

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
 Data File : BF097272.D
 Acq On : 2 Aug 2017 14:42
 Operator : SJ/JU
 Sample : I4497-09
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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	2.604	119	122	146	rBV	173614	407541	16.02%	1.575%
2	4.581	454	458	470	rBV	299084	482720	18.97%	1.865%
3	5.051	534	538	555	rBV	2230281	2542729	99.93%	9.826%
4	6.122	716	720	733	rBV	2309121	2544588	100.00%	9.833%
5	6.228	733	738	745	rVB	2468909	2514934	98.83%	9.718%
6	6.451	772	776	782	rBV	740949	707211	27.79%	2.733%
7	6.604	798	802	810	rBV	2056770	1856572	72.96%	7.174%
8	7.022	868	873	887	rBV	1561600	1575696	61.92%	6.089%
9	7.169	894	898	904	rVB	49745	54459	2.14%	0.210%
10	7.663	979	982	990	rBV	102423	107516	4.23%	0.415%
11	7.733	990	994	999	rBV	1137291	997400	39.20%	3.854%
12	8.810	1173	1177	1180	rBV	2295388	2104377	82.70%	8.132%
13	9.210	1241	1245	1248	rBV	696592	551746	21.68%	2.132%
14	9.433	1276	1283	1286	rBV3	58567	103220	4.06%	0.399%
15	9.474	1286	1290	1298	rVB	1145277	1034178	40.64%	3.996%
16	9.716	1329	1331	1335	rVB2	37118	31128	1.22%	0.120%
17	9.898	1359	1362	1365	rBV2	44358	53522	2.10%	0.207%
18	9.933	1365	1368	1372	rVB	60407	53500	2.10%	0.207%
19	10.151	1400	1405	1407	rBV2	38708	46317	1.82%	0.179%
20	10.263	1420	1424	1428	rBV	1490462	1430634	56.22%	5.528%
21	10.404	1444	1448	1455	rBV	68689	108518	4.26%	0.419%
22	10.486	1459	1462	1468	rVB4	23396	34945	1.37%	0.135%
23	10.592	1474	1480	1484	rBV4	15705	26093	1.03%	0.101%
24	10.845	1520	1523	1526	rVV	63449	52031	2.04%	0.201%
25	10.874	1526	1528	1532	rVB	29518	27585	1.08%	0.107%
26	10.951	1537	1541	1544	rVB	965986	902628	35.47%	3.488%
27	11.221	1577	1587	1590	rBV9	12183	29779	1.17%	0.115%
28	11.268	1593	1595	1601	rVB	37425	37356	1.47%	0.144%
29	11.504	1630	1635	1643	rBV2	322601	381205	14.98%	1.473%
