

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
 Data File : BF088338.D
 Acq On : 24 Jun 2016 18:24
 Operator : UM/SJ
 Sample : H3676-04
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NCHC-011

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-BF060716.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	1.713	9	11	51	rVB	873022	1937009	100.00%	10.761%
2	4.719	271	274	287	rBV	42035	84877	4.38%	0.472%
3	5.176	312	314	332	rBV	803916	1492258	77.04%	8.290%
4	6.250	406	408	415	rBV	1176875	1477241	76.26%	8.207%
5	6.353	415	417	435	rVB	1454291	1629694	84.13%	9.054%
6	6.582	435	437	447	rBV	392972	466106	24.06%	2.589%
7	6.742	449	451	453	rBV	907203	1243401	64.19%	6.908%
8	7.153	485	487	499	rBV	619606	995620	51.40%	5.531%
9	7.873	548	550	552	rBV	552606	619170	31.97%	3.440%
10	8.948	641	644	651	rBV	1903491	1877891	96.95%	10.433%
11	9.348	677	679	683	rVB	249060	232026	11.98%	1.289%
12	9.565	696	698	700	rBV	26842	27443	1.42%	0.152%
13	9.611	700	702	705	rBV2	613051	699662	36.12%	3.887%
14	10.056	739	741	745	rVB	31057	28352	1.46%	0.158%
15	10.399	769	771	781	rBV2	760669	1017945	52.55%	5.655%
16	10.525	781	782	786	rVB	36159	52574	2.71%	0.292%
17	10.971	819	821	823	rBV	65329	67328	3.48%	0.374%
18	11.085	830	831	835	rBV	452471	661905	34.17%	3.677%
19	11.154	835	837	841	rVB3	21708	42064	2.17%	0.234%
20	11.394	857	858	861	rBV	29922	29726	1.53%	0.165%
21	12.297	935	937	945	rVB	20498	27231	1.41%	0.151%
22	12.525	954	957	959	rBV	16895	21267	1.10%	0.118%
23	12.674	967	970	972	rBV	1426082	1422705	73.45%	7.904%
24	12.914	988	991	993	rBV	13103	20296	1.05%	0.113%
25	13.577	1047	1049	1054	rBV2	43115	84251	4.35%	0.468%
26	13.714	1059	1061	1064	rBV	505557	563870	29.11%	3.133%
27	14.194	1101	1103	1104	rBV	17088	22441	1.16%	0.125%
28	14.491	1127	1129	1133	rBV3	22417	53754	2.78%	0.299%
29	14.548	1133	1134	1136	rVV	22022	25549	1.32%	0.142%
