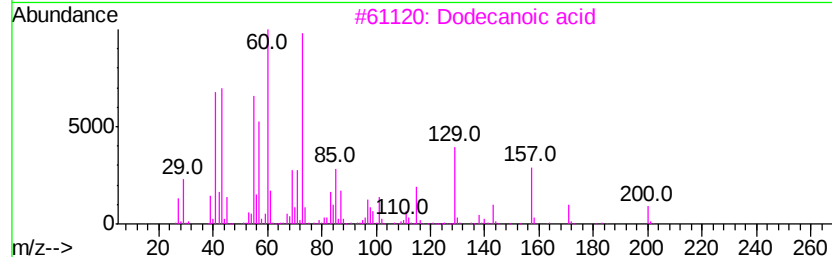
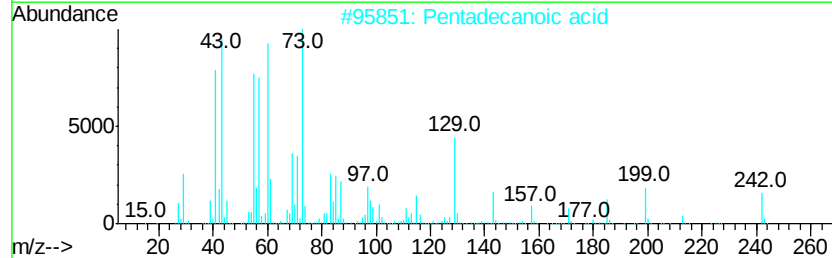
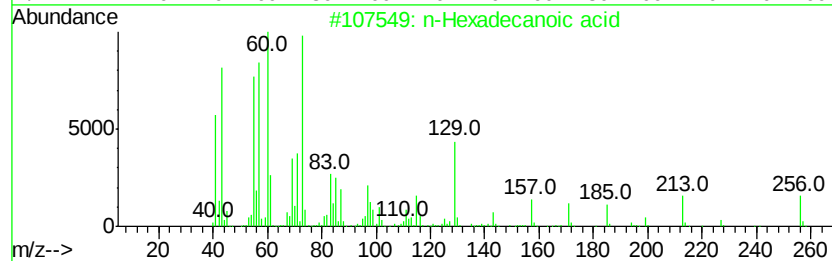
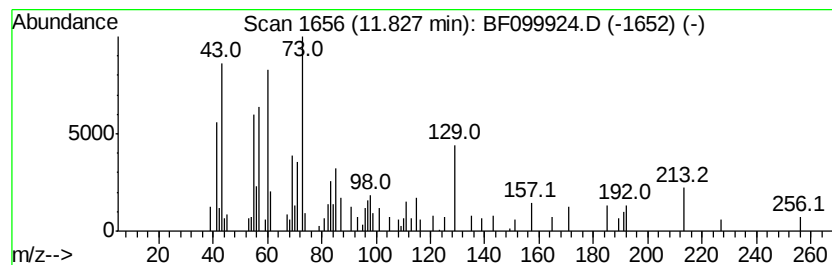
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.46 ng	90731	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3		Dodecanoic acid	200	C12H24O2	000143-07-7	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Tridecanoic acid	214	C13H26O2	000638-53-9	72



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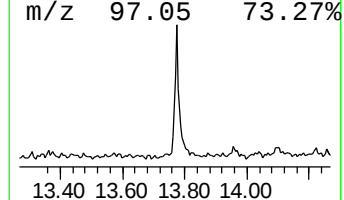
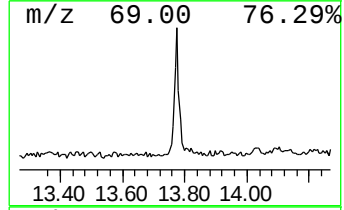
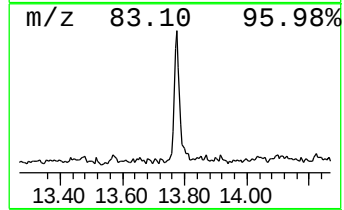
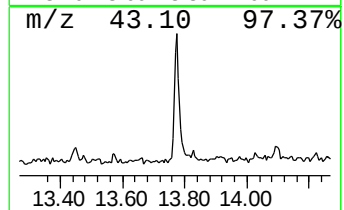
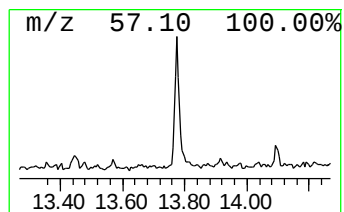
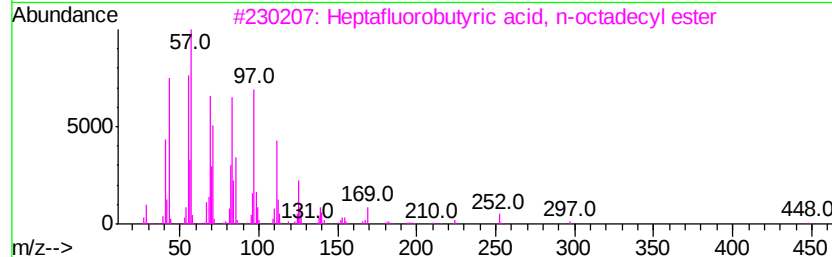
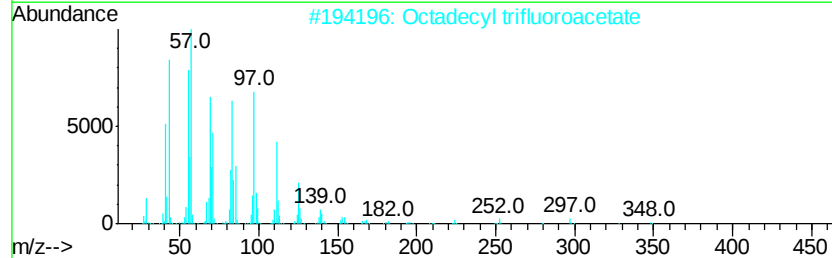
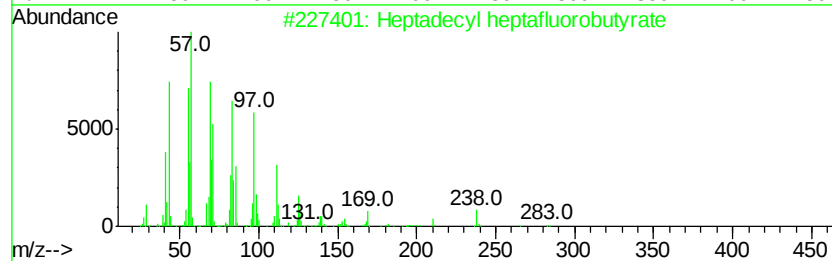
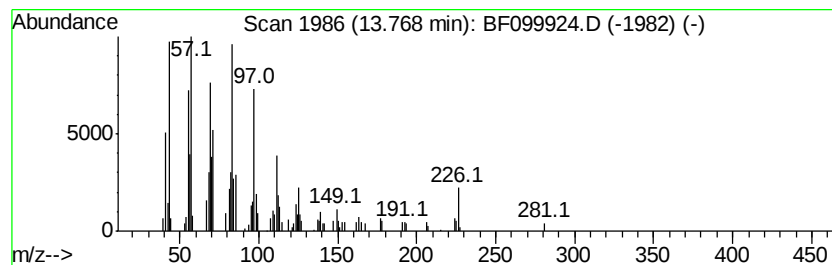
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	5.73 ng	165576	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