30	11.645	1656	1659	1662	rBV4	28786	33684	1.32%	0.130%
31	11.674	1662	1664	1669	rVB3	25819	27217	1.07%	0.105%
32	12.210	1753	1755	1761	rVB4	21622	29158	1.15%	0.113%
33	12.286	1762	1768	1779	rVV	371581	420626	16.53%	1.625%
34	12.374	1781	1783	1790	rVB2	22053	31274	1.23%	0.121%

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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	12.533	1805	1810	1813	rBV	1950366	1912611	75.16%	7.391%
36	13.451	1962	1966	1974	rBV	133553	176378	6.93%	0.682%
37	13.568	1979	1986	1994	rVB	943685	967320	38.01%	3.738%
38	14.221	2092	2097	2104	rBV	46101	90520	3.56%	0.350%
39	14.333	2111	2116	2119	rBV	102745	124330	4.89%	0.480%
40	14.362	2119	2121	2124	rVB	56831	50174	1.97%	0.194%
41	14.645	2166	2169	2172	rBV	85263	86043	3.38%	0.332%
42	14.768	2185	2190	2197	rBV2	41331	82707	3.25%	0.320%
43	14.909	2210	2214	2219	rBV	457698	553750	21.76%	2.140%
44	14.956	2219	2222	2227	rVB	84224	102272	4.02%	0.395%
45	15.074	2237	2242	2247	rBV9	29990	67380	2.65%	0.260%
46	15.309	2277	2282	2287	rBV	76909	119437	4.69%	0.462%
47	15.362	2287	2291	2297	rVB2	28600	57075	2.24%	0.221%
48	15.709	2345	2350	2358	rVB2	51590	89323	3.51%	0.345%
49	16.180	2426	2430	2436	rVB3	30296	57455	2.26%	0.222%

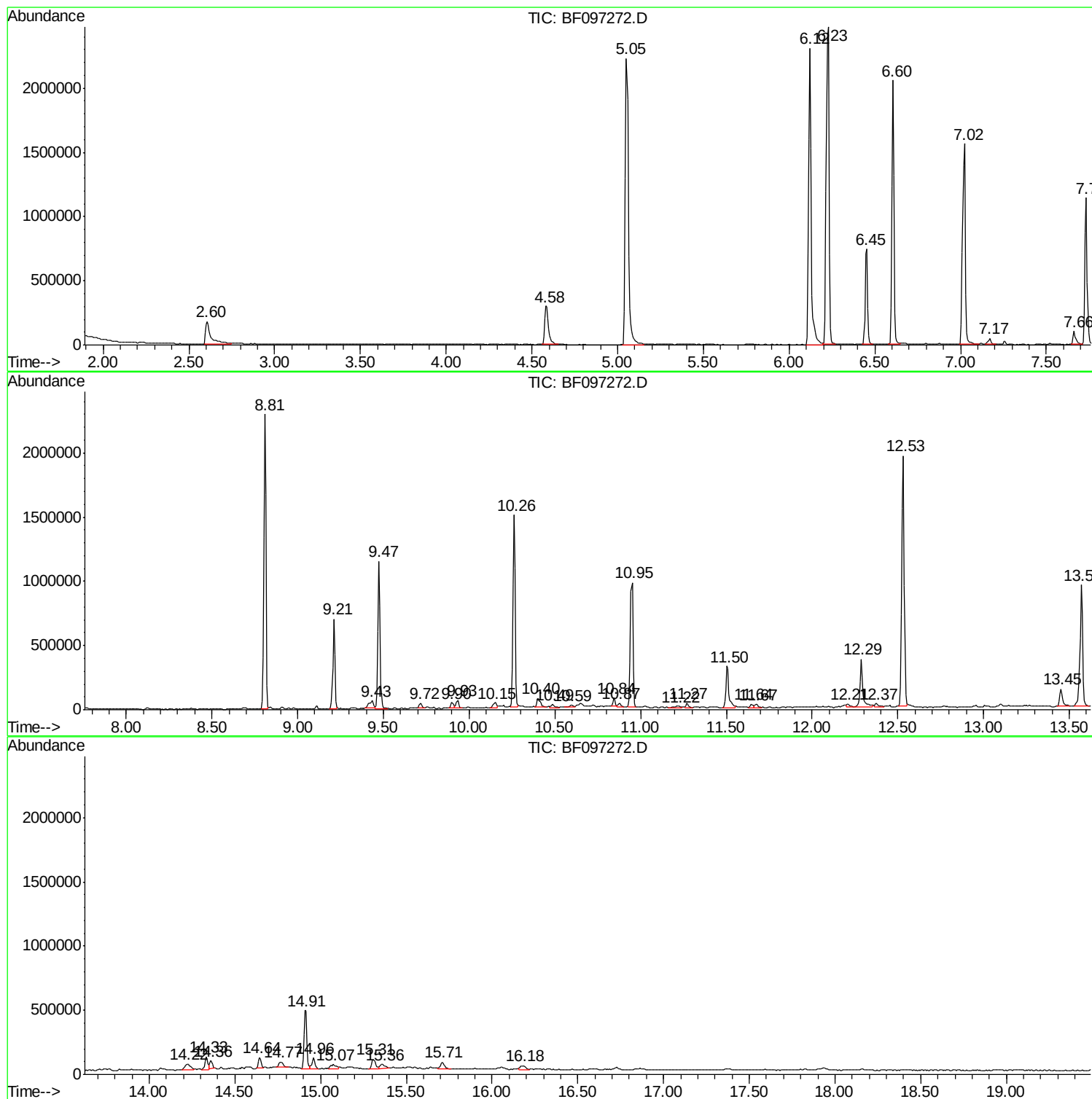
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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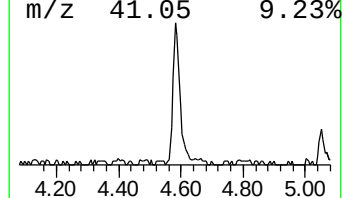
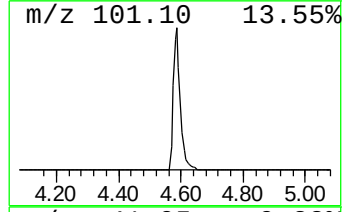
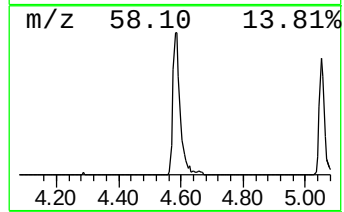
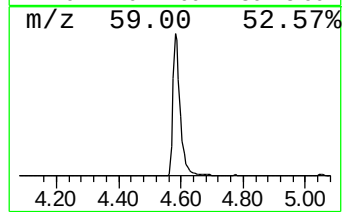
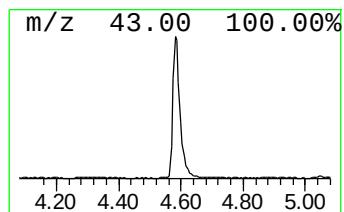
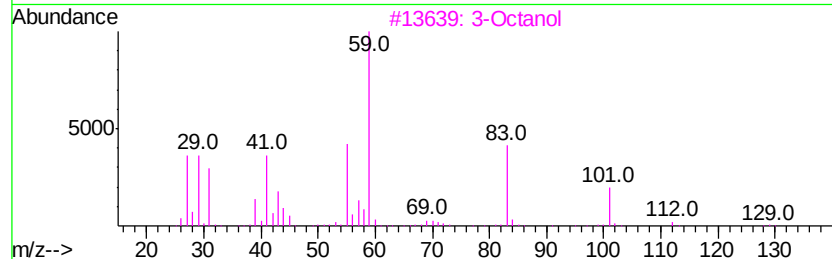
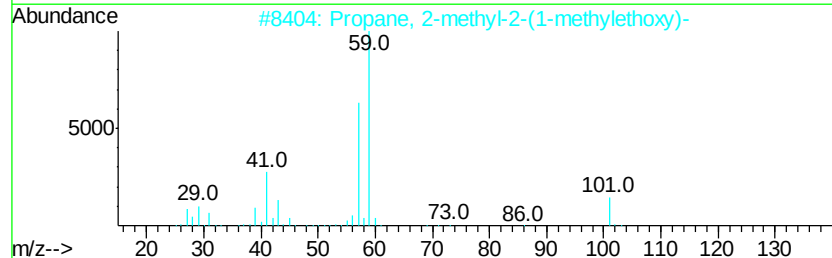
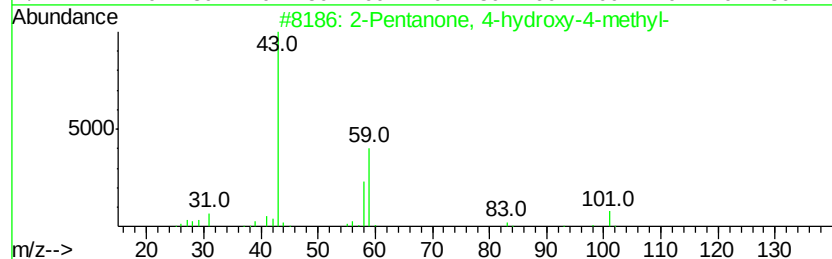
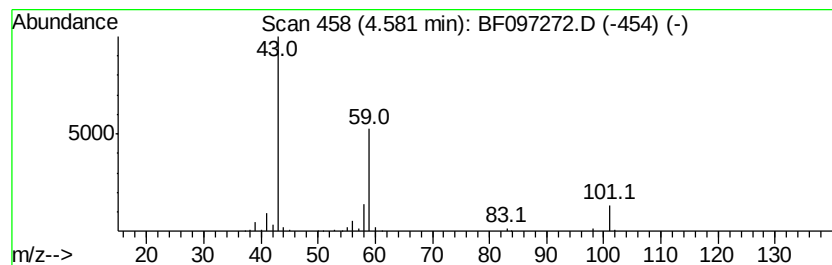
