

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052717\
 Data File : BF095515.D
 Acq On : 28 May 2017 1:01
 Operator : SJ/MA
 Sample : I3244-11
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM13-COMP-0-6

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-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	5.095	533	537	554	rBV2	74156	198276	8.78%	1.107%
2	5.701	637	640	674	rBV	636472	1845204	81.73%	10.303%
3	7.283	905	909	925	rBV	692586	1686873	74.72%	9.419%
4	7.401	925	929	952	rVB	1209850	2257562	100.00%	12.605%
5	7.736	982	986	1005	rVB	419234	544701	24.13%	3.041%
6	7.972	1021	1026	1040	rBV	1101343	1435717	63.60%	8.017%
7	8.642	1136	1140	1157	rBV	455422	1017343	45.06%	5.680%
8	9.766	1327	1331	1360	rBV	294280	701251	31.06%	3.916%
9	11.530	1626	1631	1652	rBV	932145	1811528	80.24%	10.115%
10	12.242	1748	1752	1769	rBV	107035	207293	9.18%	1.157%
11	12.601	1808	1813	1833	rBV2	416324	780850	34.59%	4.360%
12	13.424	1947	1953	1959	rBV	24029	29081	1.29%	0.162%
13	13.895	2029	2033	2064	rVB	448733	961426	42.59%	5.368%
14	14.195	2080	2084	2088	rBV	19381	25344	1.12%	0.142%
15	15.001	2217	2221	2227	rBV2	292834	502559	22.26%	2.806%
16	15.489	2299	2304	2315	rBV3	15828	38817	1.72%	0.217%
17	15.848	2360	2365	2370	rBV3	25881	44740	1.98%	0.250%
18	15.895	2370	2373	2378	rVV2	18471	29451	1.30%	0.164%
19	15.953	2379	2383	2396	rVB4	53767	110894	4.91%	0.619%
20	16.795	2522	2526	2532	rVV	88447	133338	5.91%	0.745%
21	16.853	2533	2536	2543	rVB2	25149	35034	1.55%	0.196%
22	17.095	2572	2577	2591	rVB	88477	132705	5.88%	0.741%
23	17.312	2610	2614	2624	rBV	860808	1041963	46.15%	5.818%
24	18.553	2820	2825	2834	rBV8	27117	67845	3.01%	0.379%
25	18.677	2840	2846	2862	rBV2	373743	722847	32.02%	4.036%
26	19.341	2955	2959	2962	rBV4	16644	24614	1.09%	0.137%
27	19.783	3030	3034	3037	rBV	26760	31684	1.40%	0.177%
28	19.865	3044	3048	3052	rVB6	18412	25691	1.14%	0.143%
29	19.953	3059	3063	3066	rBV	68259	93699	4.15%	0.523%