30	14.617	1138	1140	1143	rVV2	22255	31283	1.62%	0.174%
31	14.777	1152	1154	1156	rVB	31544	31500	1.63%	0.175%
32	14.811	1156	1157	1165	rBV6	18098	45152	2.33%	0.251%
33	15.074	1178	1180	1185	rBV	418411	544797	28.13%	3.027%
34	15.268	1195	1197	1201	rVB3	28934	47866	2.47%	0.266%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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35	15.463	1211	1214	1215	rBV	37530	58808	3.04%	0.327%
36	15.623	1226	1228	1234	rVB5	41149	93704	4.84%	0.521%
37	15.988	1257	1260	1265	rVB2	28116	61744	3.19%	0.343%
38	16.343	1289	1291	1294	rVB2	21218	41470	2.14%	0.230%
39	16.457	1298	1301	1303	rBV	23900	43243	2.23%	0.240%
40	17.451	1385	1388	1392	rBV5	10388	31922	1.65%	0.177%
41	17.577	1397	1399	1405	rVB4	17826	44723	2.31%	0.248%

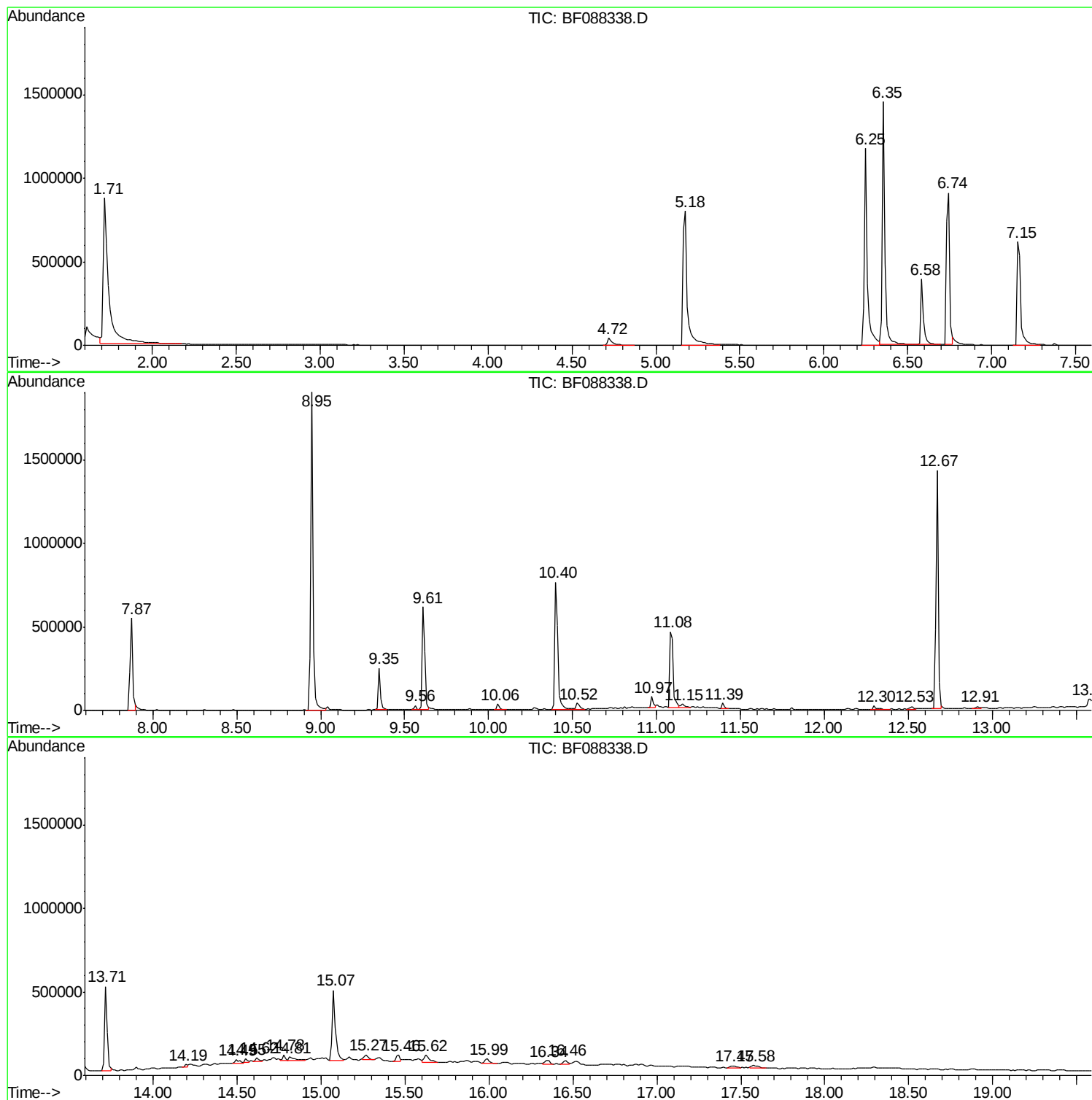
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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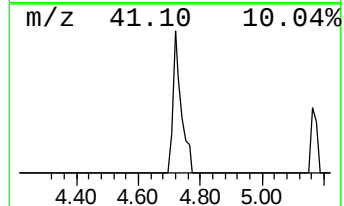