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	13.65 ng	482720	1,4-Dichlorobenzene-d4	6.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Octanol	130	C8H18O	000589-98-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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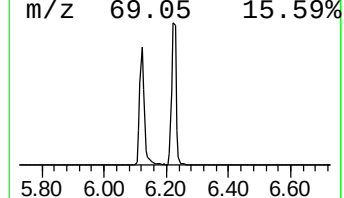
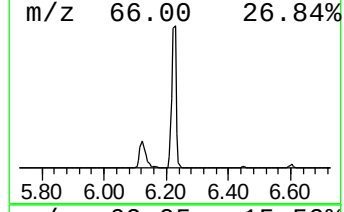
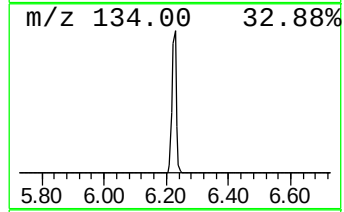
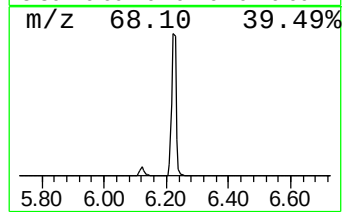
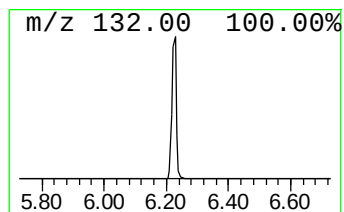
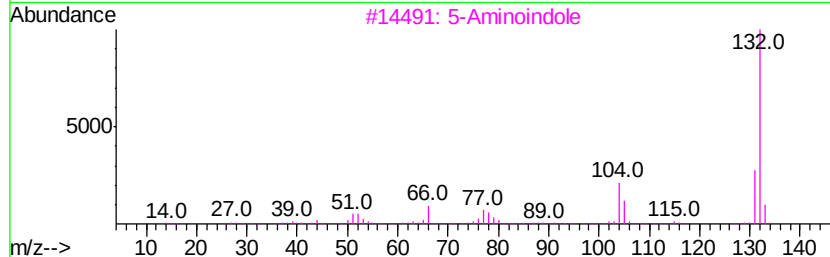
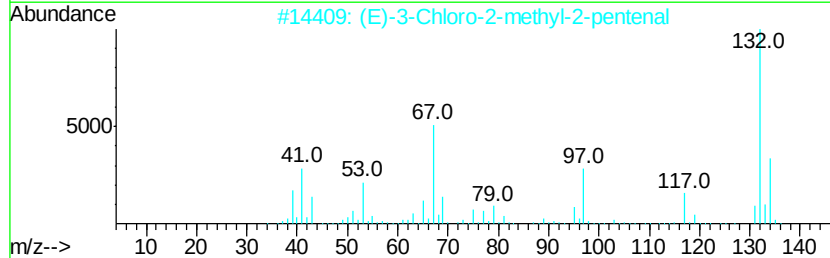
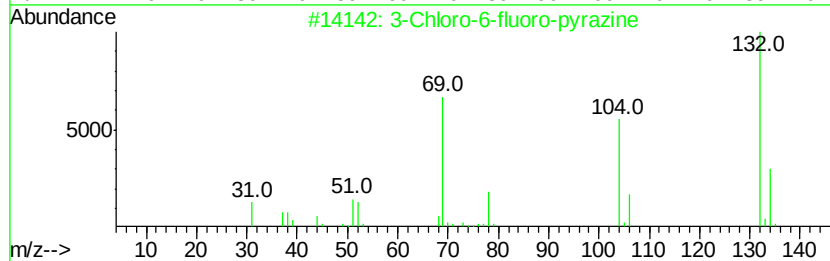
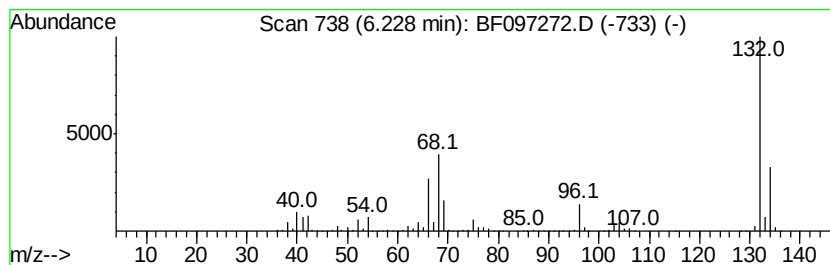
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	71.12 ng	2514930	1,4-Dichlorobenzene-d4	6.45

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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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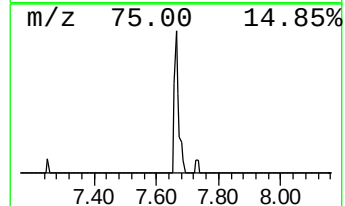
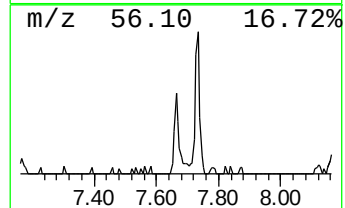
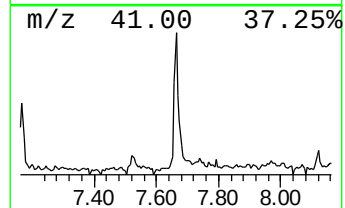
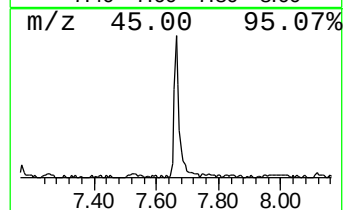
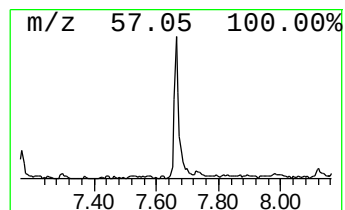
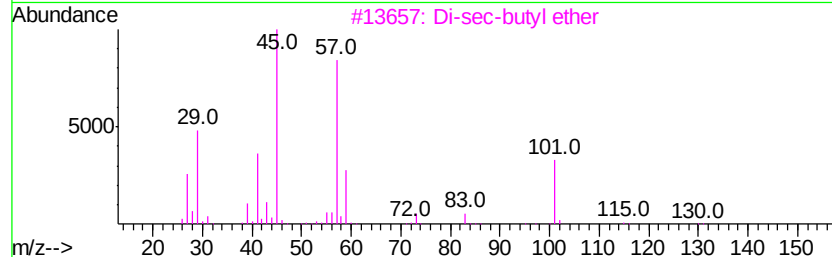
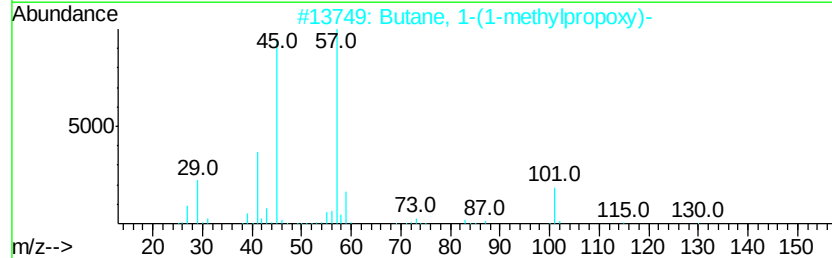
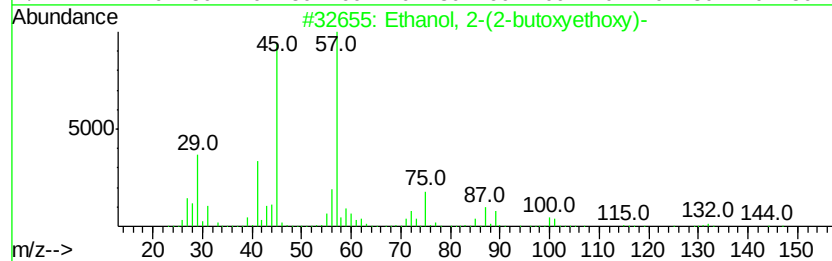
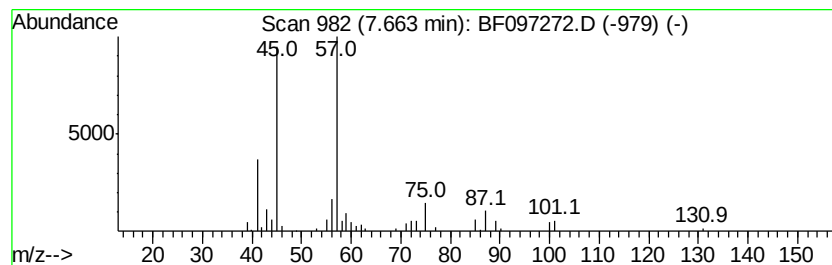
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	2.16 ng	107516	Napthalene-d8	7.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2		Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3		Di-sec-butyl ether	130	C8H18O	006863-58-7	53
4		Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
5		Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50



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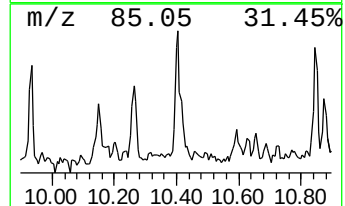
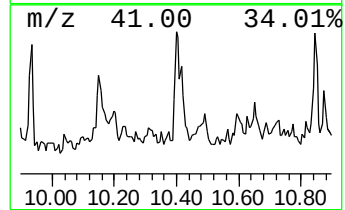
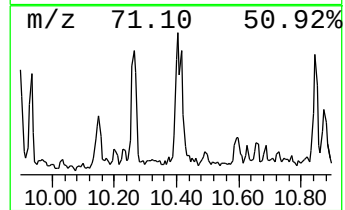
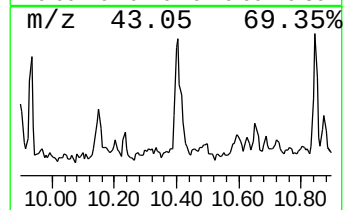
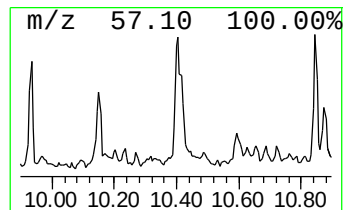
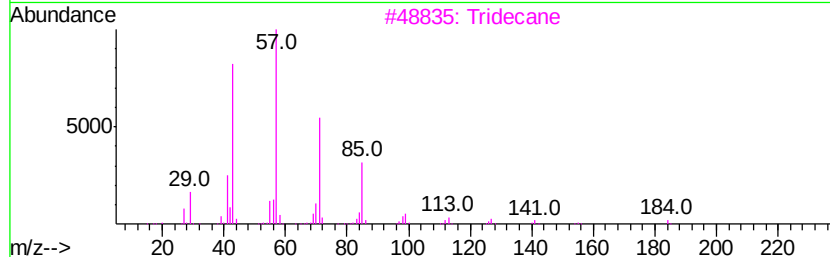
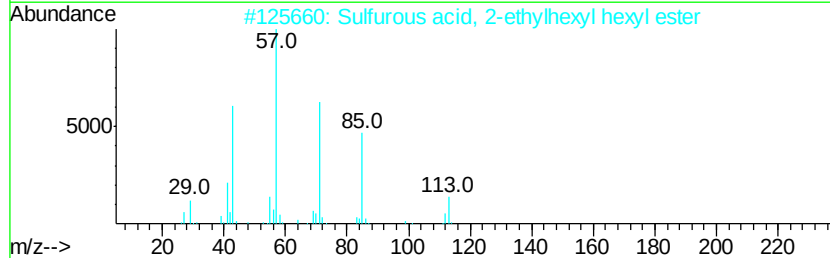
