

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051817\
 Data File : BF095224.D
 Acq On : 18 May 2017 16:05
 Operator : SJ/MA
 Sample : I3159-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3-20170515

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-BF050217.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	5.113	536	540	556	rBV	88039	175886	5.05%	0.758%
2	5.742	643	647	679	rBV	514158	1260906	36.23%	5.431%
3	7.319	911	915	930	rBV	286522	696733	20.02%	3.001%
4	7.431	930	934	952	rVB	1611751	2436748	70.02%	10.495%
5	7.766	987	991	1002	rVB	481179	576748	16.57%	2.484%
6	8.007	1026	1032	1048	rBV	1737009	2159802	62.06%	9.302%
7	8.672	1139	1145	1170	rBV	1187784	1759543	50.56%	7.578%
8	9.783	1330	1334	1353	rBV	558884	785738	22.58%	3.384%
9	11.560	1630	1636	1650	rBV	2657049	3479951	100.00%	14.988%
10	12.260	1750	1755	1763	rBV	56349	92070	2.65%	0.397%
11	12.619	1811	1816	1827	rBV2	626174	892674	25.65%	3.845%
12	13.918	2031	2037	2049	rBV	1297937	1973669	56.72%	8.501%
13	14.224	2085	2089	2092	rBV	35712	45841	1.32%	0.197%
14	15.018	2219	2224	2237	rBV	513661	741535	21.31%	3.194%
15	15.977	2381	2387	2393	rBV2	115199	174459	5.01%	0.751%
16	17.065	2567	2572	2578	rBV	76459	111193	3.20%	0.479%
17	17.342	2613	2619	2631	rBV	2102114	2677228	76.93%	11.531%
18	17.830	2687	2702	2716	rVB5	47357	213289	6.13%	0.919%
19	18.577	2826	2829	2839	rBV5	17545	36390	1.05%	0.157%
20	18.695	2844	2849	2862	rBV	457467	663368	19.06%	2.857%
21	18.918	2878	2887	2901	rBV3	104999	395101	11.35%	1.702%
22	19.689	3009	3018	3026	rBV3	89581	246081	7.07%	1.060%
23	20.318	3119	3125	3130	rBV	106607	201467	5.79%	0.868%
24	20.371	3130	3134	3144	rVV	235491	360613	10.36%	1.553%