3		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	93
4		Pentafluoropropionic acid, heptafluorobutyl ester	402	C20H35F5O2	959218-78-1	93
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93



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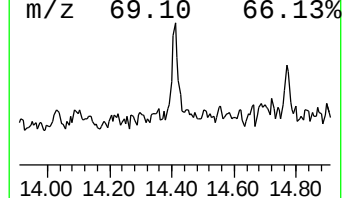
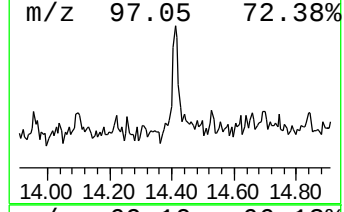
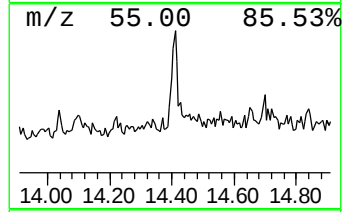
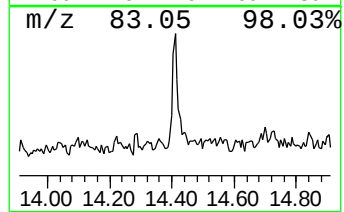
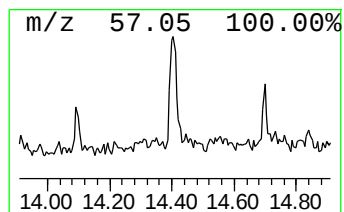
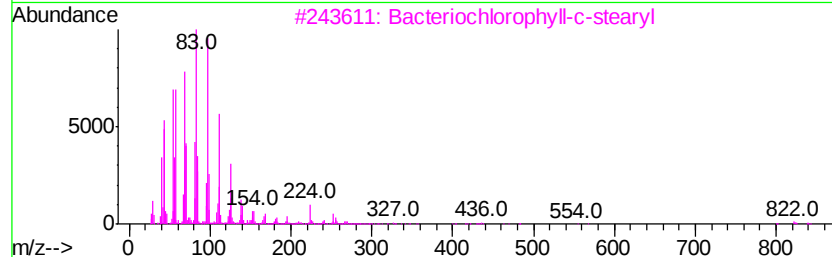
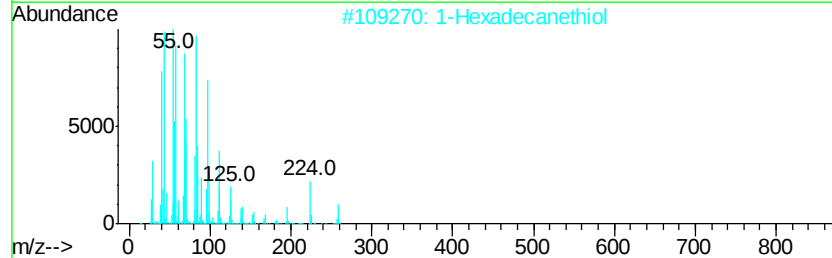
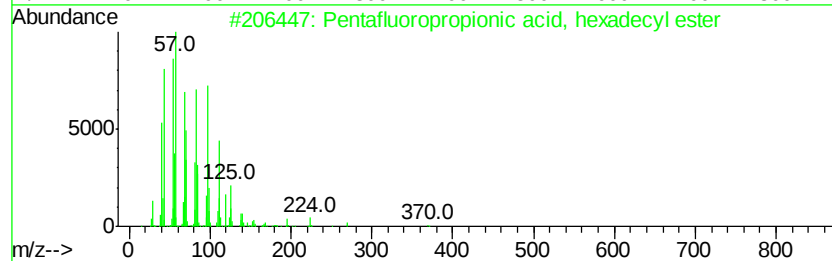
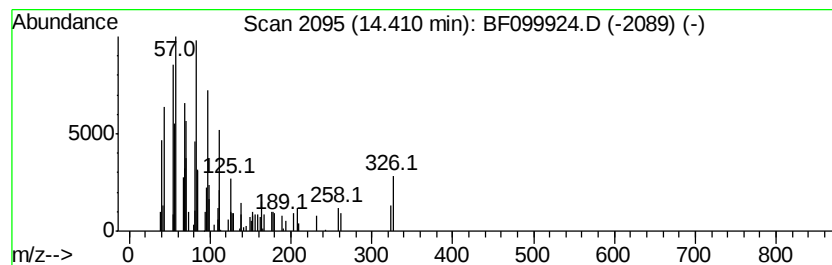
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	3.09 ng	89178	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93
2		1-Hexadecanethiol	258	C16H34S	002917-26-2	91
3		Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	76
4		2-Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	76
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099924.D
Acq On : 28 Oct 2017 18:26