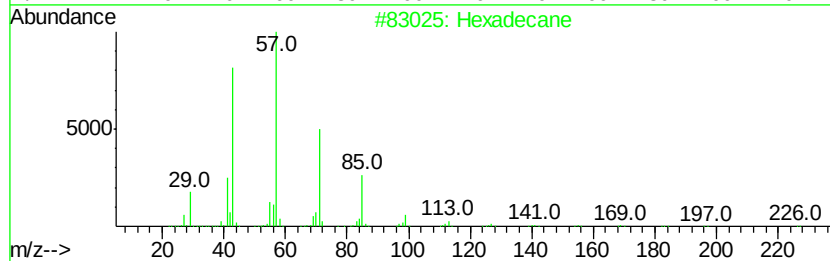
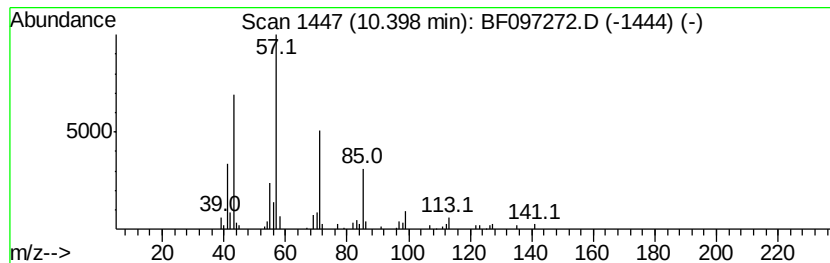
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.40	2.40 ng	108518	Phenanthrene-d10	10.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
3	Tridecane	184	C13H28	000629-50-5	78
4	Pentadecane	212	C15H32	000629-62-9	78
5	Decane, 3-methyl-	156	C11H24	013151-34-3	59



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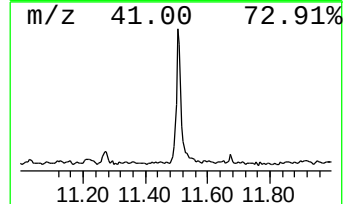
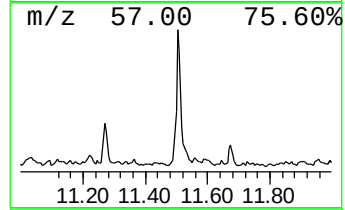
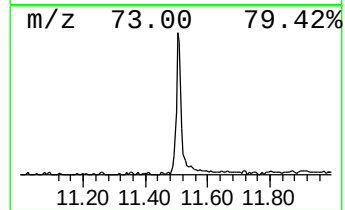
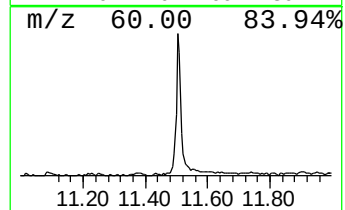
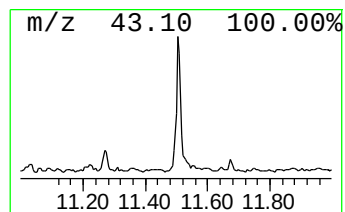
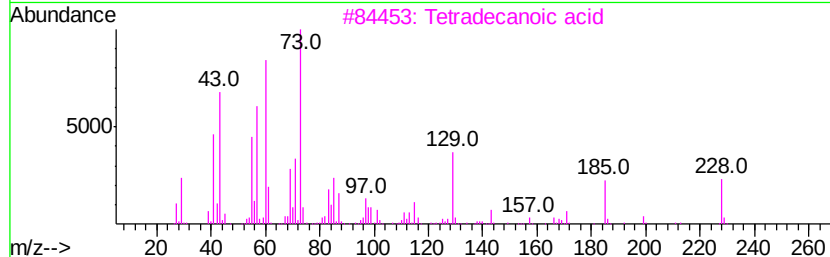
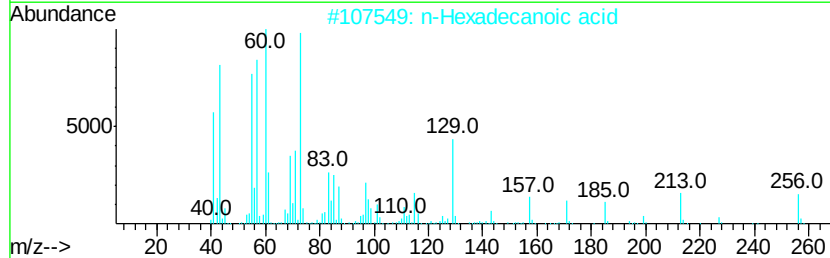
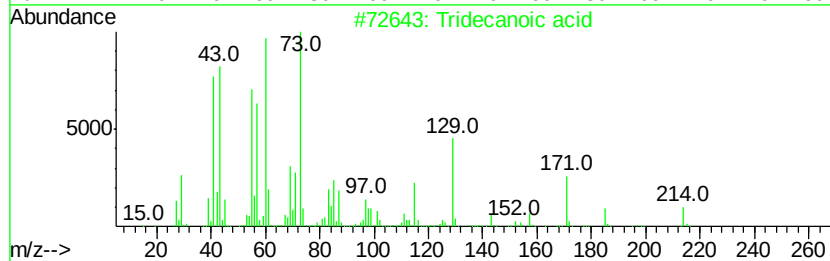
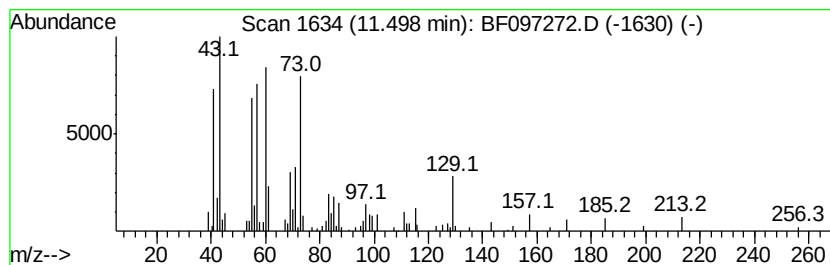
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.50	8.45 ng	381205	Phenanthrene-d10	10.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
Data File : BF097272.D
Acq On : 2 Aug 2017 14:42
Operator : SJ/JU
Sample : I4497-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

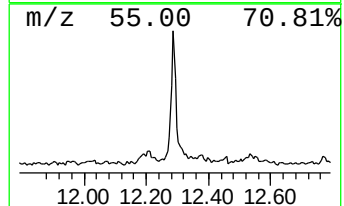
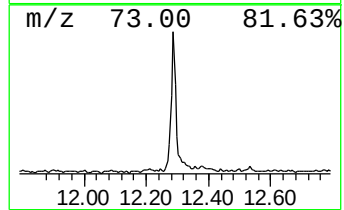
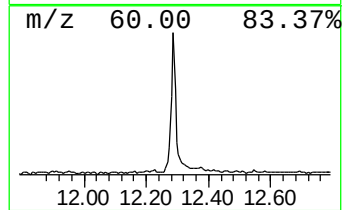
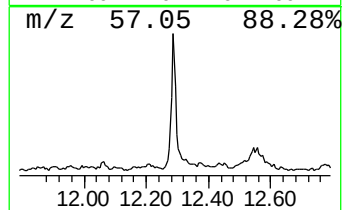
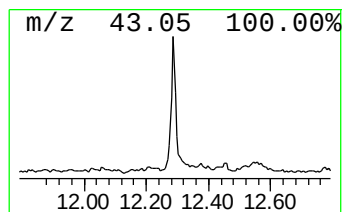
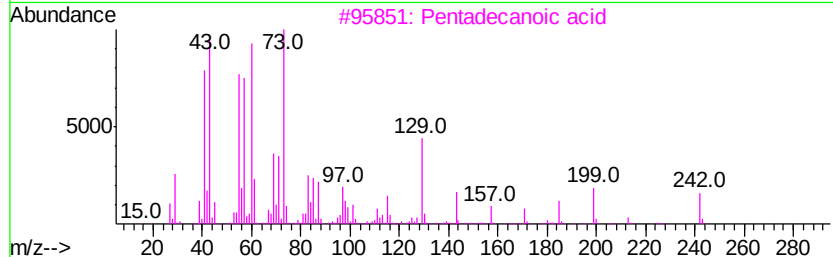
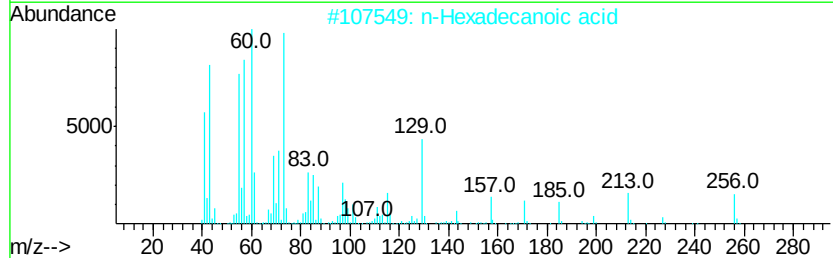
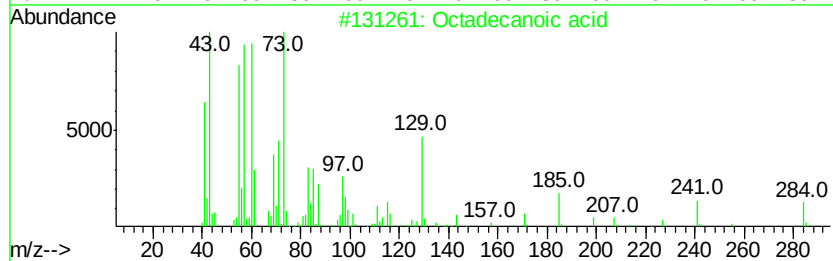
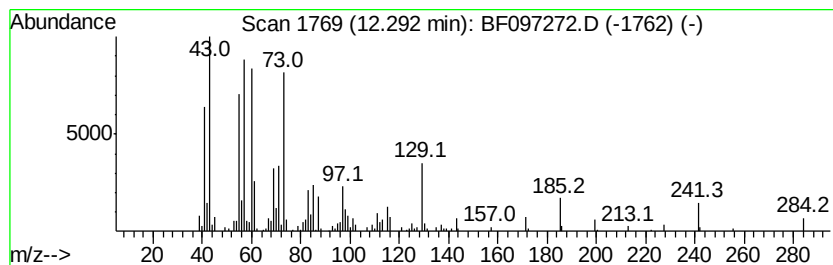
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	8.70 ng	420626	Chrysene-d12	13.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
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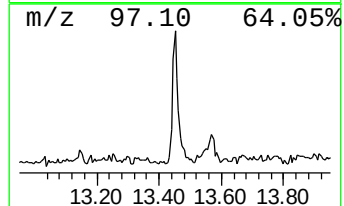
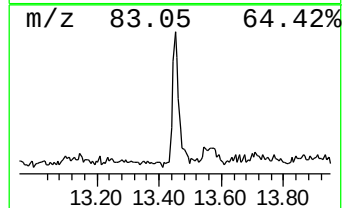
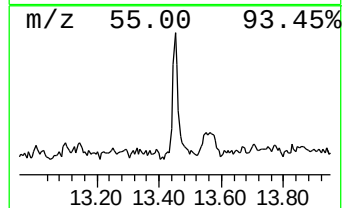
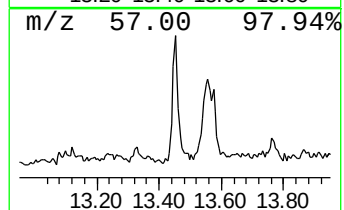
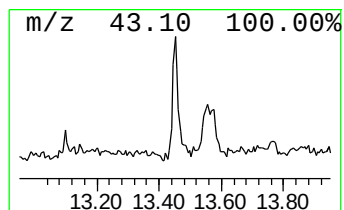
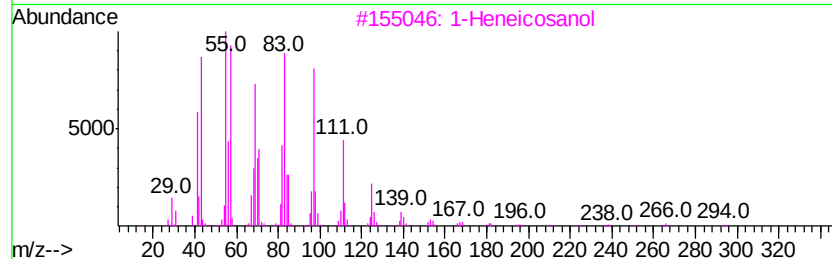