25	20.630	3173	3178	3190	rBV	61058	195630	5.62%	0.843%
26	20.942	3224	3231	3240	rBV2	65387	158089	4.54%	0.681%
27	21.083	3248	3255	3261	rVB4	29985	66909	1.92%	0.288%
28	21.265	3279	3286	3293	rBV6	26584	67312	1.93%	0.290%
29	21.677	3348	3356	3364	rBV3	50605	134555	3.87%	0.580%
30	22.524	3492	3500	3510	rVB6	33611	103596	2.98%	0.446%
31	23.300	3621	3632	3644	rVB5	104474	334946	9.63%	1.443%

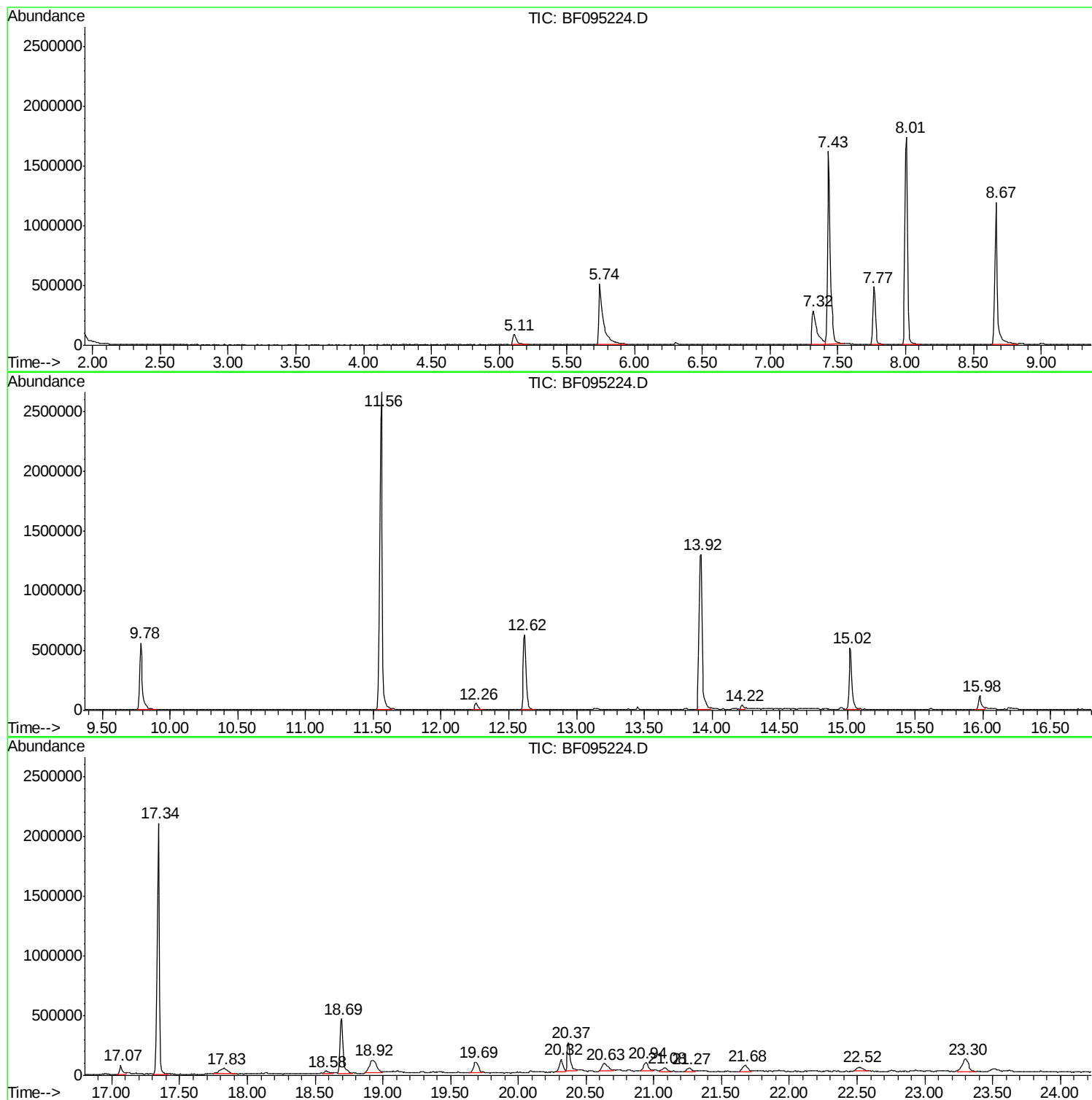
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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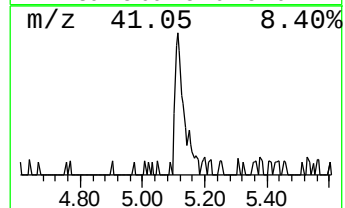
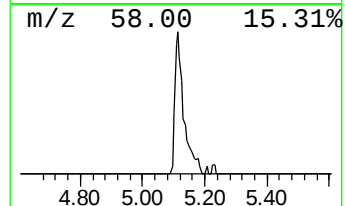
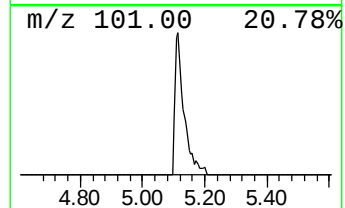
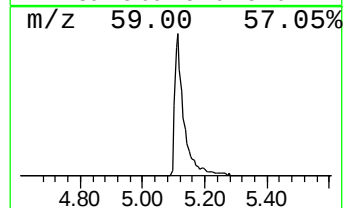
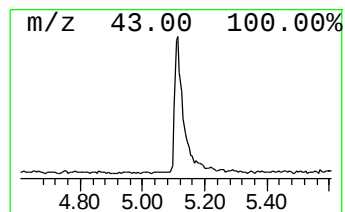
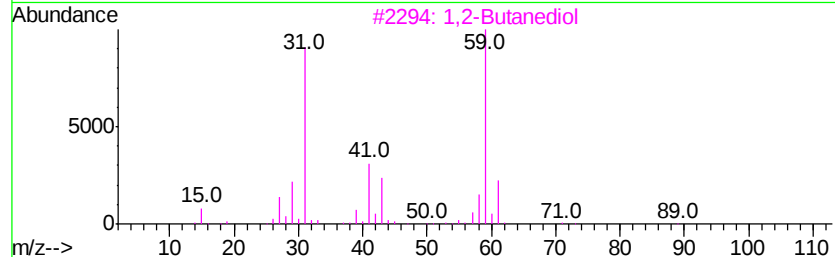
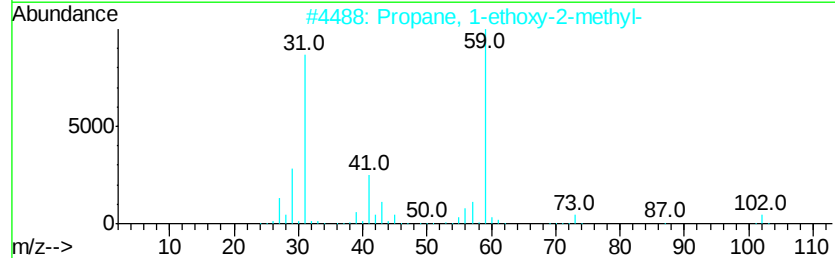
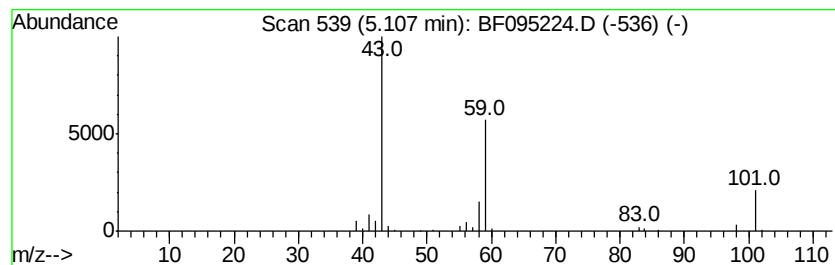
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	6.10 ng	175886	1,4-Dichlorobenzene-d4	7.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
3			1,2-Butanediol	90	C4H10O2	000584-03-2	23
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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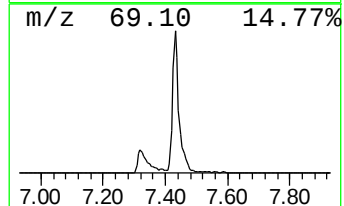
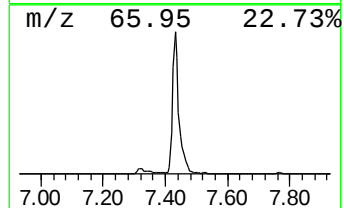
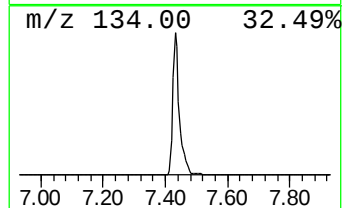
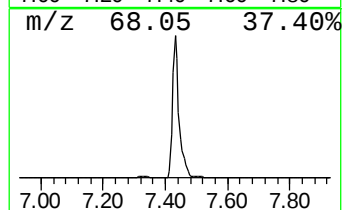
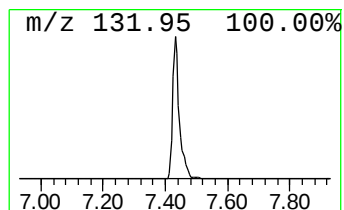
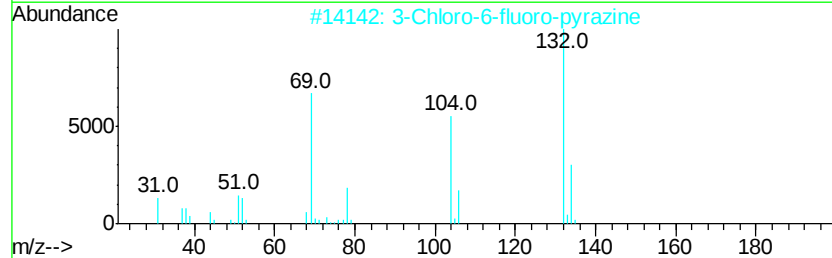
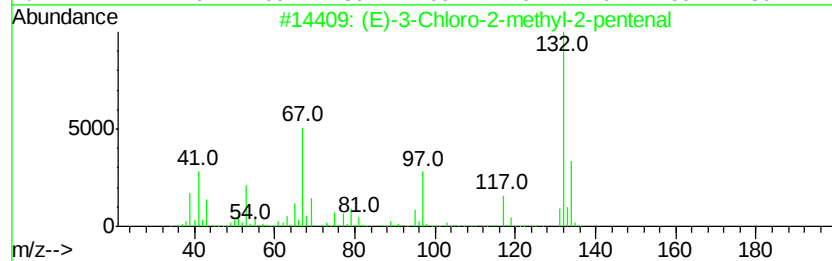
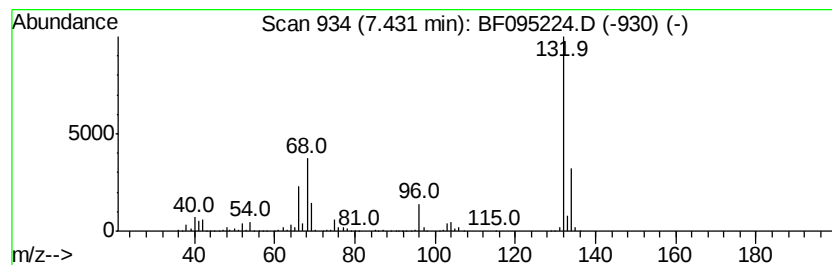