Operator : SJ/JU
Sample : I6141-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-A-COMP

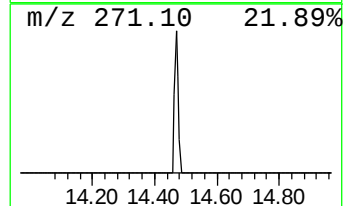
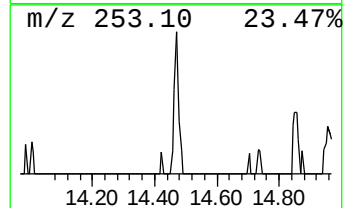
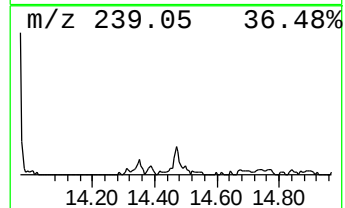
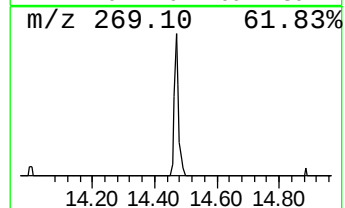
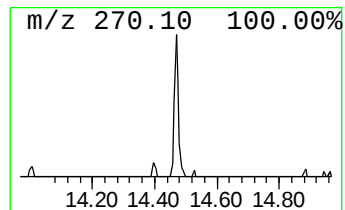
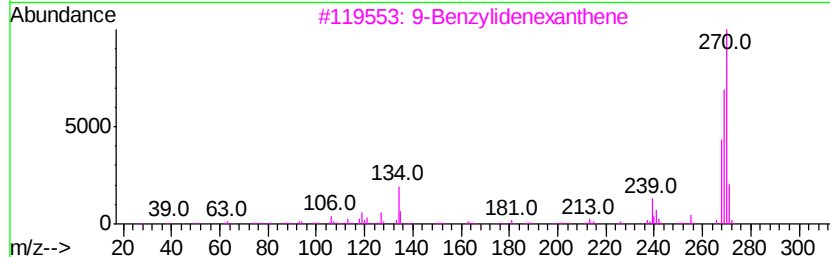
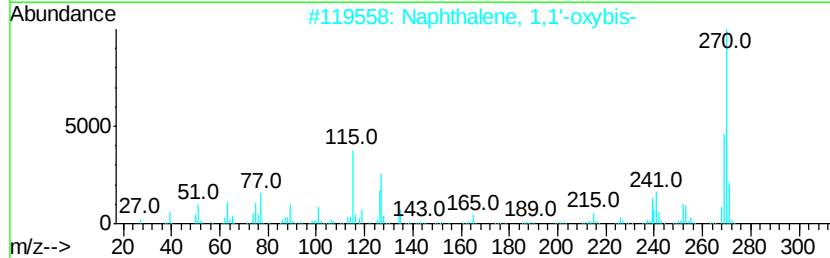
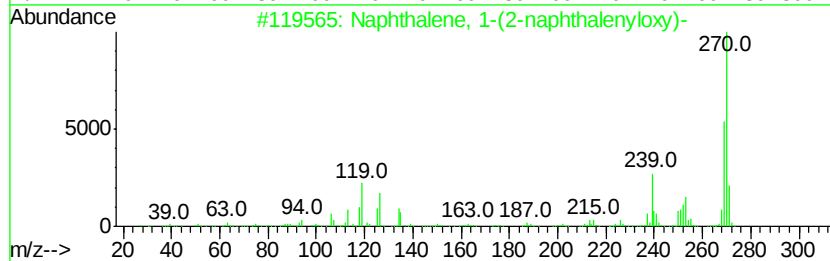
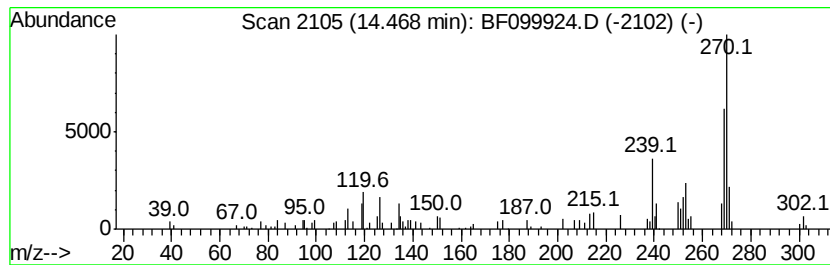
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Naphthalene, 1-(2-naphthale... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.85 ng	82354	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-(2-naphthalenyloxy)-	270	C20H14O	000611-49-4	93
2		Naphthalene, 1,1'-oxybis-	270	C20H14O	000607-52-3	64
3		9-Benzylidenexanthene	270	C20H14O	027980-52-5	64
4		Benzofran-3-one, 2-[3,4-dihydrox...	270	C15H10O5	1000128-63-2	47
5		4-Azafluorenone, 3-methylphenyli...	270	C19H14N2	1000301-74-7	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099924.D