30	20.065	3077	3082	3086	rBV2	80352	101507	4.50%	0.567%
31	20.241	3110	3112	3119	rVB	34992	39008	1.73%	0.218%
32	20.306	3119	3123	3127	rBV	44765	60500	2.68%	0.338%
33	20.353	3127	3131	3139	rBV	264700	430914	19.09%	2.406%
34	20.583	3166	3170	3176	rBV7	30484	50809	2.25%	0.284%

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ALS Vial : 14 Sample Multiplier: 1

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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	20.788	3199	3205	3211	rBV	255001	343457	15.21%	1.918%
36	21.459	3313	3319	3323	rBV9	16364	31803	1.41%	0.178%
37	21.530	3325	3331	3333	rBV6	14789	26743	1.18%	0.149%
38	21.718	3357	3363	3372	rBV4	72303	144341	6.39%	0.806%
39	21.865	3383	3388	3393	rBV8	13715	29362	1.30%	0.164%
40	22.112	3425	3430	3437	rBV6	24231	59797	2.65%	0.334%
41	22.965	3570	3575	3578	rBV7	15469	27349	1.21%	0.153%
42	23.300	3626	3632	3635	rBV7	11145	25522	1.13%	0.143%

Sum of corrected areas: 17909442

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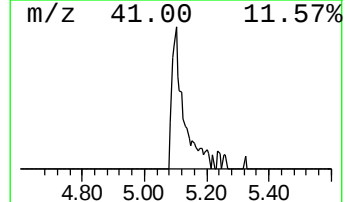
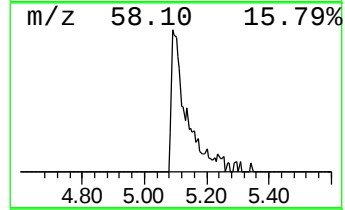
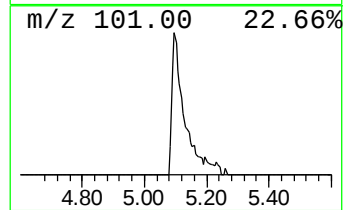
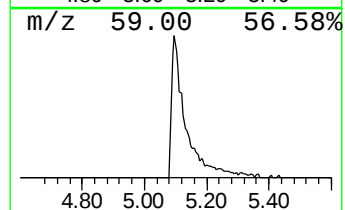
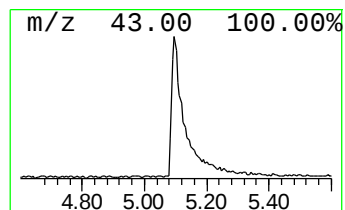
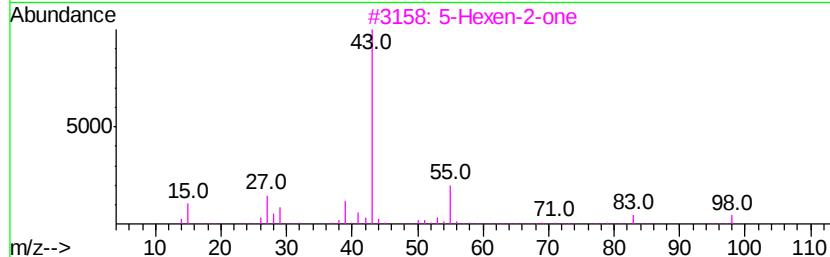
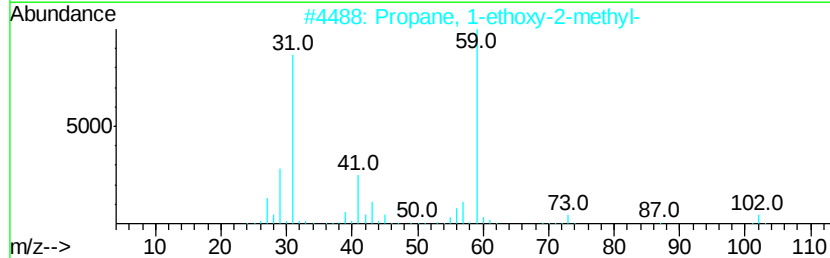
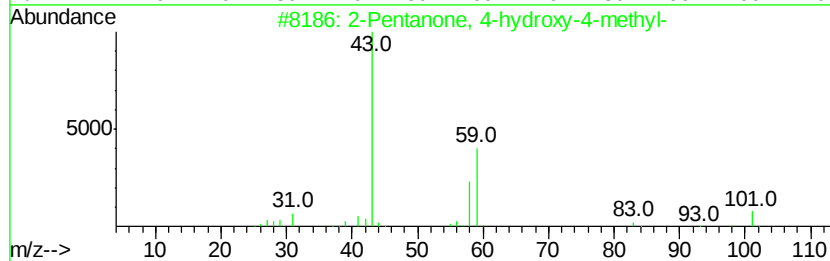
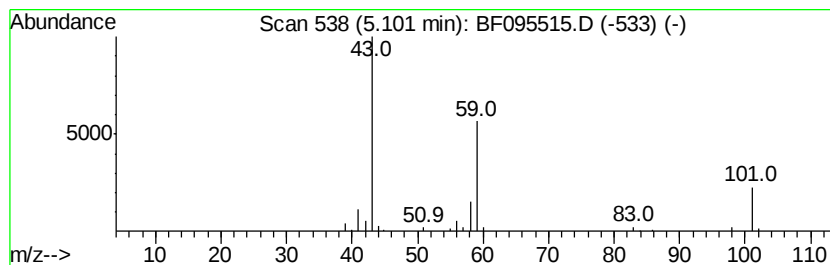
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	7.28 ng	198276	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
3		5-Hexen-2-one	98	C6H10O	000109-49-9	14
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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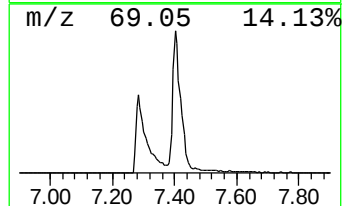
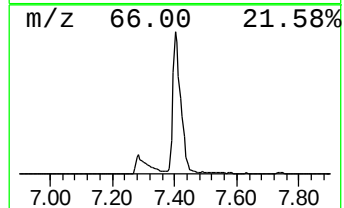
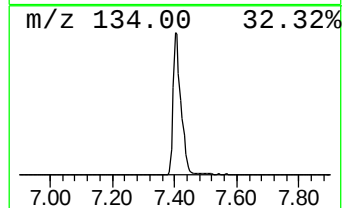
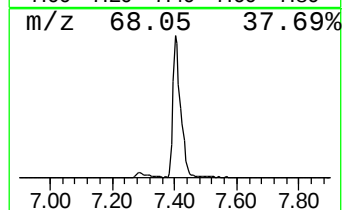
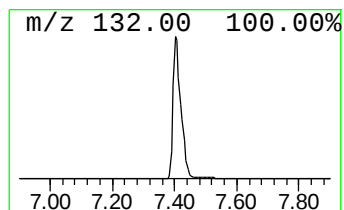
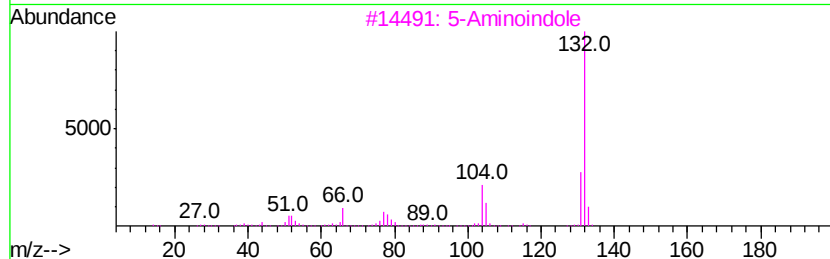