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Peak Number 2 unknown7.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	84.50 ng	2436750	1,4-Dichlorobenzene-d4	7.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Benzeneethanamine, .alpha.-methy...	223	C16H17N	002980-02-1	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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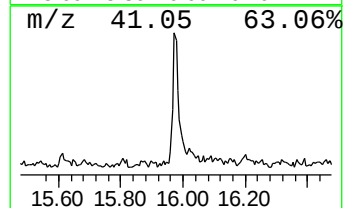
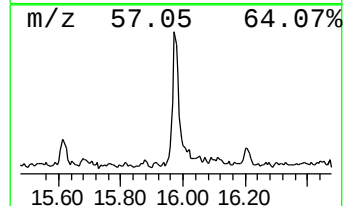
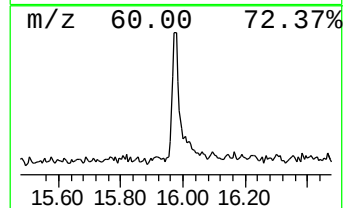
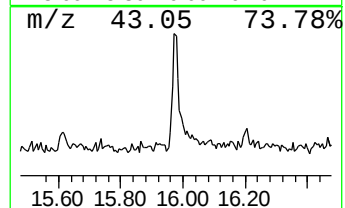
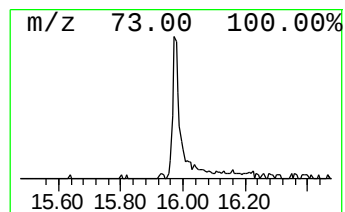
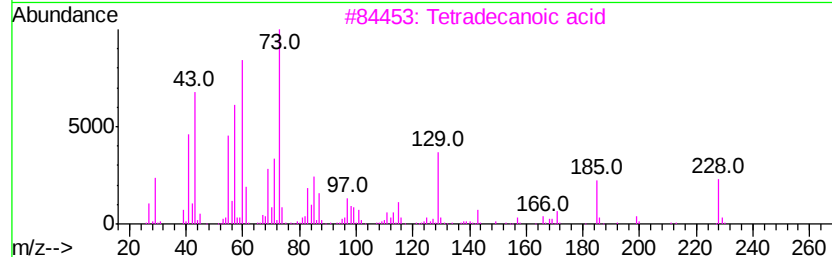
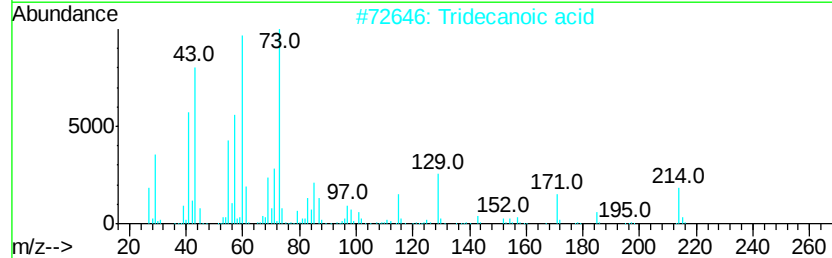
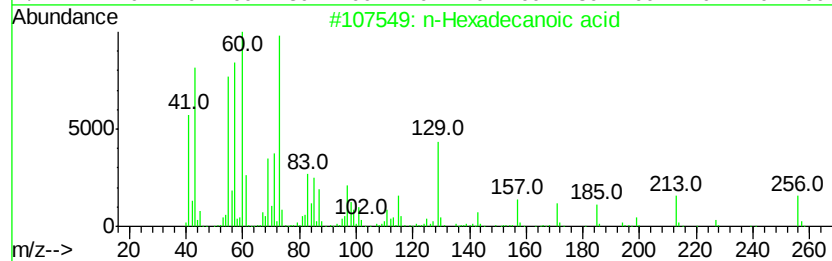
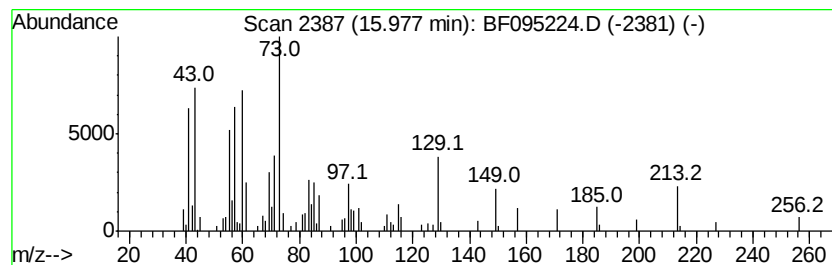
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.98	4.71 ng	174459	Phenanthrene-d10	15.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20



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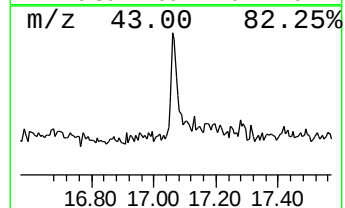
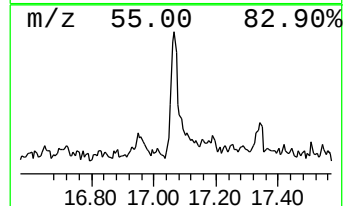
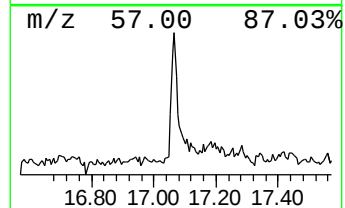
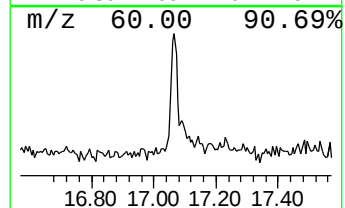
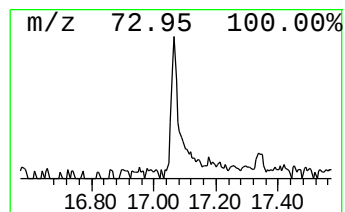
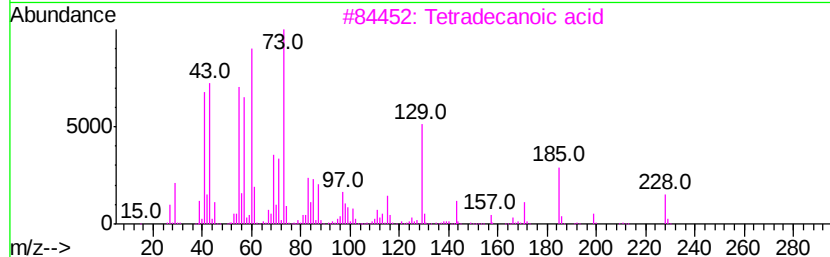
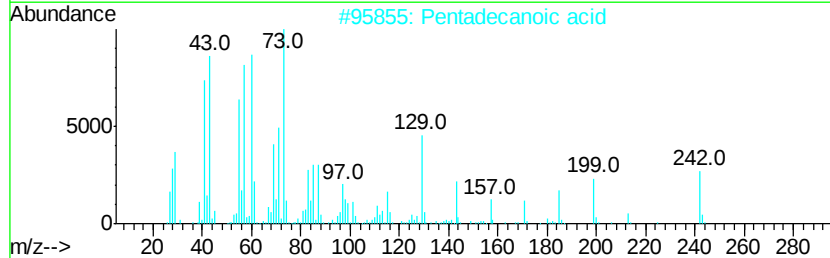
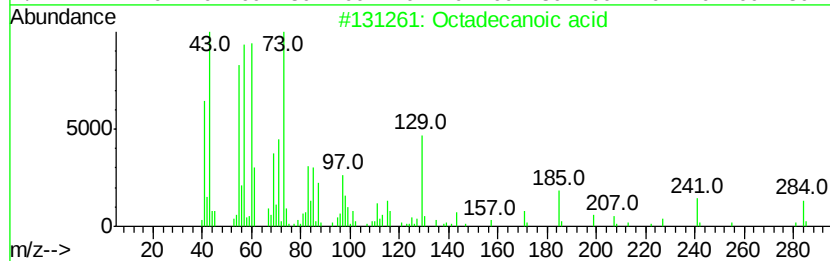
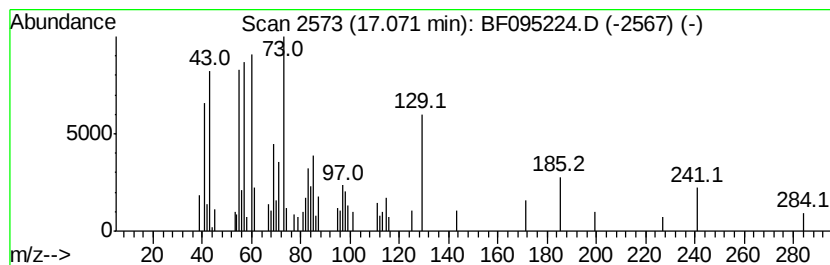
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Peak Number 5 Octadecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.07	3.35 ng	111193	Chrysene-d12	18.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	47
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25



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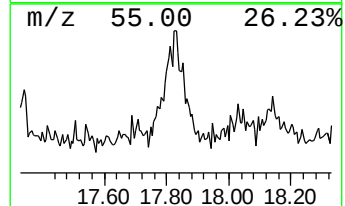
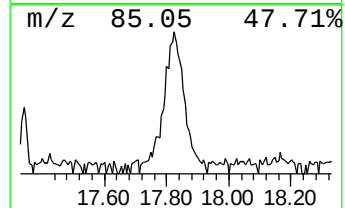
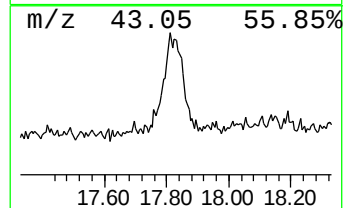