Acq On : 28 Oct 2017 18:26
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ClientSampleId :
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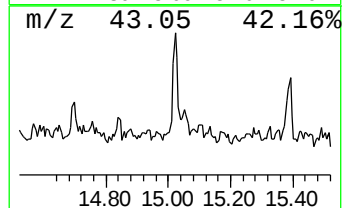
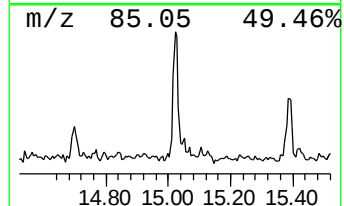
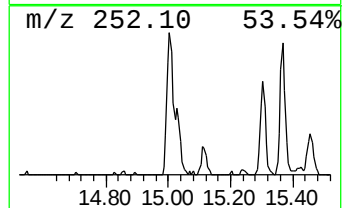
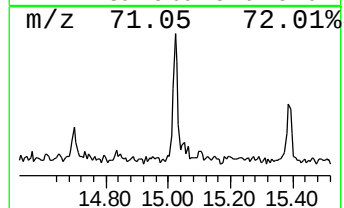
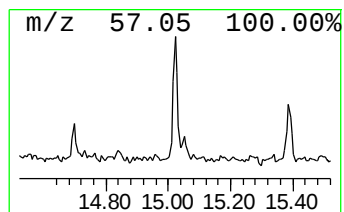
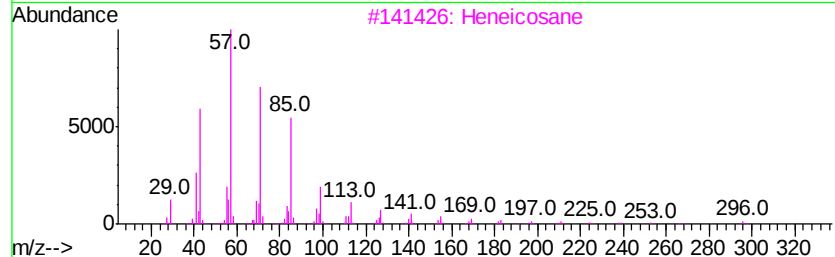
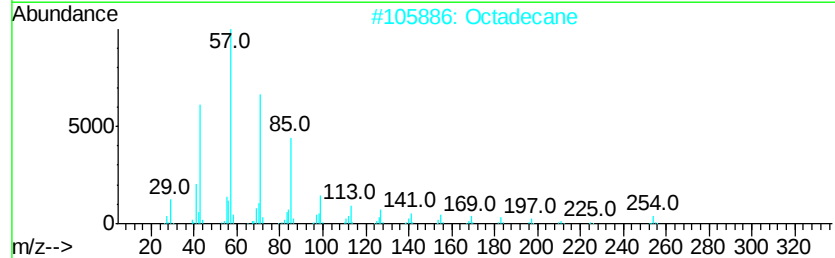
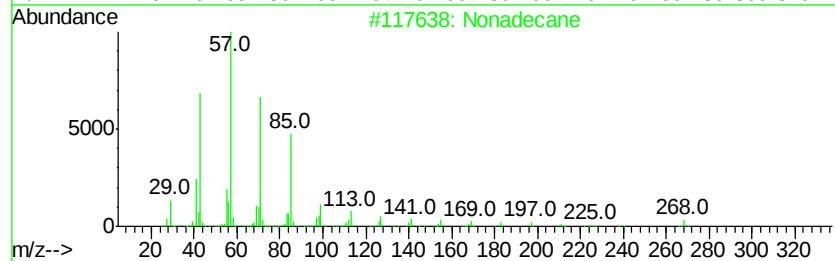
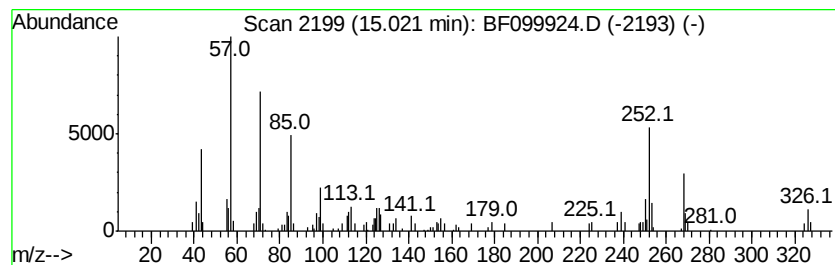
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	4.79 ng	144226	Perylene-d12	15.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	91
2	Octadecane		254	C18H38	000593-45-3	90
3	Heneicosane		296	C21H44	000629-94-7	50
4	Octacosane		394	C28H58	000630-02-4	46
5	Pentacosane		352	C25H52	000629-99-2	46



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099924.D
Acq On : 28 Oct 2017 18:26
Operator : SJ/JU