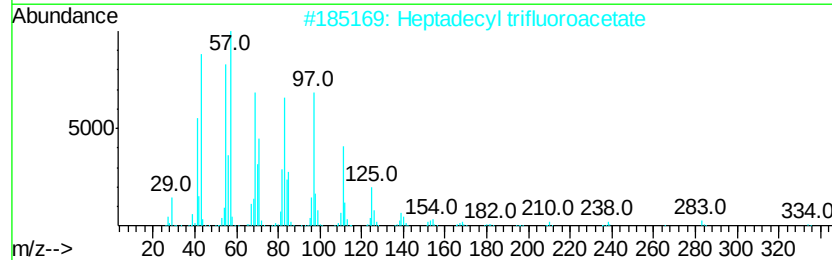
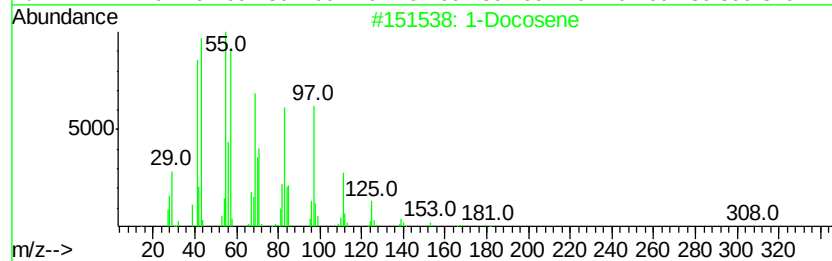
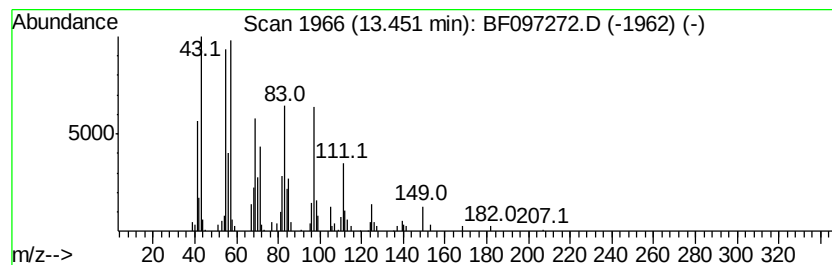
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Docosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	3.65 ng	176378	Chrysene-d12	13.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene		308 C22H44	001599-67-3 94
2	Heptadecyl trifluoroacetate		352 C19H35F3O2	1000351-87-0 94
3	1-Heneicosanol		312 C21H44O	015594-90-8 93
4	Trichloroacetic acid, pentadecyl...		372 C17H31Cl3O2	074339-53-0 91
5	n-Tetracosanol-1		354 C24H50O	000506-51-4 91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080217\
Data File : BF097272.D
Acq On : 2 Aug 2017 14:42
Operator : SJ/JU
Sample : I4497-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

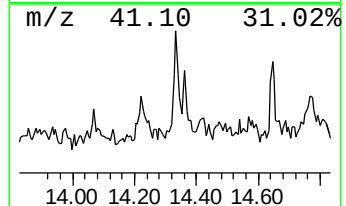
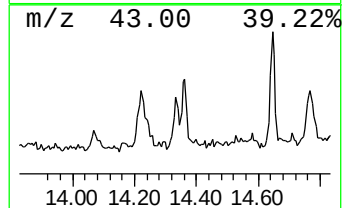
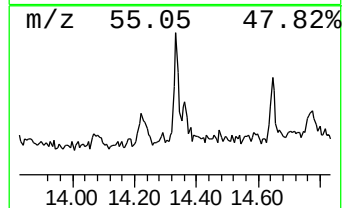
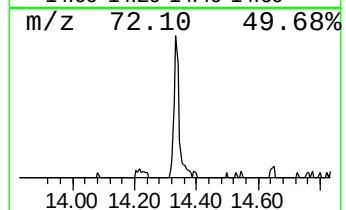
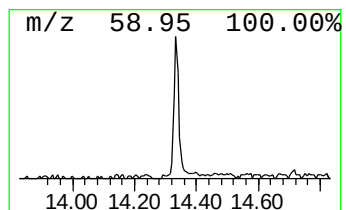
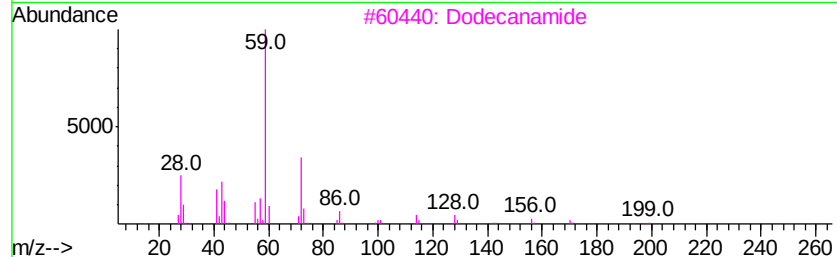
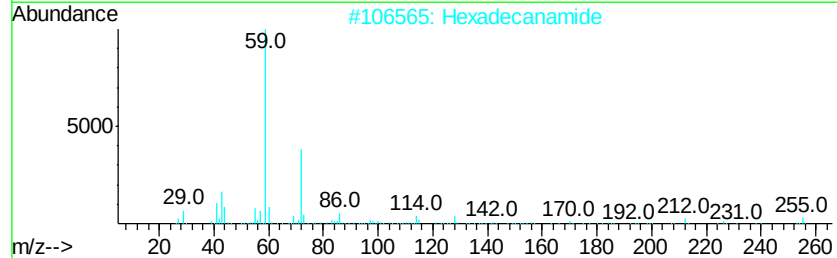
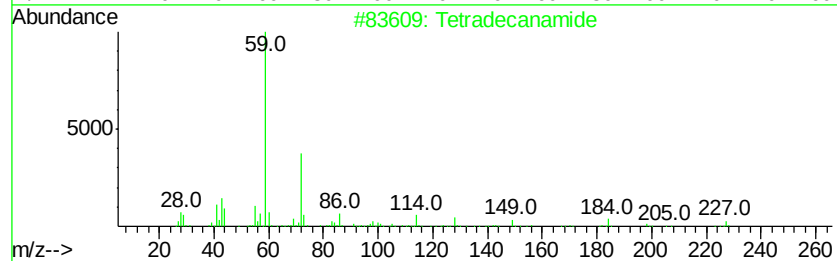
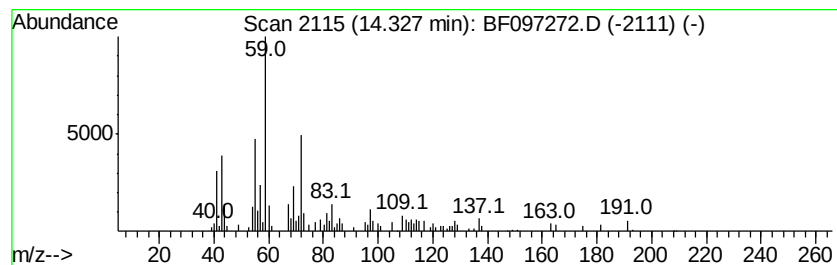
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetradecanamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.33	4.49 ng	124330	Perylene-d12		14.92		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanamide	227	C14H29NO	000638-58-4	72
2			Hexadecanamide	255	C16H33NO	000629-54-9	72
3			Dodecanamide	199	C12H25NO	001120-16-7	53
4			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	52
5			Octanamide	143	C8H17NO	000629-01-6	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
Data File : BF097272.D
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Operator : SJ/JU
Sample : I4497-09
Misc :
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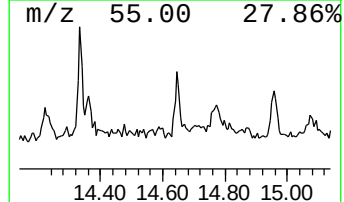