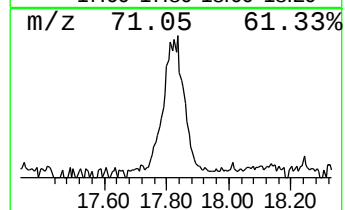
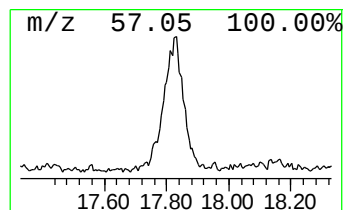
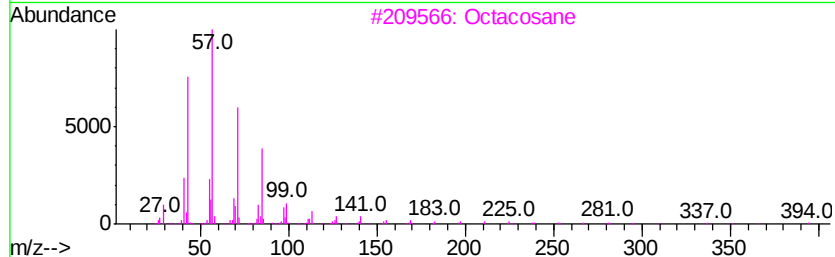
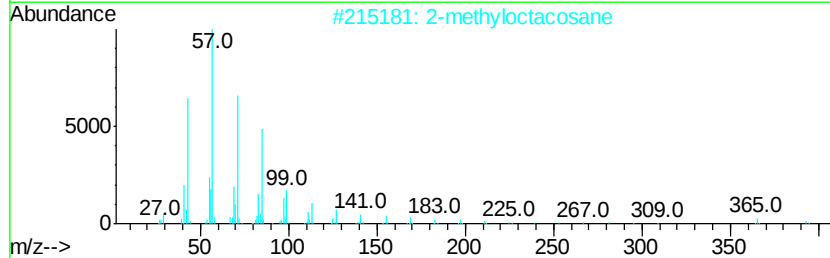
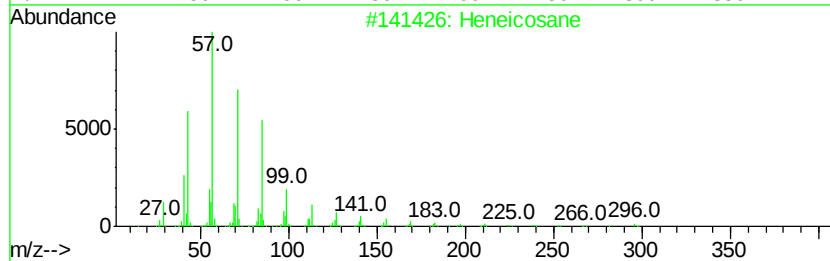
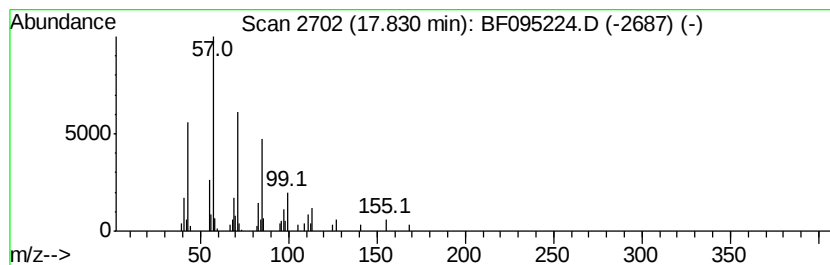
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Peak Number 6 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	6.43 ng	213289	Chrysene-d12	18.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	86
3	Octacosane		394	C28H58	000630-02-4	78
4	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	72
5	Heptadecane		240	C17H36	000629-78-7	59



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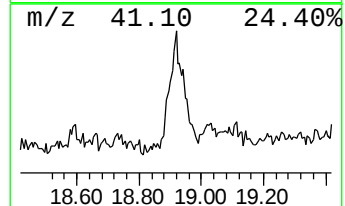
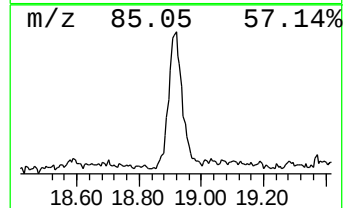
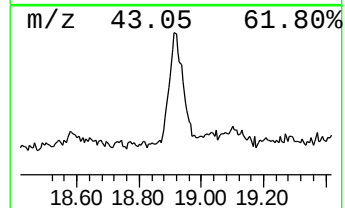
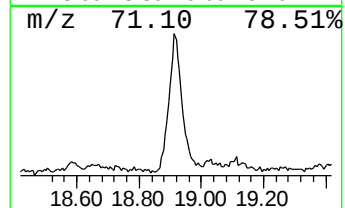
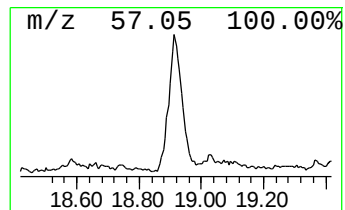
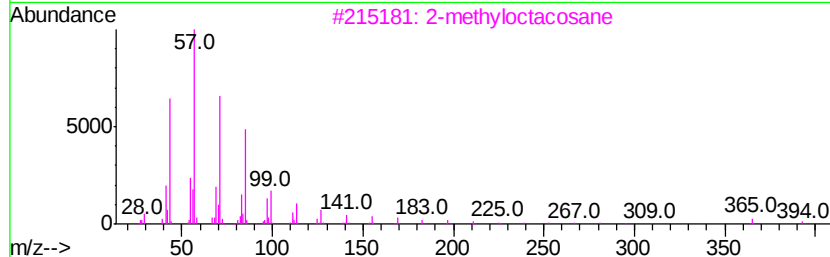
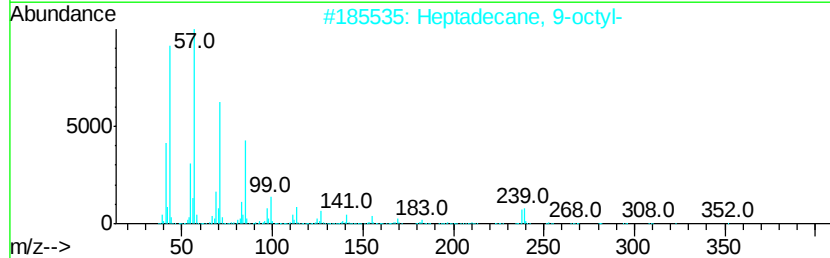
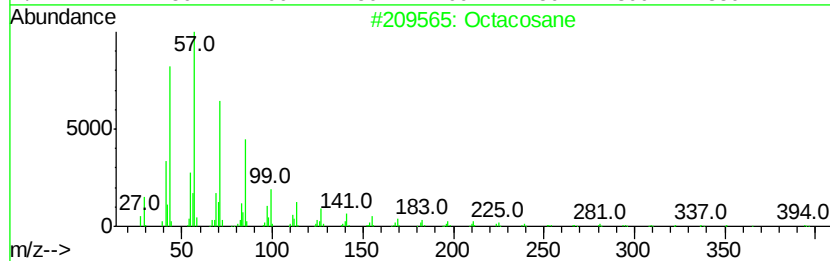
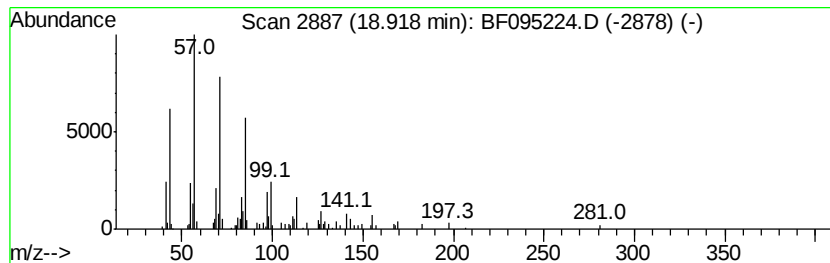
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.92	11.91 ng	395101	Chrysene-d12	18.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Heneicosane	296	C21H44	000629-94-7	87
5		Triacontane	422	C30H62	000638-68-6	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051817\
Data File : BF095224.D
Acq On : 18 May 2017 16:05
Operator : SJ/MA
Sample : I3159-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-3-20170515

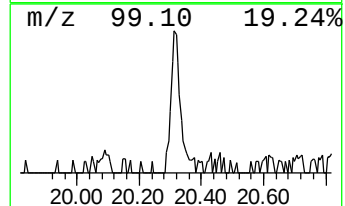
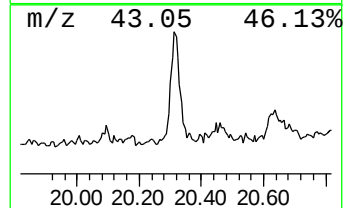
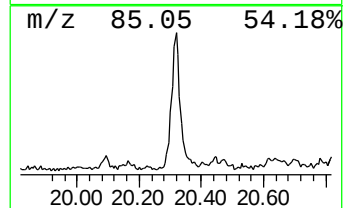
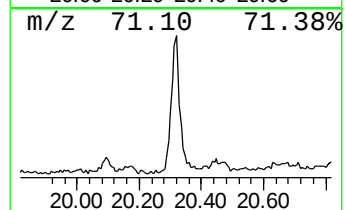
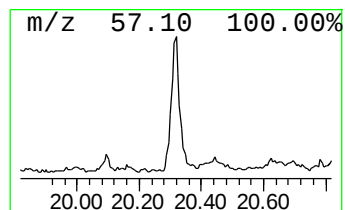