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Misc :
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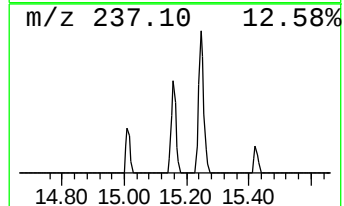
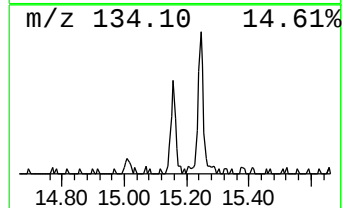
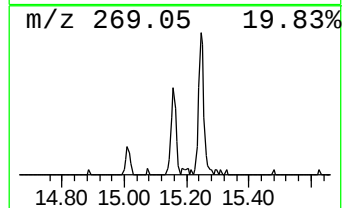
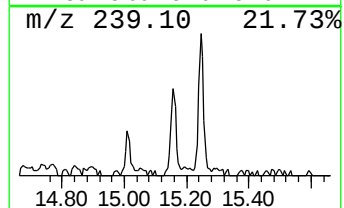
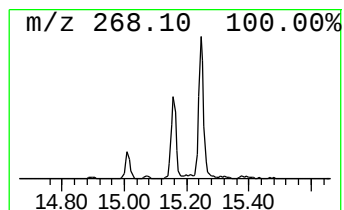
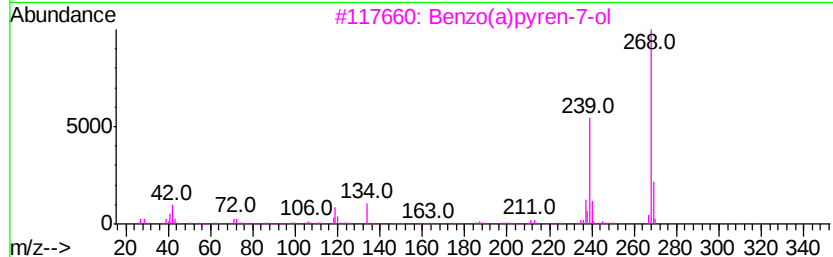
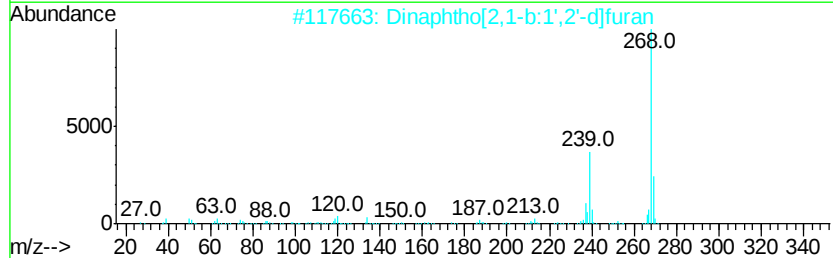
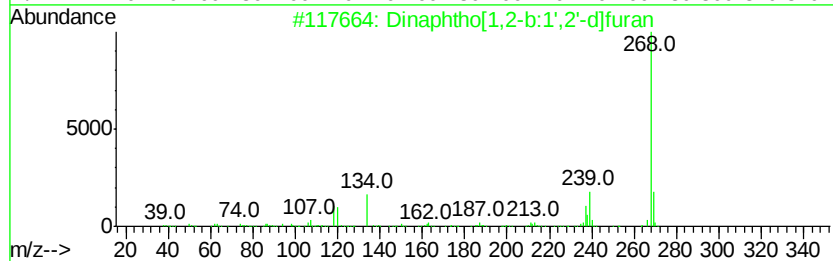
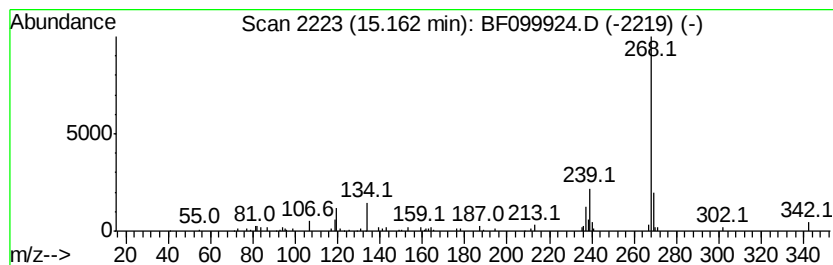
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dinaphtho[1,2-b:1',2'-d]furan Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.08 ng	62541	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dinaphtho[1,2-b:1',2'-d]furan	268	C20H12O	000207-93-2	93
2		Dinaphtho[2,1-b:1',2'-d]furan	268	C20H12O	000194-63-8	72
3		Benzo(a)pyren-7-ol	268	C20H12O	037994-82-4	59
4		4H-1-Benzopyran-4-one, 5-hydroxy...	268	C16H12O4	000520-28-5	59
5		9,10-Dihydro-8-methylbenzo[a]pyrene	268	C21H16	089524-72-1	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099924.D