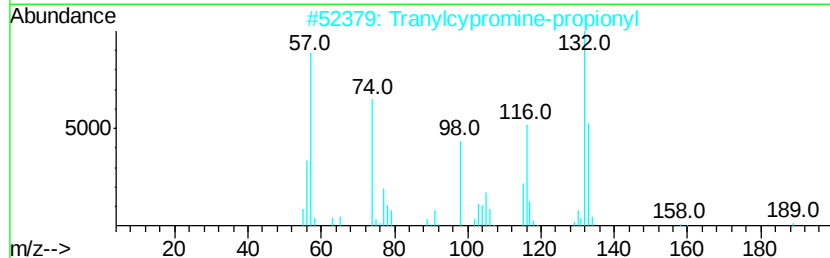
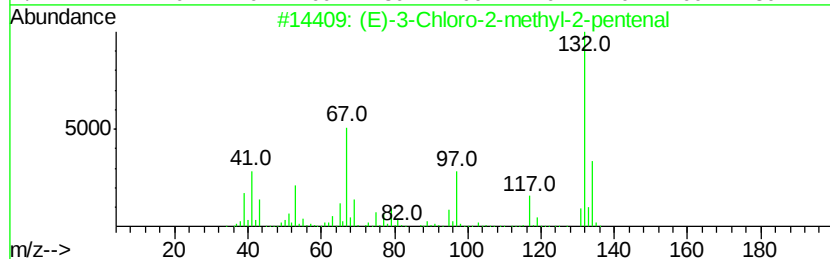
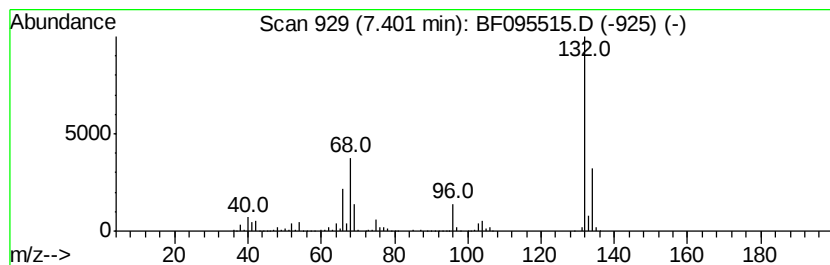
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	82.89 ng	2257560	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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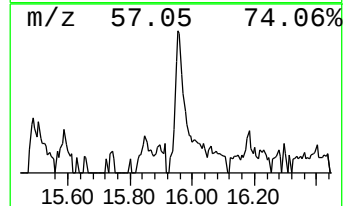
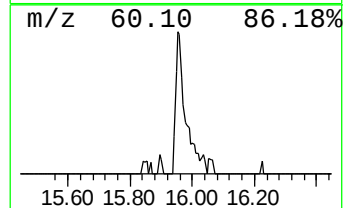
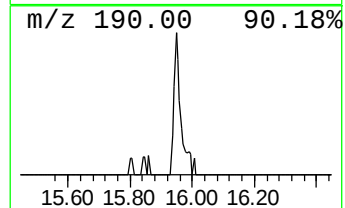
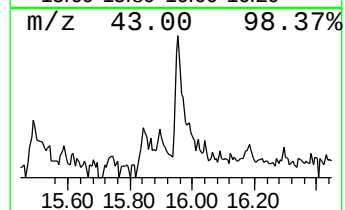
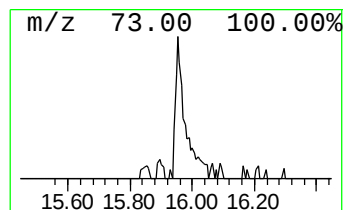
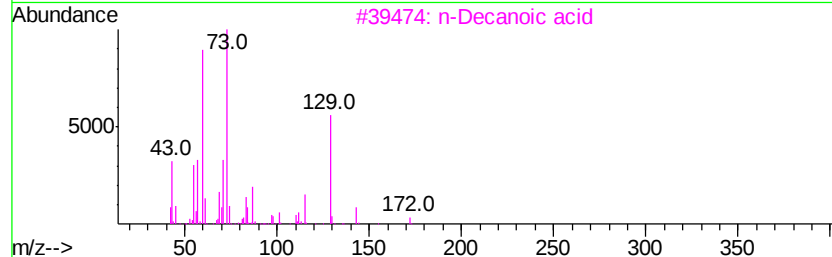
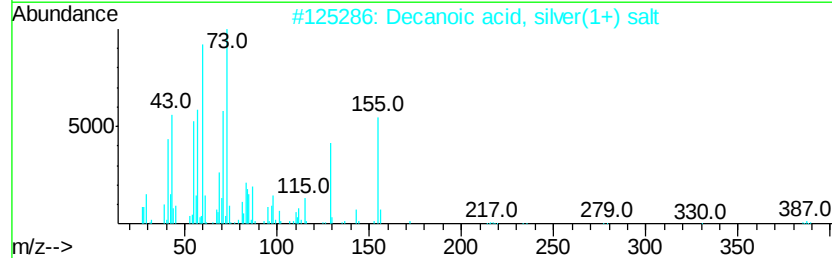
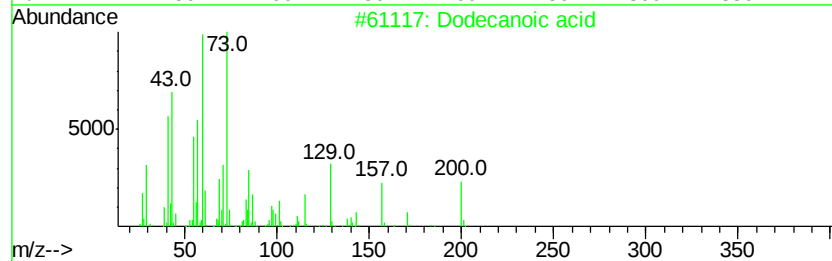
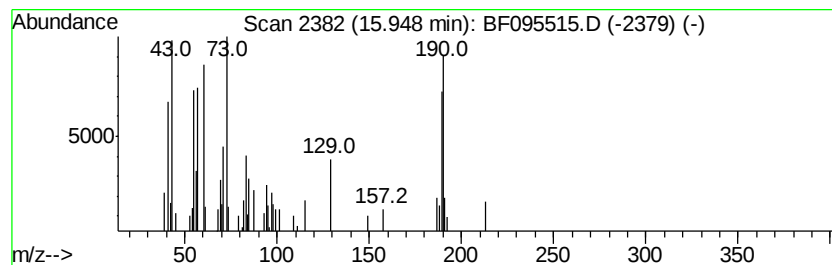
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.95 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.95	4.41 ng	110894	Phenanthrene-d10	15.00	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	38
2	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	37
3	n-Decanoic acid	172	C10H20O2	000334-48-5	35