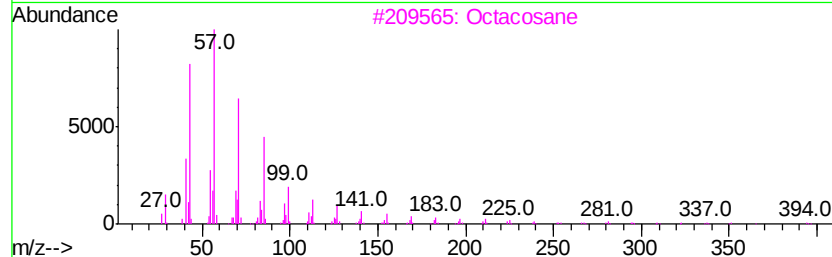
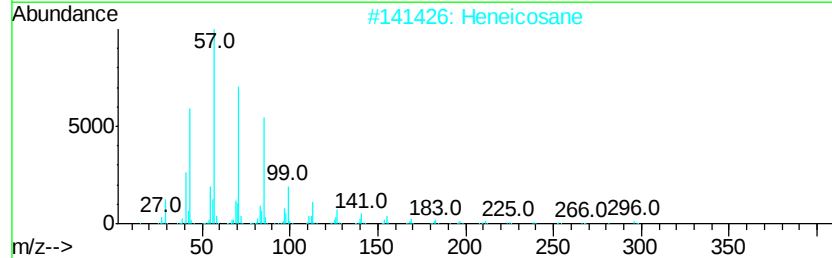
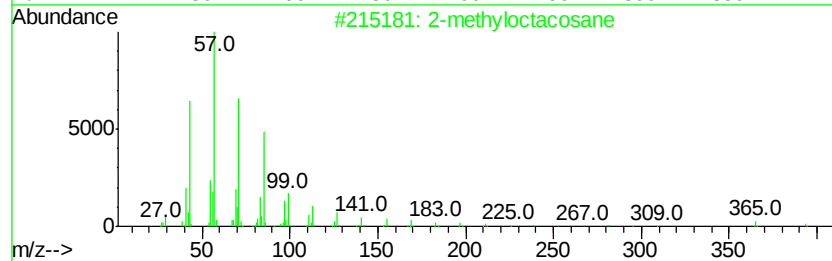
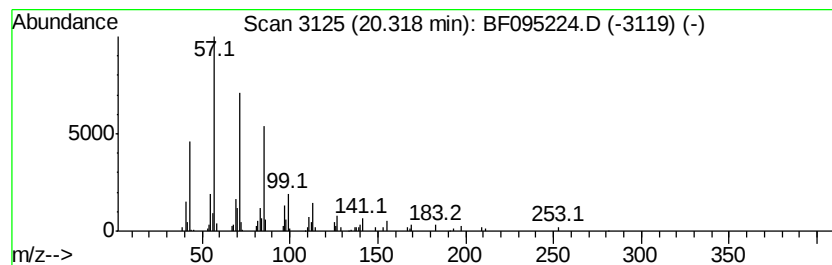
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.32	11.17 ng	201467	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051817\
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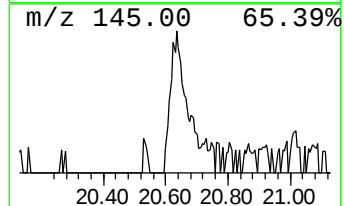
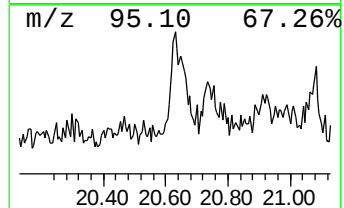
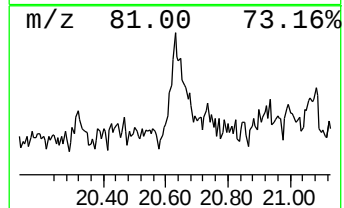
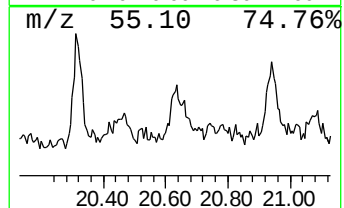
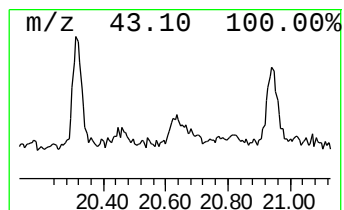
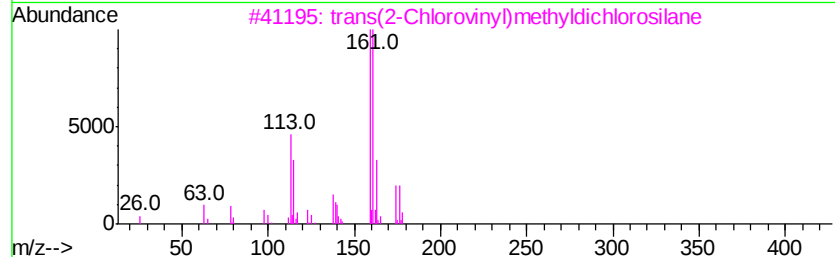
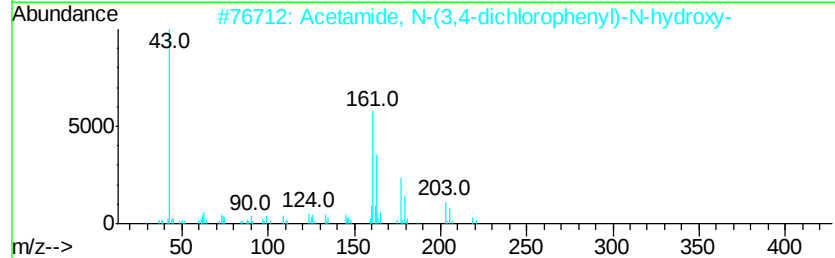
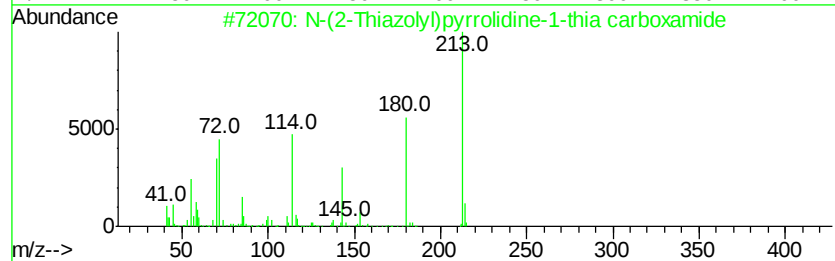
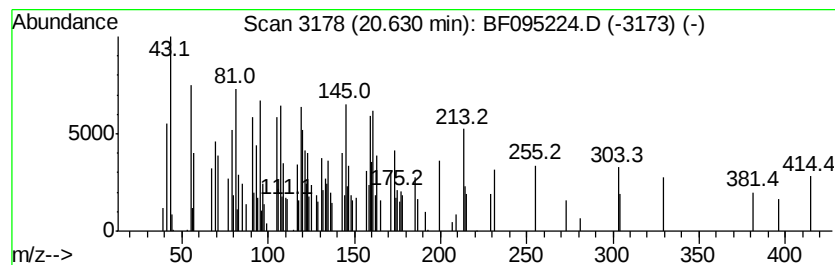
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown20.63 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.63	10.85 ng	195630	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-(2-Thiazolyl)pyrrolidine-1-thi...	213	C8H11N3S2	036241-35-7	10
2		Acetamide, N-(3,4-dichlorophenyl...	219	C8H7Cl2N02	086412-49-9	10
3		trans(2-Chlorovinyl)methylidichlo...	174	C3H5Cl3Si	079629-94-0	10
4		N-(2-Chloroethyl) endothalimide	229	C10H12ClN03	1000290-21-1	9
5		Carbamic acid, (4-chlorophenyl)-...	213	C10H12ClN02	002239-92-1	9



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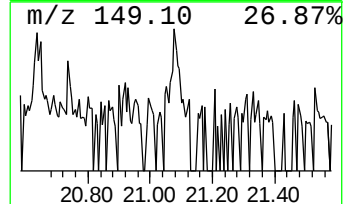
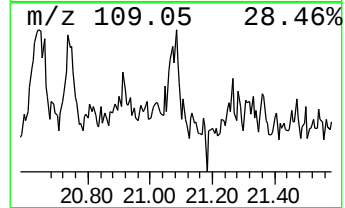
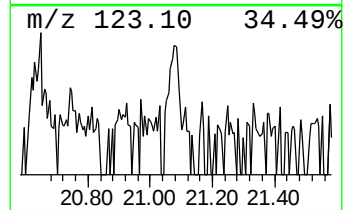
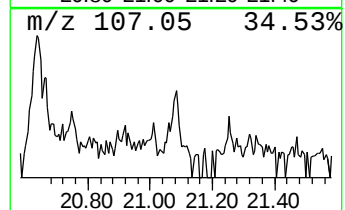
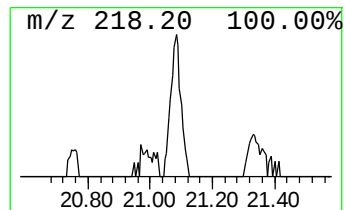
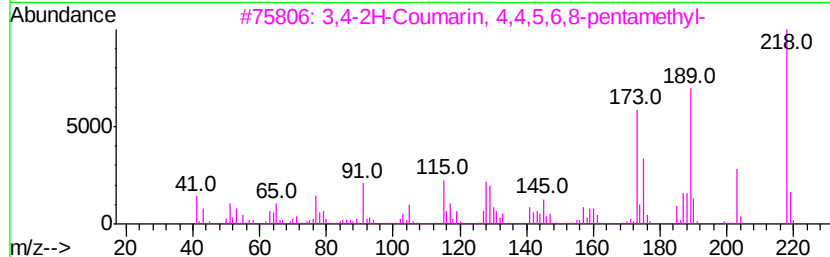
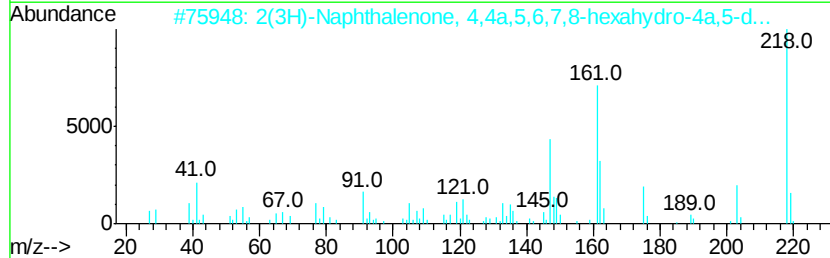
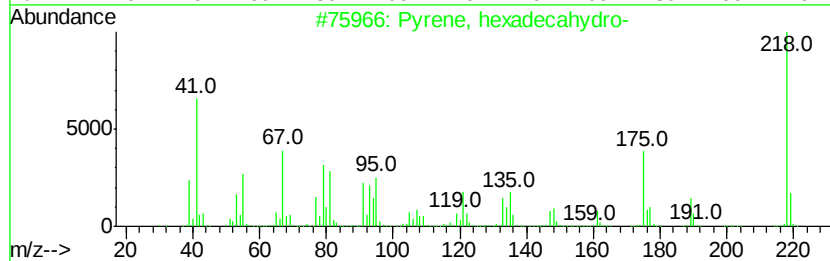
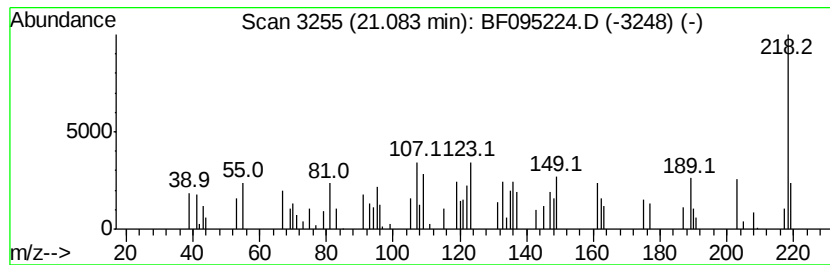