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Operator : SJ/JU
Sample : I6141-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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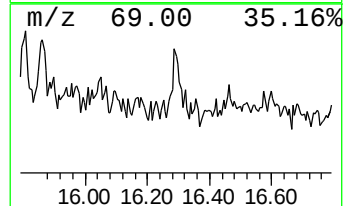
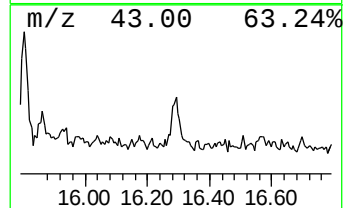
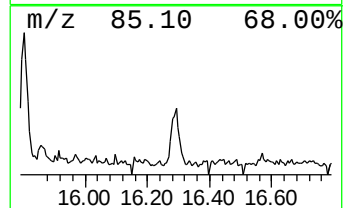
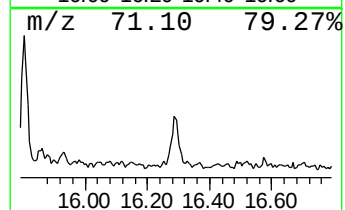
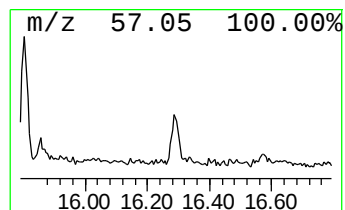
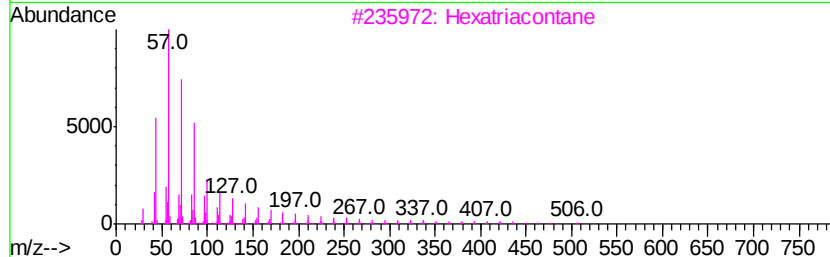
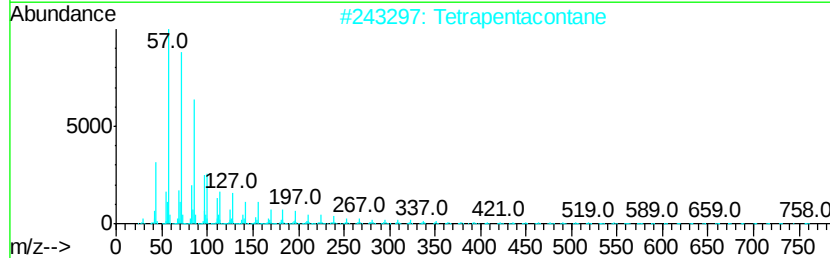
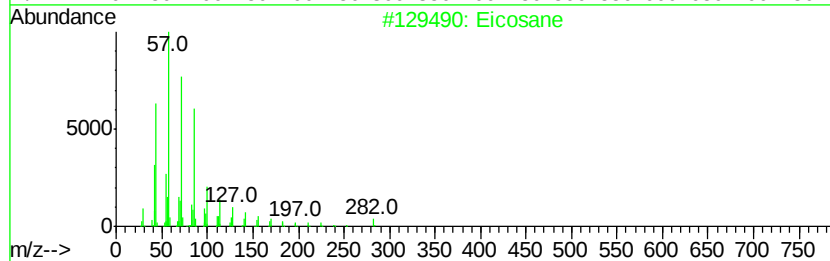
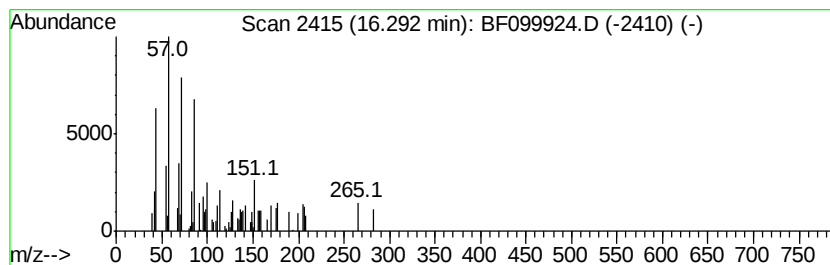
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.29	2.04 ng	61312	Perylene-d12	15.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	89
2			Tetrapentacontane	759	C54H110	005856-66-6	58
3			Hexatriacontane	507	C36H74	000630-06-8	53
4			Tetracosane	338	C24H50	000646-31-1	53
5			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
Data File : BF099924.D
Acq On : 28 Oct 2017 18:26