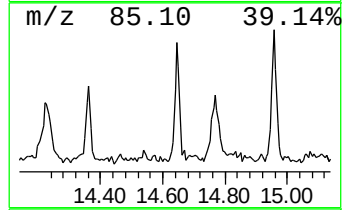
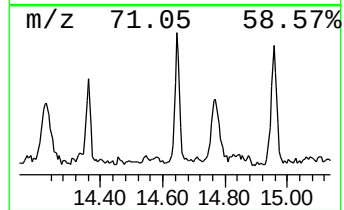
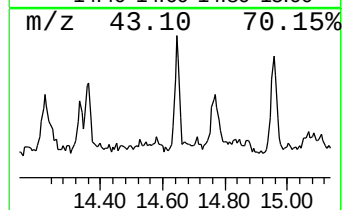
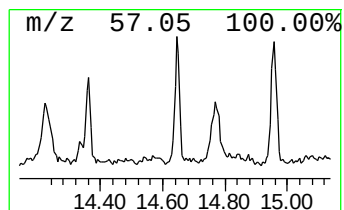
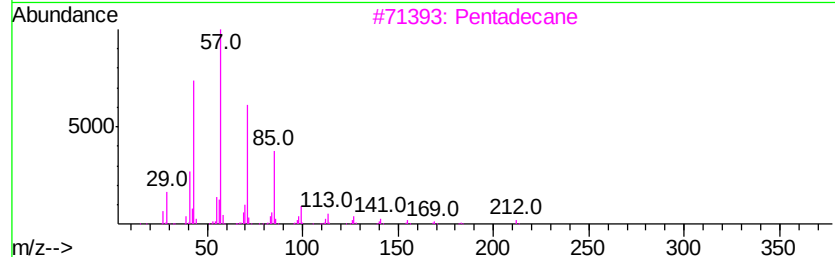
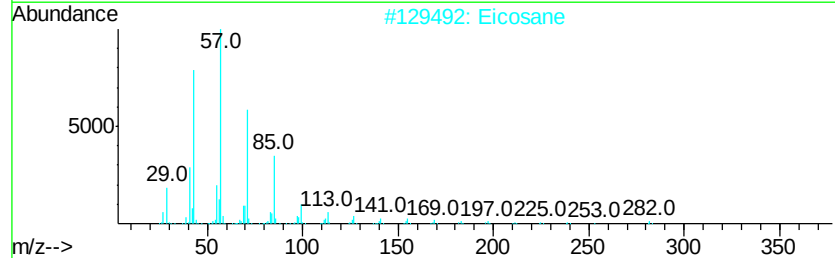
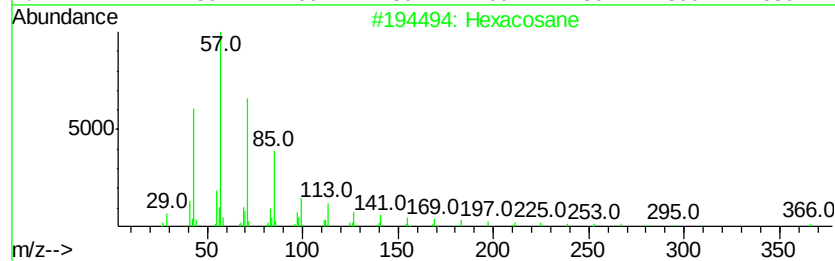
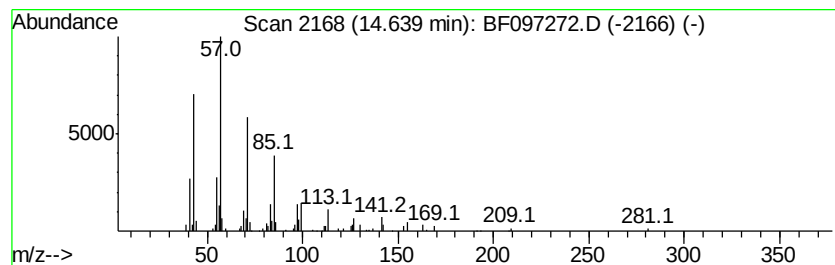
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.64	3.11 ng	86043	Perylene-d12		14.92
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Eicosane	282	C20H42	000112-95-8	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Heptacosane	380	C27H56	000593-49-7	86
5	Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
Data File : BF097272.D
Acq On : 2 Aug 2017 14:42
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Sample : I4497-09
Misc :
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Instrument :
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ClientSampleId :
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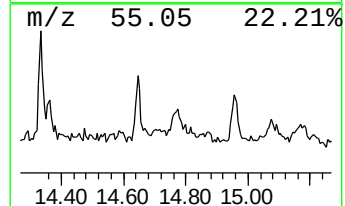
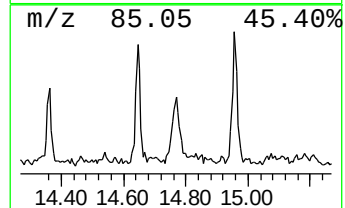
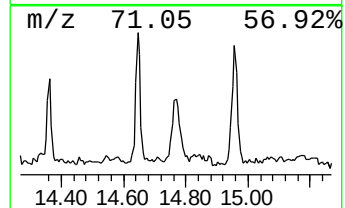
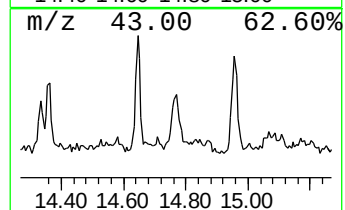
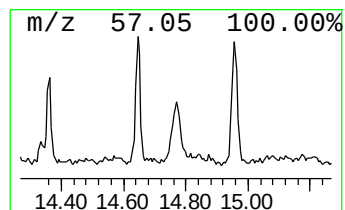
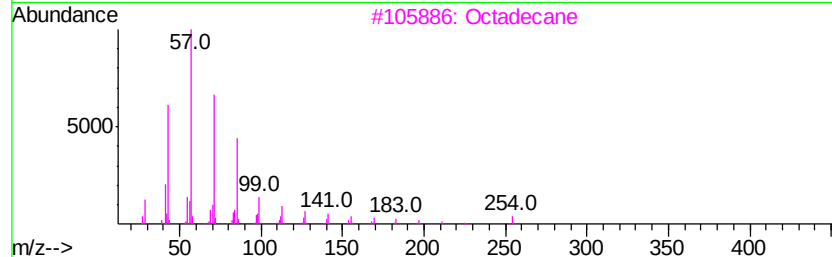
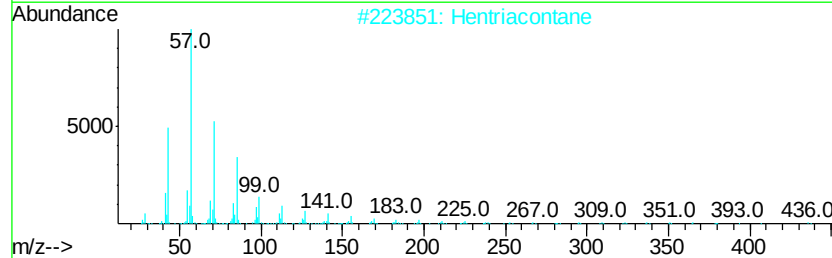
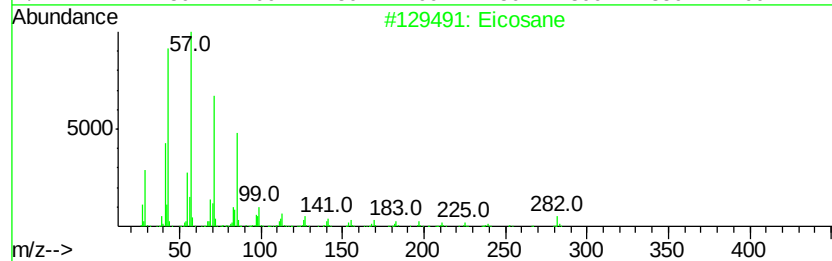
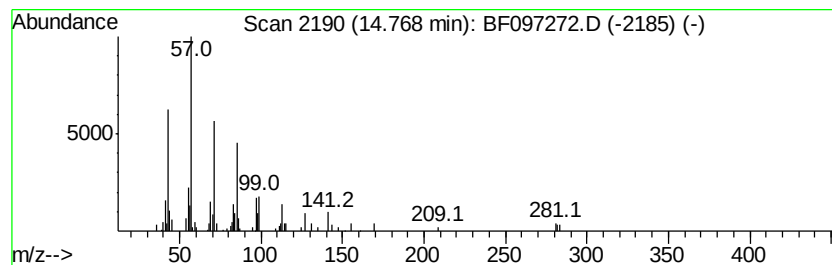
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	2.99 ng	82707	Perylene-d12	14.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	90
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Octadecane	254	C18H38	000593-45-3	83
4			2-methyloctacosane	408	C29H60	1000376-72-8	80
5			Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
Data File : BF097272.D
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Misc :
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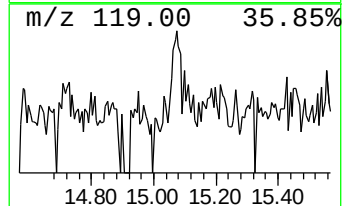