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pyrene, hexadecahydro- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	3.71 ng	66909	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	50
2		2(3H)-Naphthalenone, 4,4a,5,6,7,...	218	C15H22O	019598-45-9	49
3		3,4-2H-Coumarin, 4,4,5,6,8-penta...	218	C14H18O2	1000129-70-7	38
4		D-Norandrostane-16-one, (5.alpha.)-	260	C18H28O	032319-06-5	38
5		Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	35



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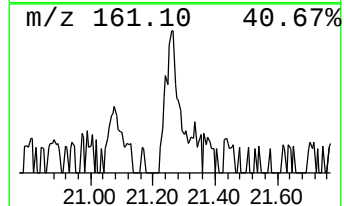
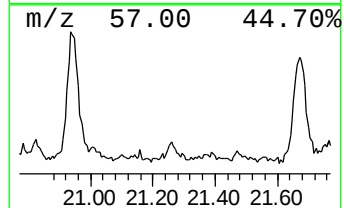
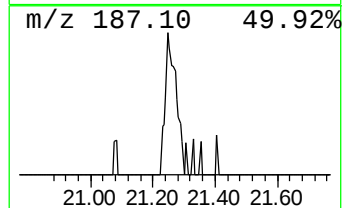
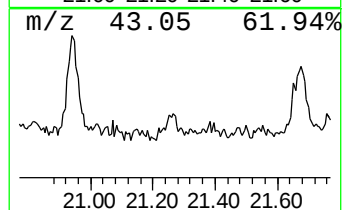
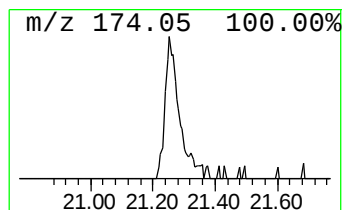
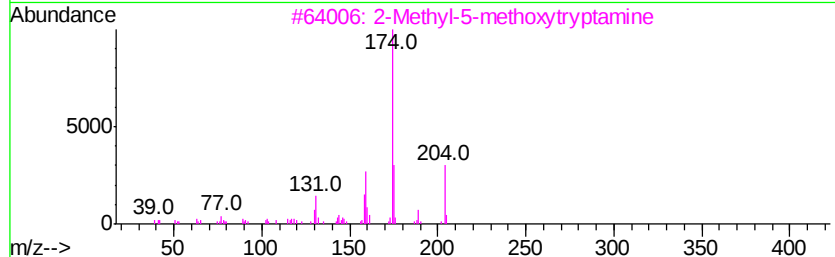
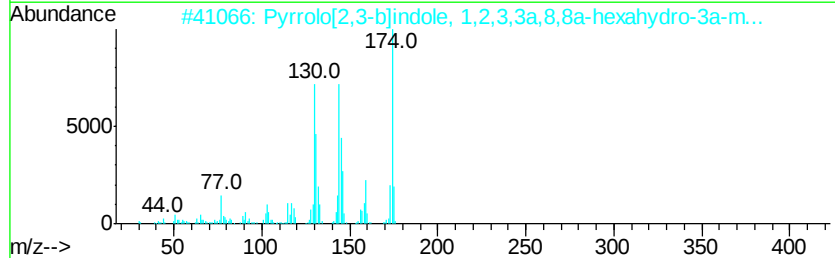
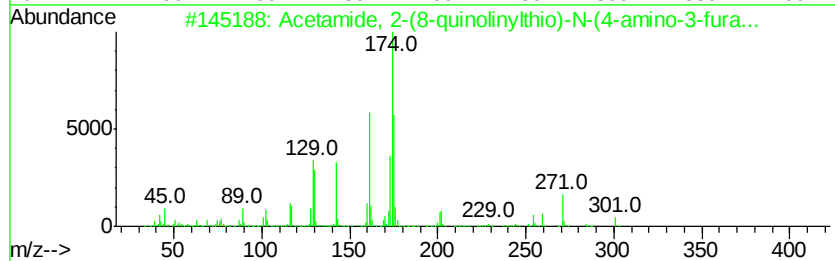
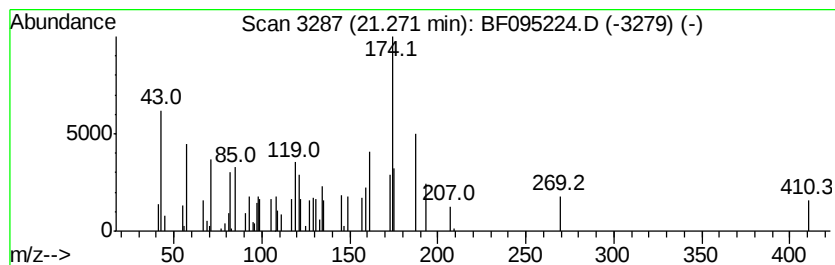
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown21.27 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	3.73 ng	67312	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetamide, 2-(8-quinolinylthio)-...	301	C13H11N5O2S	329780-80-5	17
2		Pyrrolo[2,3-b]indole, 1,2,3,3a,8...	174	C11H14N2	055255-88-4	16
3		2-Methyl-5-methoxytryptamine	204	C12H16N2O	003143-97-3	16
4		5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	12
5		N-(6-Methoxy-4-methyl-quinazolin...	380	C18H16N6O4	1000275-15-0	10



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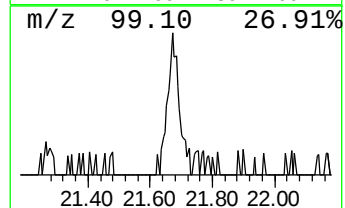
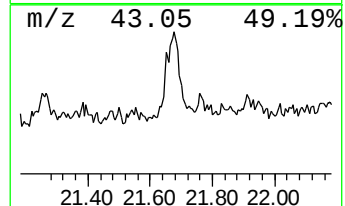
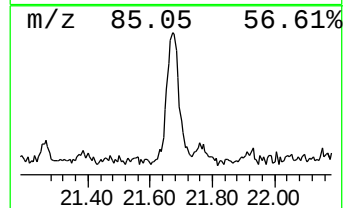
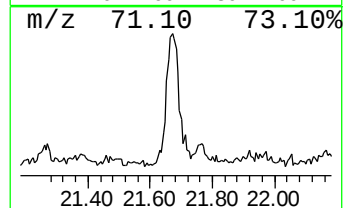
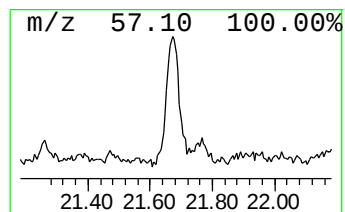