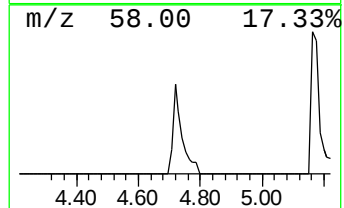
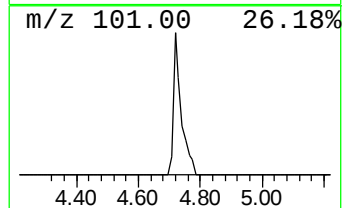
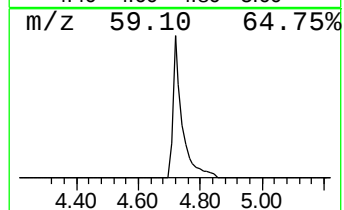
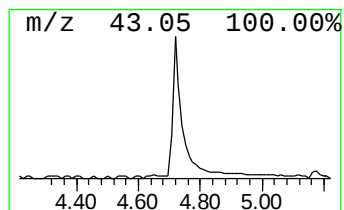
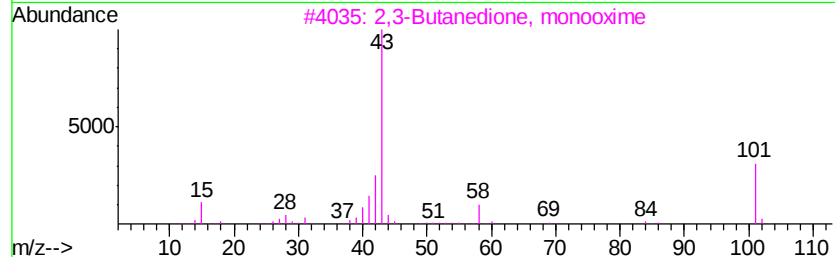
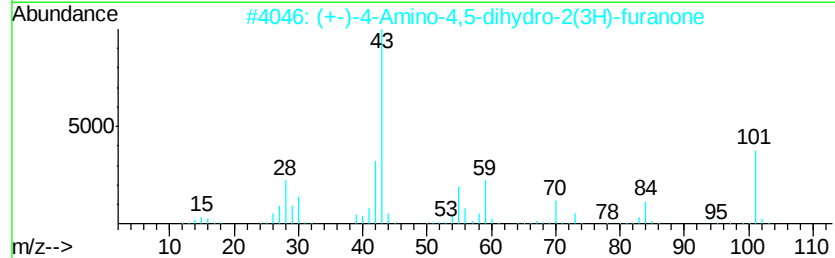
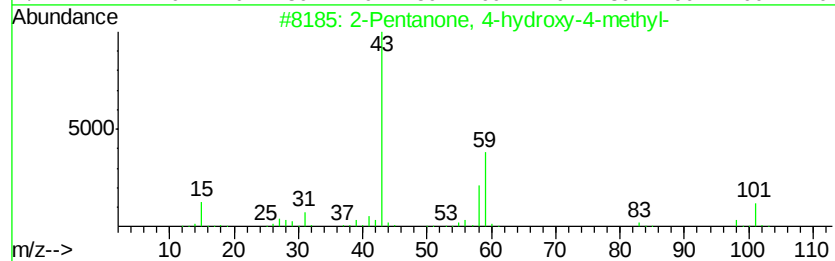
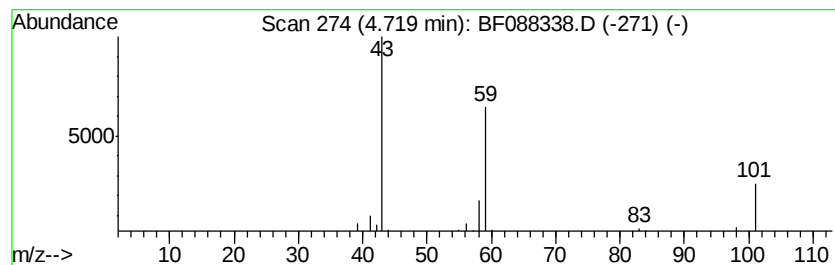
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	3.64 ng	84877	1,4-Dichlorobenzene-d4	6.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9



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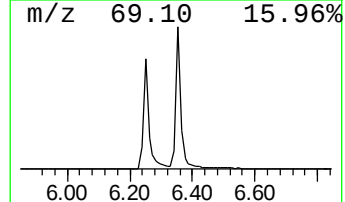
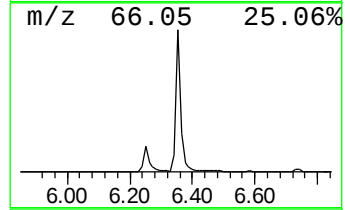
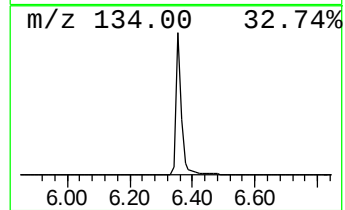
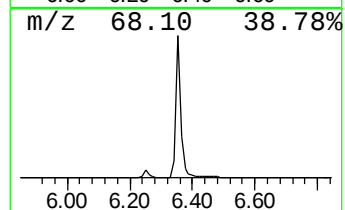
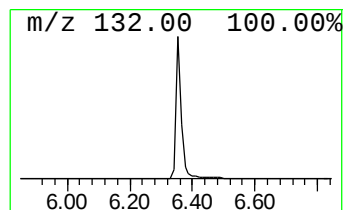
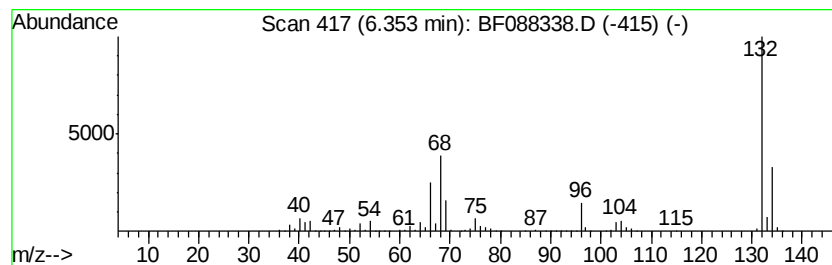
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.35 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	69.93 ng	1629690	1,4-Dichlorobenzene-d4	6.58