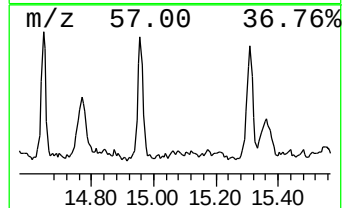
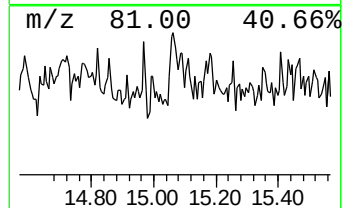
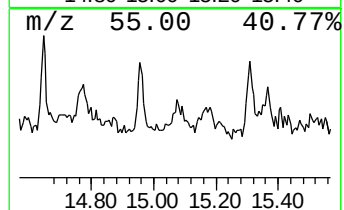
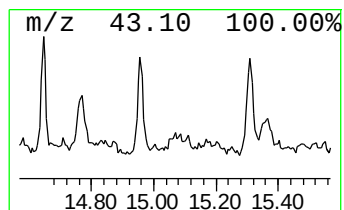
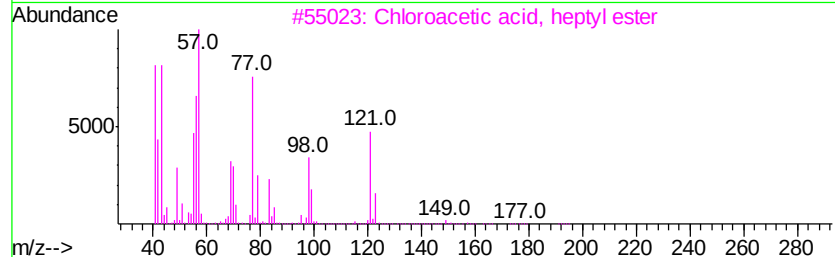
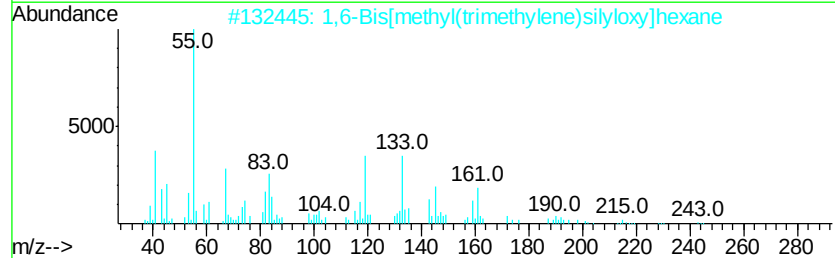
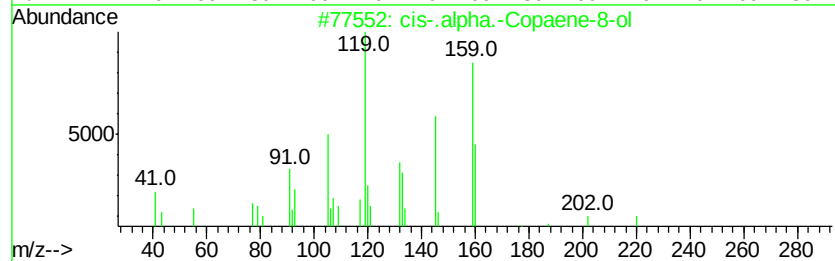
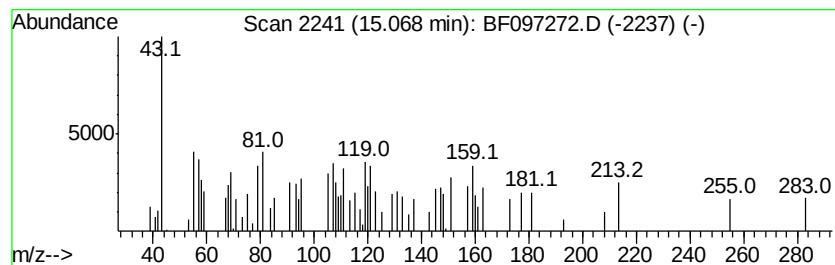
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown15.07 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.43 ng	67380	Perylene-d12	14.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-.alpha.-Copaene-8-ol	220	C15H24O	058569-25-8	22
2		1,6-Bis[methyl(trimethylene)silyl]hexane	286	C14H30O2Si2	1000217-00-5	12
3		Chloroacetic acid, heptyl ester	192	C9H17ClO2	034589-22-5	10
4		Carbonic acid, chloromethyl (4-methylphenyl) ester	200	C9H9ClO3	132905-79-4	10
5		2-Ethyl-1-(4-(pyridin-2-yl)piperidin-1-yl)ethan-1-ol	289	C17H27N3O	1000368-48-7	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
Data File : BF097272.D
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Misc :
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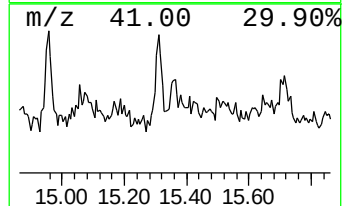
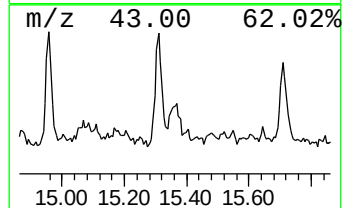
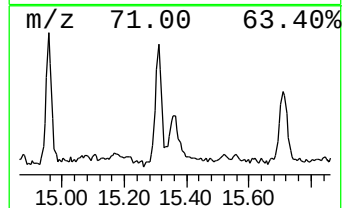
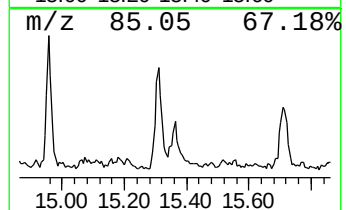
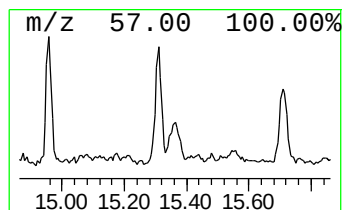
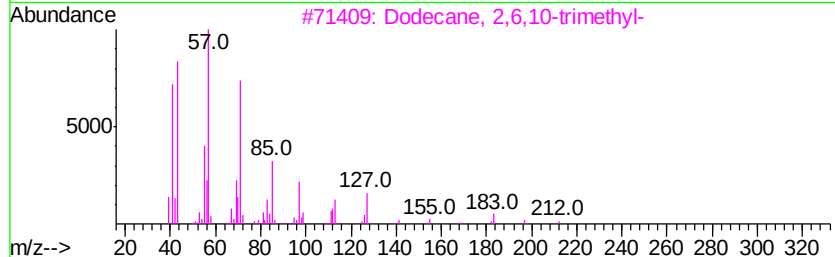
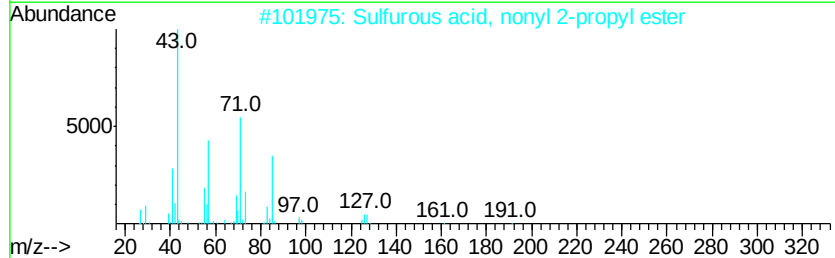
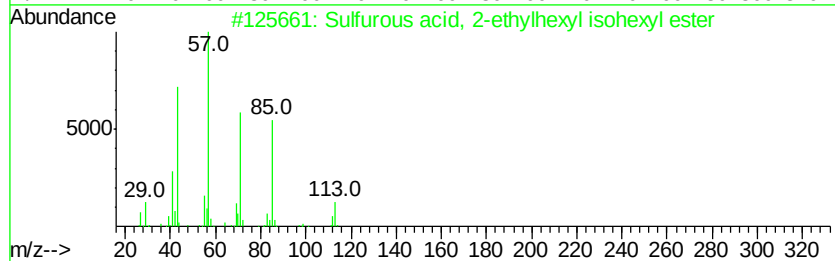
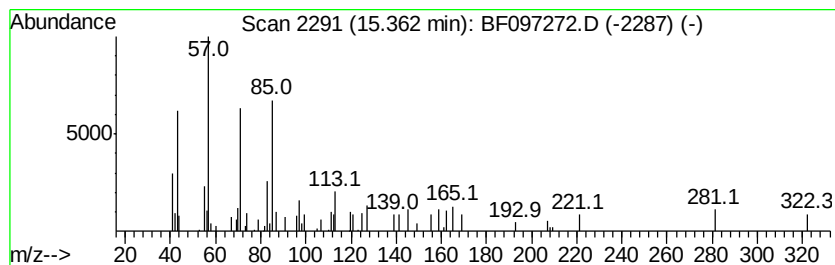
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown15.36 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.06 ng	57075	Perylene-d12	14.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	43
2			Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	38
3			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	35
4			Sulfurous acid, pentadecyl penty...	362	C20H42O3S	1000309-14-8	27