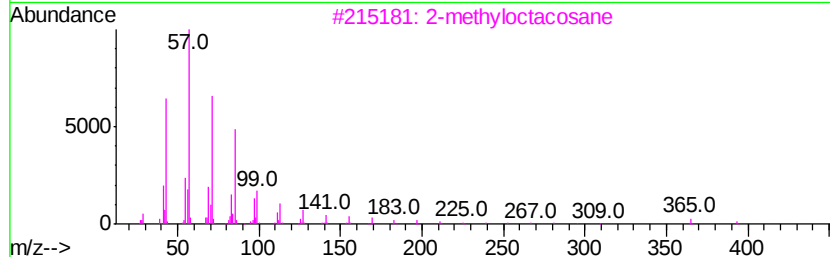
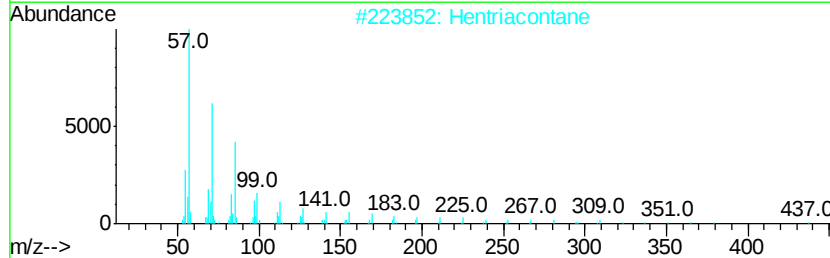
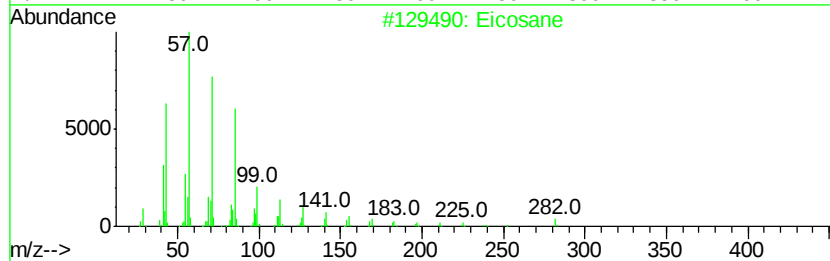
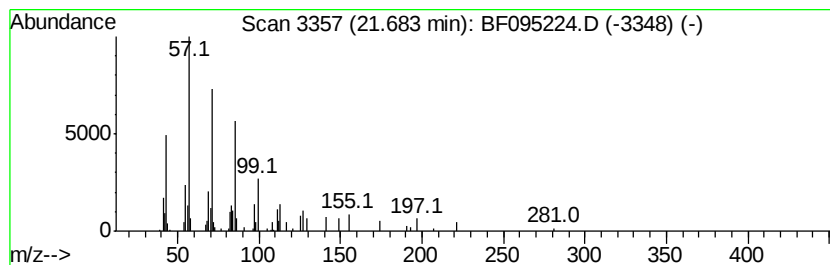
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.68	7.46 ng	134555	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	98
2		Hentriacontane	437	C31H64	000630-04-6	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	87
4		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



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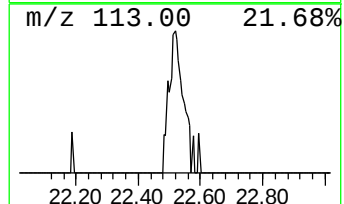
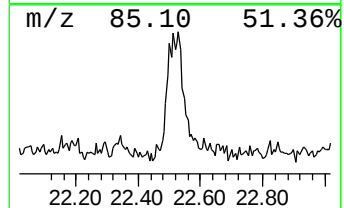
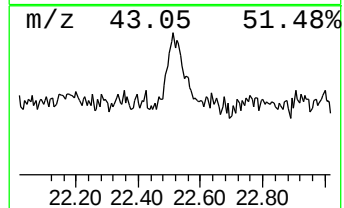
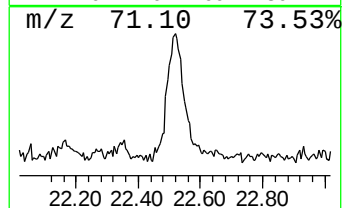
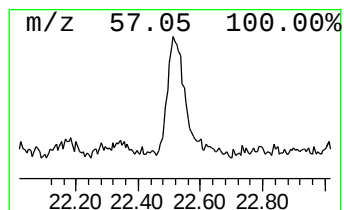
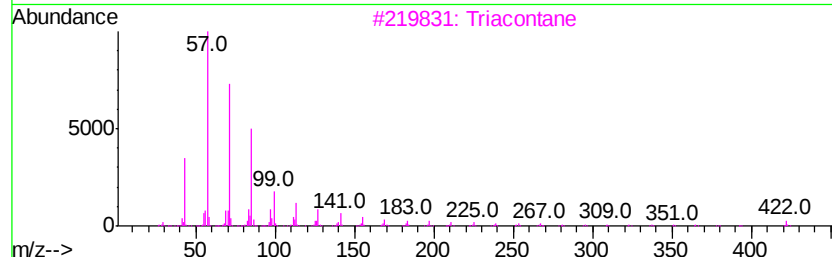
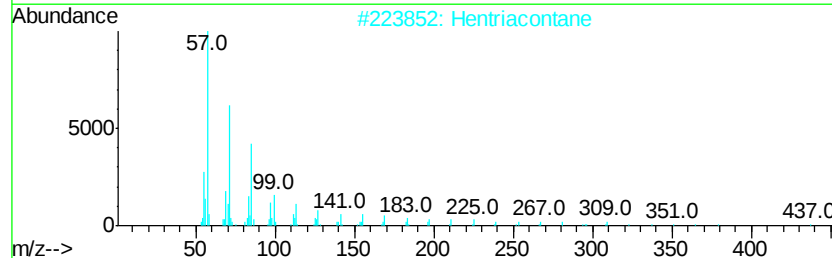
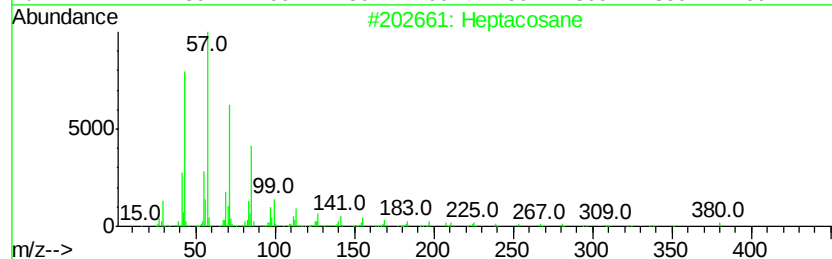
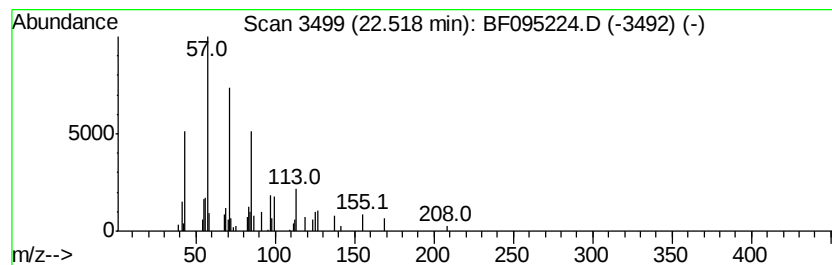
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.52	5.75 ng	103596	Perylene-d12	20.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	80
2			Hentriacontane	437	C31H64	000630-04-6	80
3			Triacontane	422	C30H62	000638-68-6	72
4			Pentacosane	352	C25H52	000629-99-2	72
5			10-Methylnonadecane	282	C20H42	056862-62-5	64



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ALS Vial : 3 Sample Multiplier: 1

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ClientSampleId :
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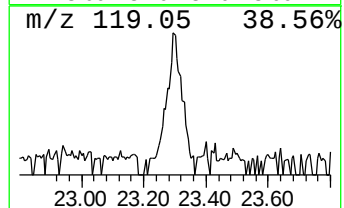
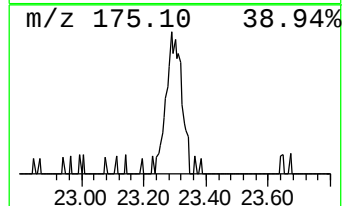
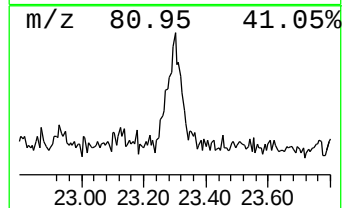
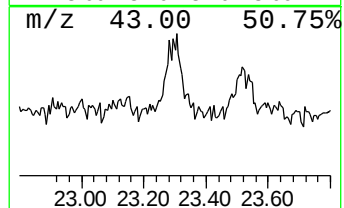
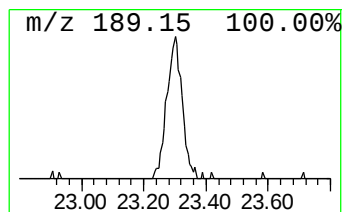