4	Undecanoic acid	186	C11H22O2	000112-37-8	35
5	.beta.-l-Rhamnofuranoside, 5-O-a...	334	C16H30O5S	1000153-79-3	27



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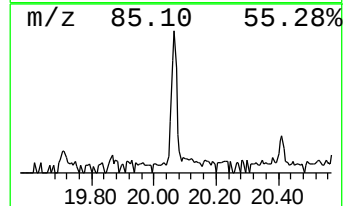
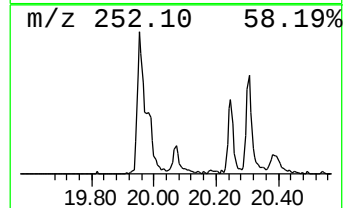
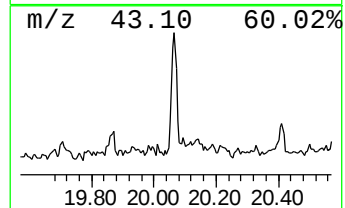
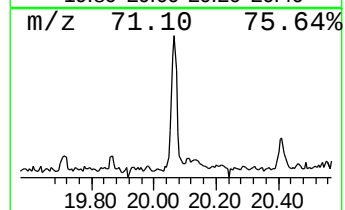
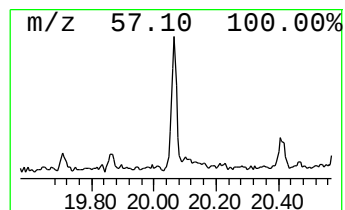
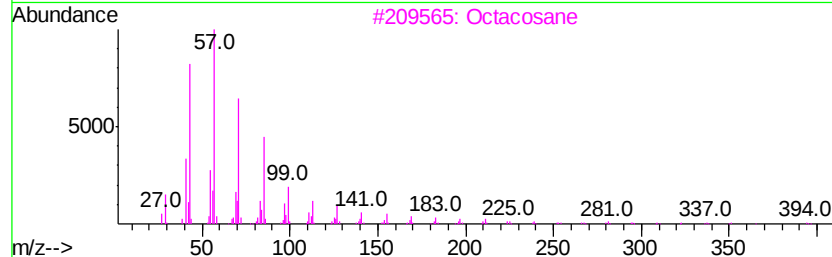
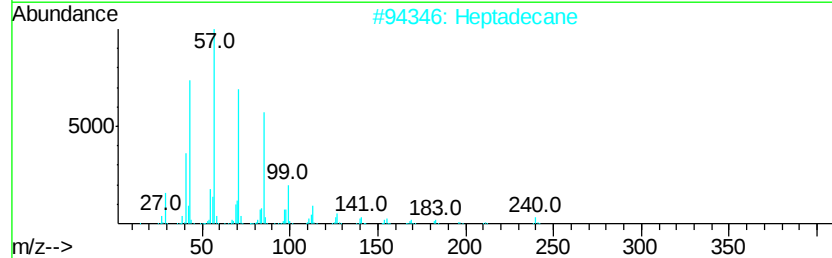
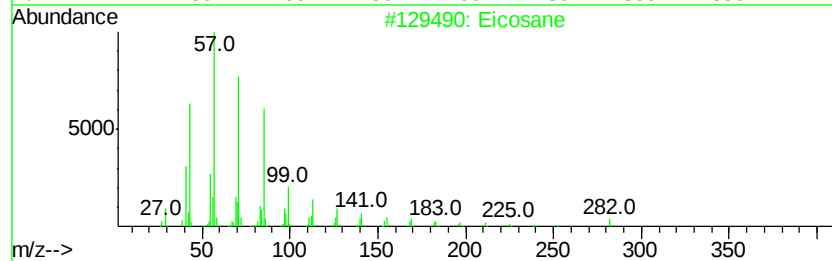
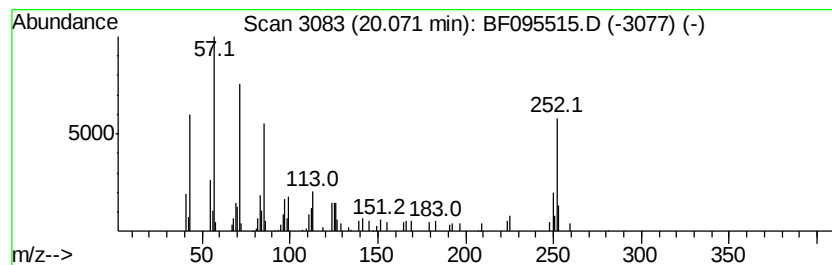
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	4.71 ng	101507	Perylene-d12	20.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Heptadecane		240	C17H36	000629-78-7	91
3	Octacosane		394	C28H58	000630-02-4	58
4	Hentriacontane		437	C31H64	000630-04-6	58
5	2-methyloctacosane		408	C29H60	1000376-72-8	58



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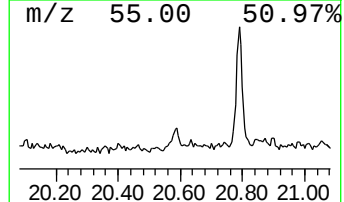