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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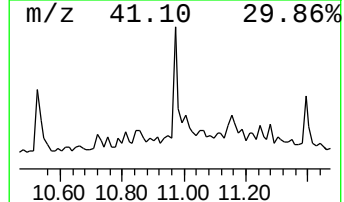
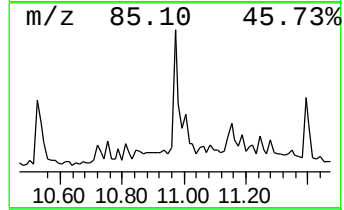
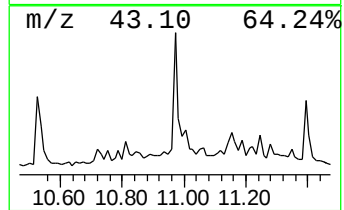
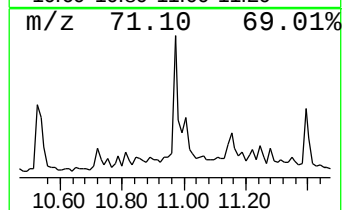
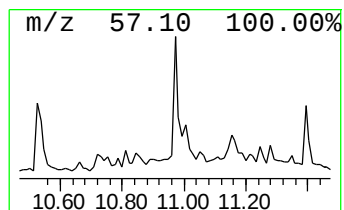
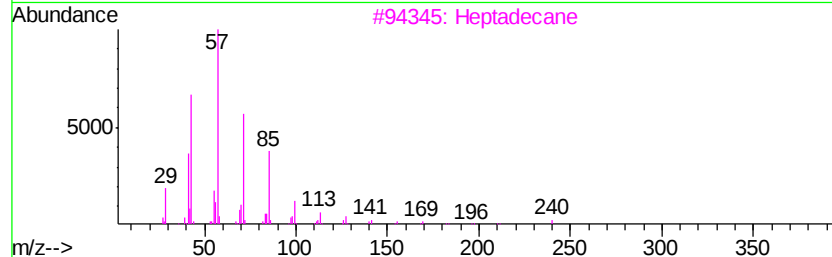
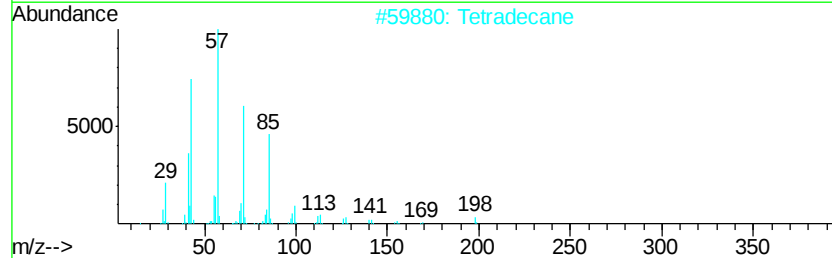
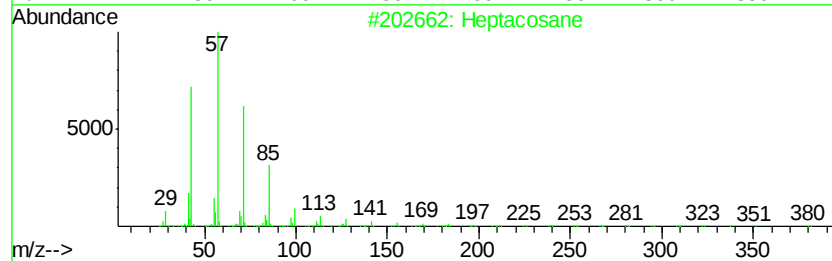
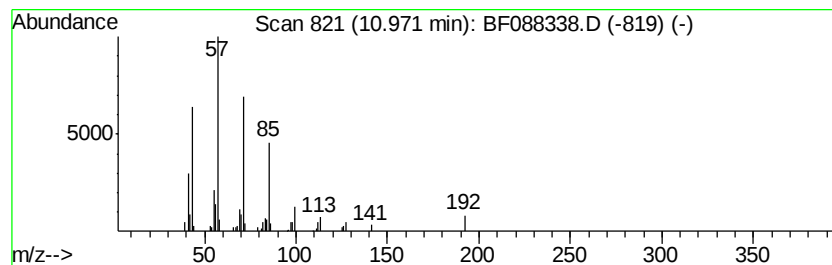
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.97	2.03 ng	67328	Phenanthrene-d10	11.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	90
2		Tetradecane	198	C14H30	000629-59-4	90
3		Heptadecane	240	C17H36	000629-78-7	90
4		Octadecane	254	C18H38	000593-45-3	90
5		Hexadecane	226	C16H34	000544-76-3	90



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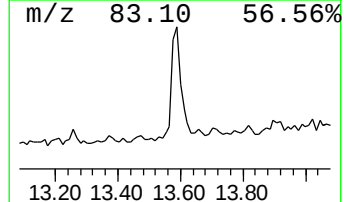