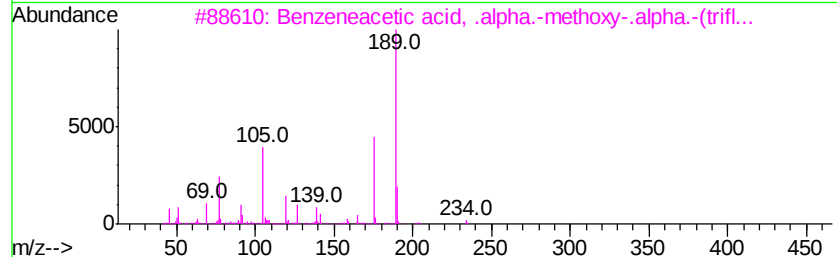
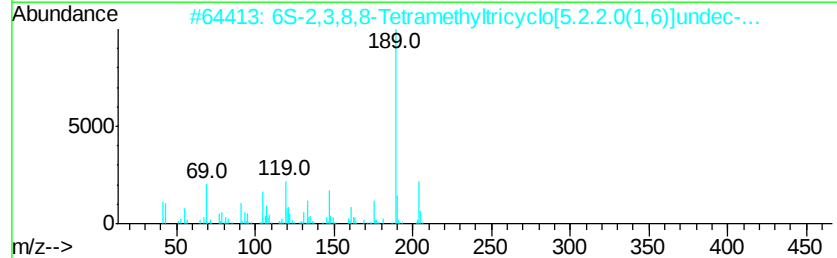
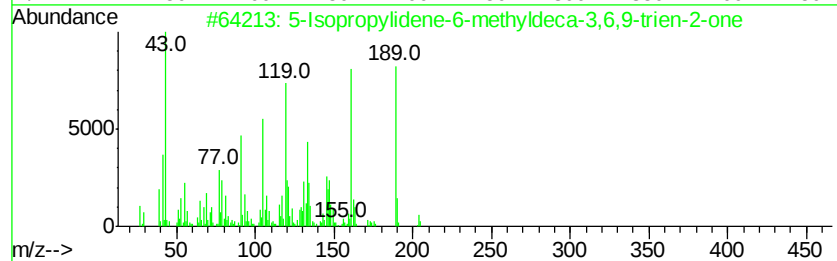
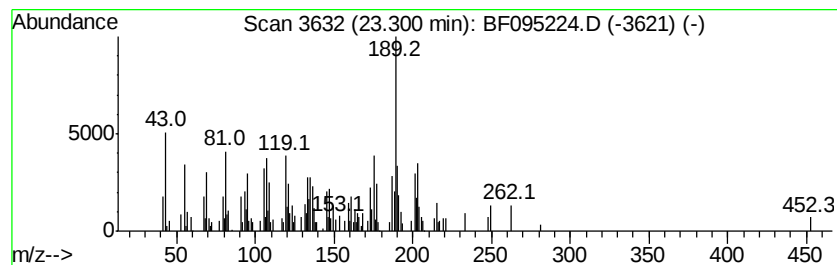
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 5-Isopropylidene-6-methylde... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	18.58 ng	334946	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Isopropylidene-6-methyldeca-3,...	204	C14H20O	1000197-84-7	62
2		6S-2,3,8,8-Tetramethyltricyclo[5...	204	C15H24	137235-48-4	50
3		Benzeneacetic acid, .alpha.-meth...	234	C10H9F3O3	020445-31-2	32
4		1H-[1,4]Oxazino[4,3-a][1,3]benzi...	189	C10H11N3O	1000362-54-6	27
5		9-Methyltetracyclo[7.3.1.0(2,7)...	204	C15H24	1000215-30-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051817\
 Data File : BF095224.D
 Acq On : 18 May 2017 16:05
 Operator : SJ/MA
 Sample : I3159-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3-20170515

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.11	6.1 ng		175886	1	7.77	576748	20.0
unknown7.43	7.43	84.5 ng		2436750	1	7.77	576748	20.0
n-Hexadecanoic acid	15.98	4.7 ng		174459	4	15.02	741535	20.0
Octadecanoic acid	17.07	3.4 ng		111193	5	18.69	663368	20.0
Heneicosane	17.83	6.4 ng		213289	5	18.69	663368	20.0
Octacosane	18.92	11.9 ng		395101	5	18.69	663368	20.0
2-methyloctacosane	20.32	11.2 ng		201467	6	20.37	360613	20.0
unknown20.63	20.63	10.9 ng		195630	6	20.37	360613	20.0
Pyrene, hexadecah...	21.08	3.7 ng		66909	6	20.37	360613	20.0
unknown21.27	21.27	3.7 ng		67312	6	20.37	360613	20.0
Eicosane	21.68	7.5 ng		134555	6	20.37	360613	20.0
Heptacosane	22.52	5.8 ng		103596	6	20.37	360613	20.0
5-Isopropylidene-...	23.30	18.6 ng		334946	6	20.37	360613	20.0