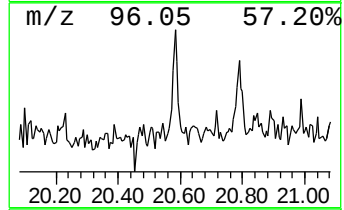
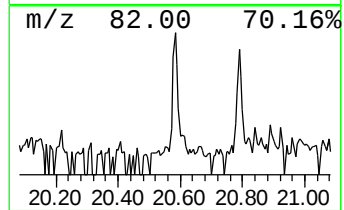
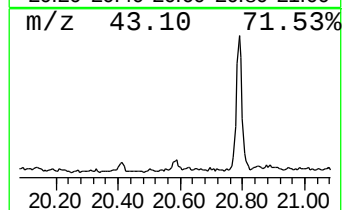
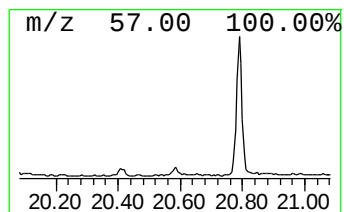
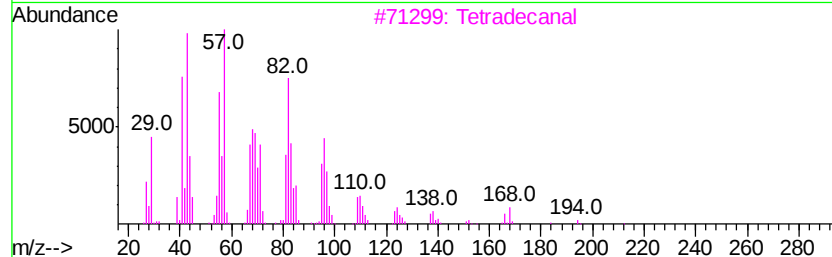
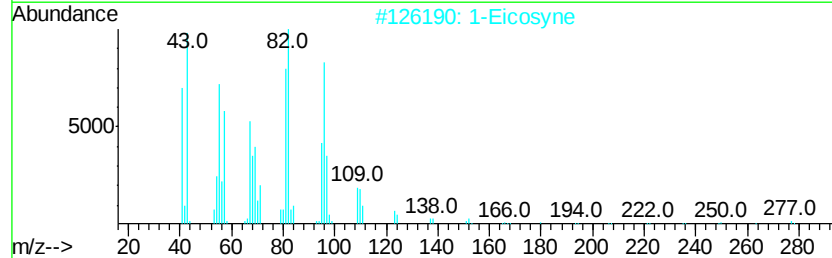
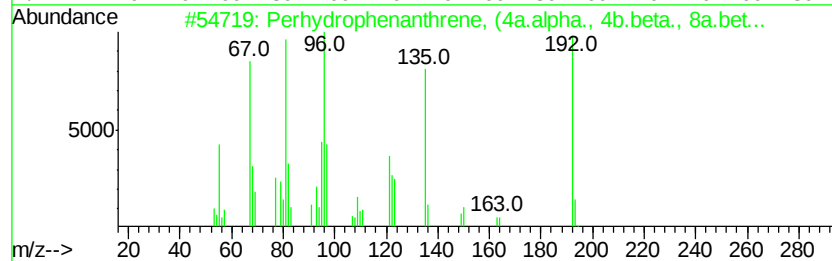
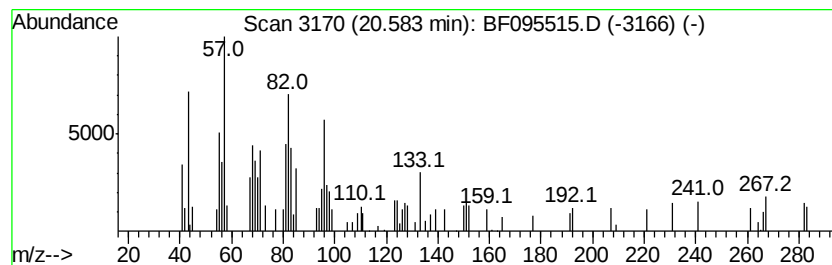
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown20.58 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.58	2.36 ng	50809	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perhydrophenanthrene, (4a.alpha....	192	C14H24	027389-74-8	43
2		1-Eicosyne	278	C20H38	000765-27-5	35
3		Tetradecanal	212	C14H28O	000124-25-4	30
4		Heptadecanal	254	C17H34O	1000376-70-0	27
5		Tridecanal	198	C13H26O	010486-19-8	25



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ClientSampleId :
NM13-COMP-0-6

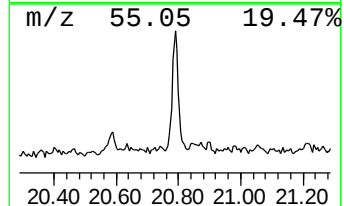
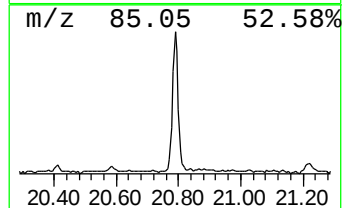
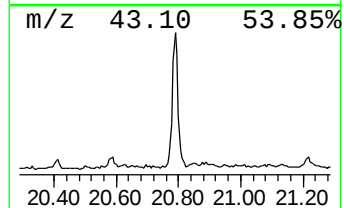