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ALS Vial : 16 Sample Multiplier: 1

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ClientSampleId :
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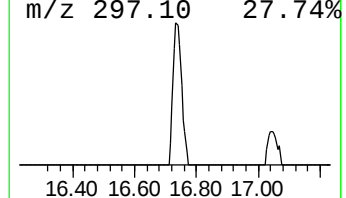
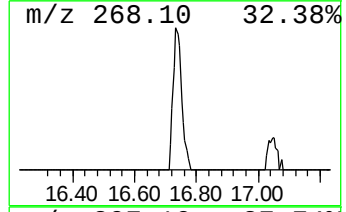
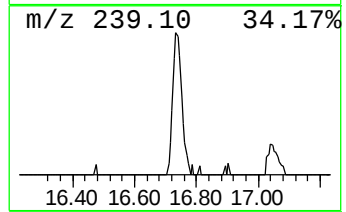
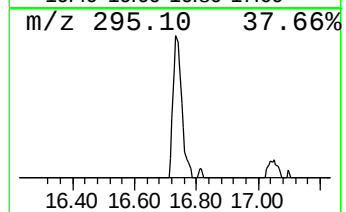
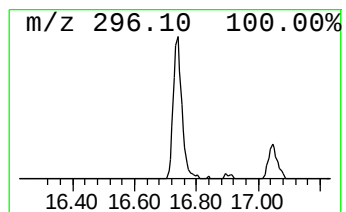
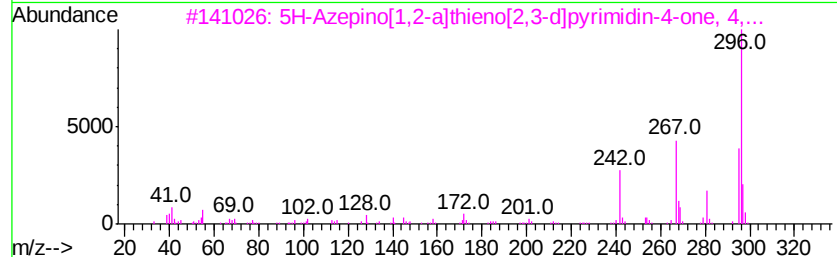
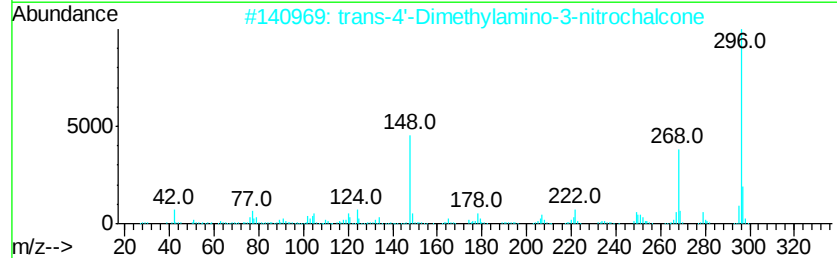
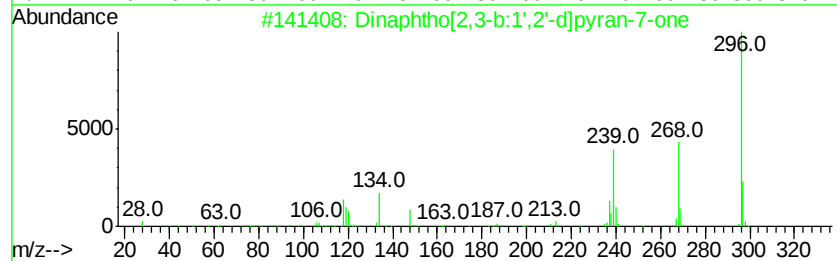
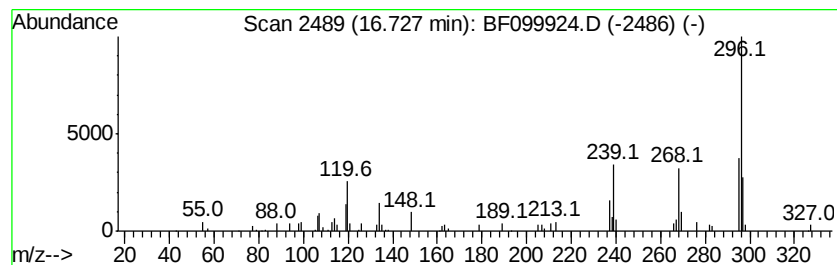
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Dinaphtho[2,3-b:1',2'-d]pyr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	3.95 ng	119051	Perylene-d12	15.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dinaphtho[2,3-b:1',2'-d]pyran-7-one	296	C21H12O2	154352-87-1	91
2			trans-4'-Dimethylamino-3-nitroch...	296	C17H16N2O3	1000234-56-7	52
3			5H-Azepino[1,2-a]thieno[2,3-d]pv...	296	C17H16N2OS	056929-66-9	50
4			Benzothiophene-3-carbonitrile, 4...	296	C17H16N2OS	069438-35-3	50
5			Benzoic acid, 4-[[[4-(dimethylam...	296	C18H20N2O2	020534-73-0	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102817\
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 Acq On : 28 Oct 2017 18:26
 Operator : SJ/JU
 Sample : I6141-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-A-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	12.7	ng	382668	1	6.79	604192	20.0
unknown6.56	6.56	77.8	ng	2351030	1	6.79	604192	20.0
n-Hexadecanoic acid	11.83	2.5	ng	90731	4	11.32	736764	20.0
Heptadecyl hepta...	13.77	5.7	ng	165576	5	13.96	577720	20.0
Pentafluoropropio...	14.41	3.1	ng	89178	5	13.96	577720	20.0
Naphthalene, 1-(2...	14.47	2.9	ng	82354	5	13.96	577720	20.0
Nonadecane	15.02	4.8	ng	144226	6	15.42	602482	20.0
Dinaphtho[1,2-b:1...	15.16	2.1	ng	62541	6	15.42	602482	20.0
Eicosane	16.29	2.0	ng	61312	6	15.42	602482	20.0
Dinaphtho[2,3-b:1...	16.73	4.0	ng	119051	6	15.42	602482	20.0