5			Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080217\
Data File : BF097272.D
Acq On : 2 Aug 2017 14:42
Operator : SJ/JU
Sample : I4497-09
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-6

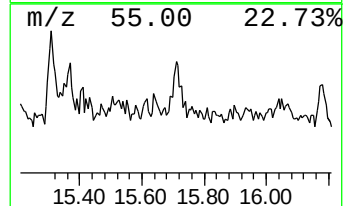
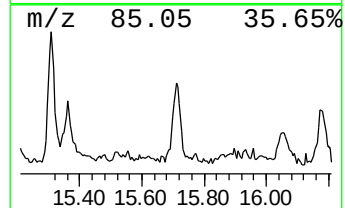
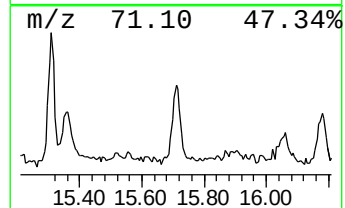
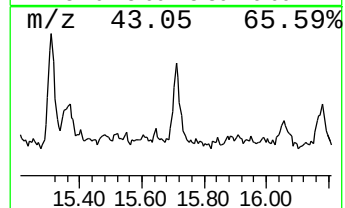
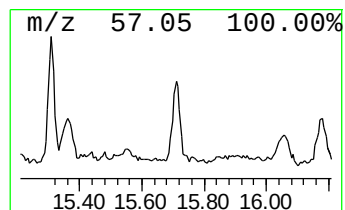
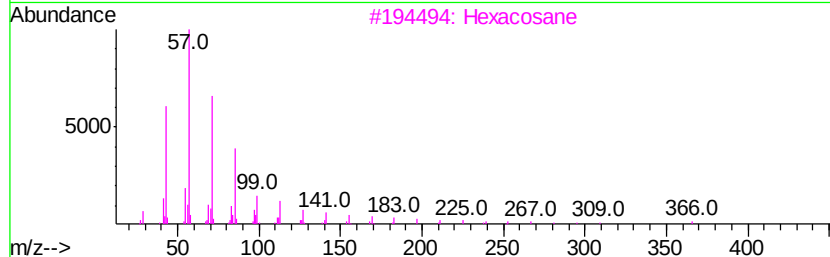
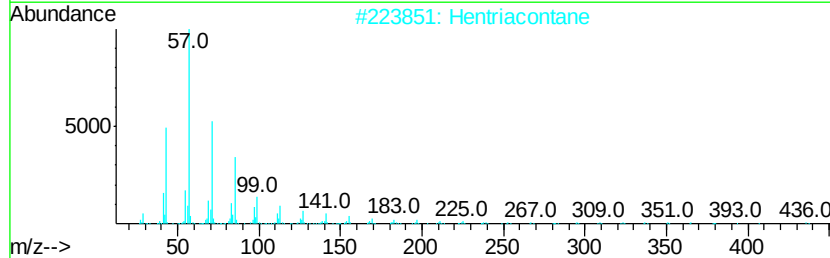
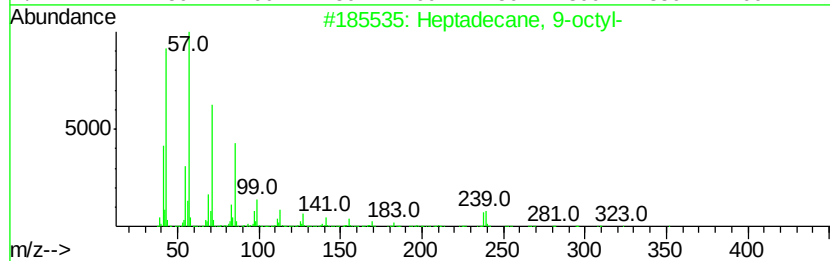
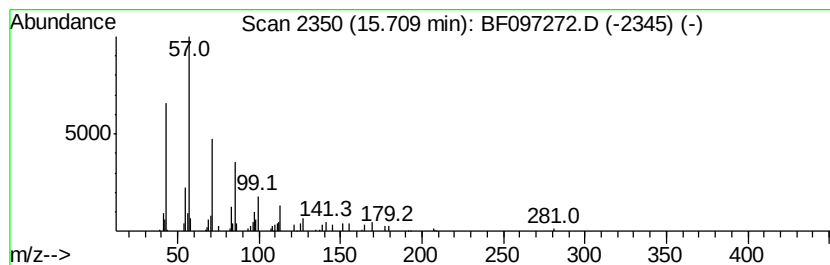
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Heptadecane, 9-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.23 ng	89323	Perylene-d12	14.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
2		Hentriacontane	437	C31H64	000630-04-6	83
3		Hexacosane	366	C26H54	000630-01-3	83
4		Tetratetracontane	619	C44H90	007098-22-8	80
5		Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080217\
 Data File : BF097272.D
 Acq On : 2 Aug 2017 14:42
 Operator : SJ/JU
 Sample : I4497-09
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-6

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.58	13.7	ng	482720	1	6.45	707211	20.0
unknown6.23	6.23	71.1	ng	2514930	1	6.45	707211	20.0
Ethanol, 2-(2-but...	7.66	2.2	ng	107516	2	7.73	997400	20.0
Hexadecane	10.40	2.4	ng	108518	4	10.95	902628	20.0
Tridecanoic acid	11.50	8.4	ng	381205	4	10.95	902628	20.0
Octadecanoic acid	12.29	8.7	ng	420626	5	13.57	967320	20.0
1-Docosene	13.45	3.6	ng	176378	5	13.57	967320	20.0
Tetradecanamide	14.33	4.5	ng	124330	6	14.92	553750	20.0
Hexacosane	14.64	3.1	ng	86043	6	14.92	553750	20.0
Eicosane	14.77	3.0	ng	82707	6	14.92	553750	20.0
unknown15.07	15.07	2.4	ng	67380	6	14.92	553750	20.0
unknown15.36	15.36	2.1	ng	57075	6	14.92	553750	20.0
Heptadecane, 9-oc...	15.71	3.2	ng	89323	6	14.92	553750	20.0