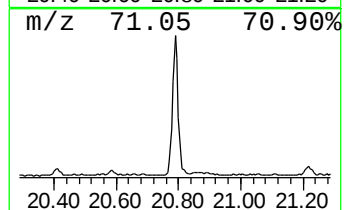
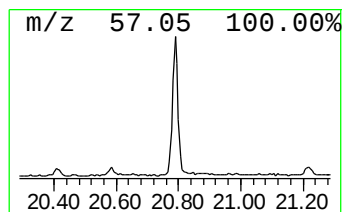
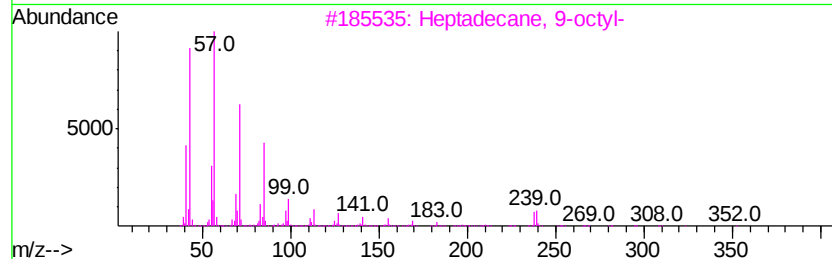
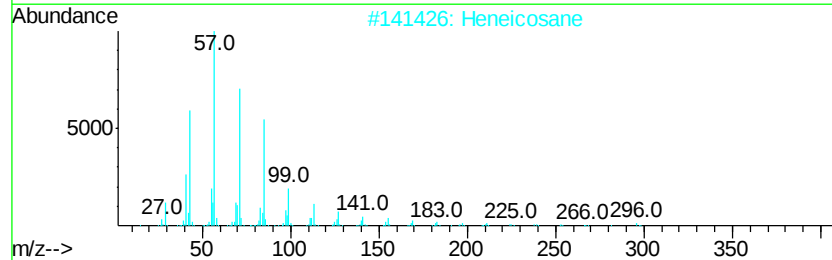
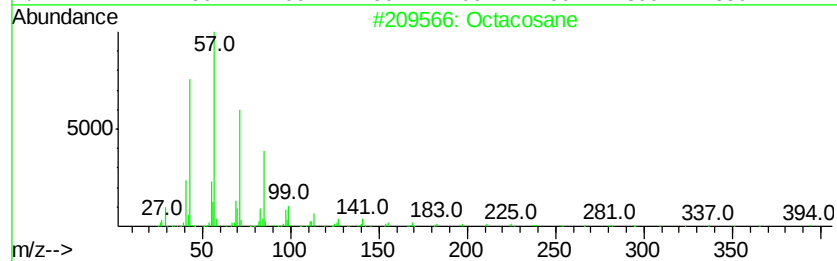
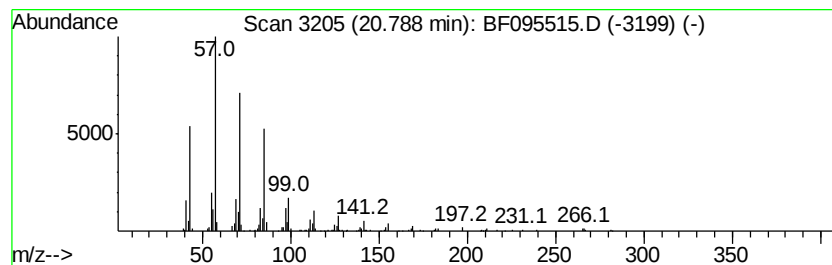
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	15.94 ng	343457	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		triacontane	422	C30H62	000638-68-6	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052717\
Data File : BF095515.D
Acq On : 28 May 2017 1:01
Operator : SJ/MA
Sample : I3244-11
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM13-COMP-0-6

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...	5.10	7.3	ng	198276	1	7.74	544701	20.0
unknown7.40	7.40	82.9	ng	2257560	1	7.74	544701	20.0
unknown15.95	15.95	4.4	ng	110894	4	15.00	502559	20.0
Eicosane	20.07	4.7	ng	101507	6	20.35	430914	20.0
unknown20.58	20.58	2.4	ng	50809	6	20.35	430914	20.0
Octacosane	20.79	15.9	ng	343457	6	20.35	430914	20.0