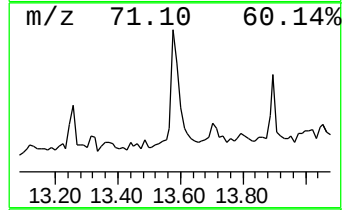
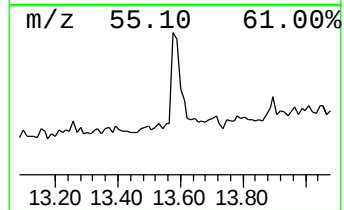
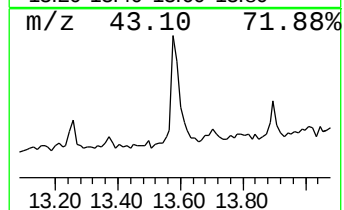
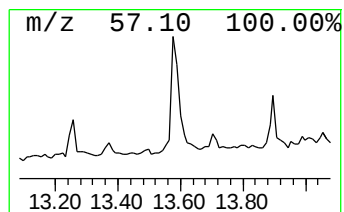
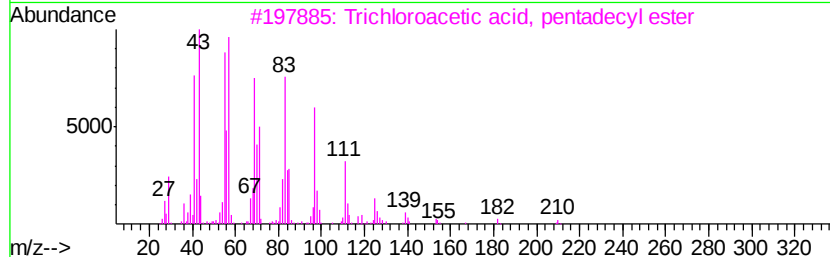
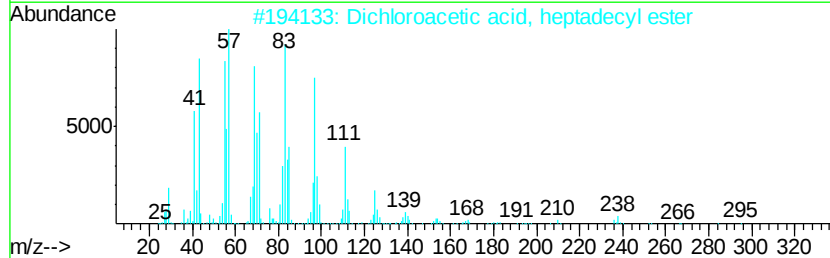
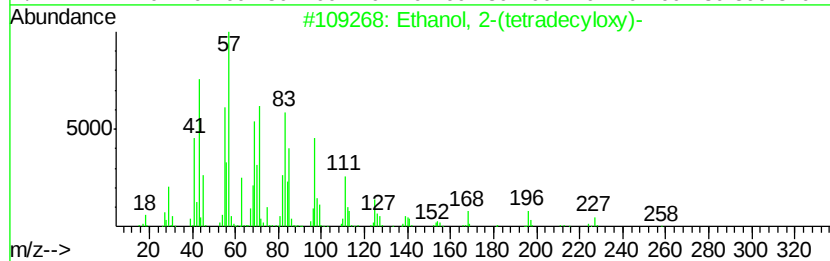
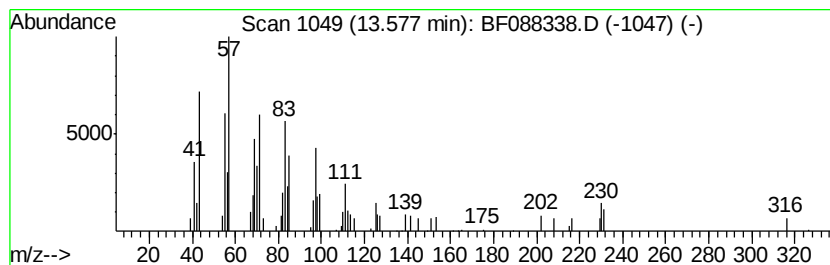
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.58	2.99 ng	84251	Chrysene-d12	13.71		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	64
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	60
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	60
5		Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	60



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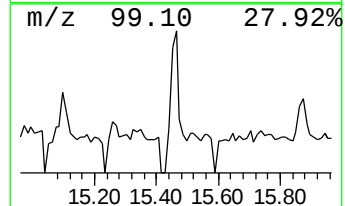
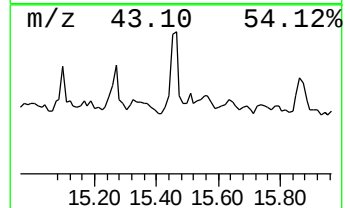
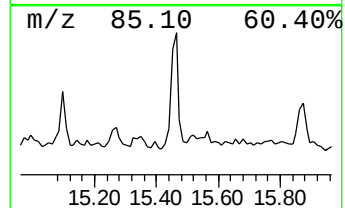
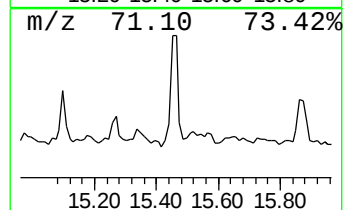
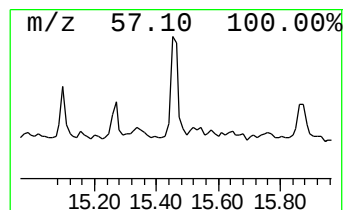
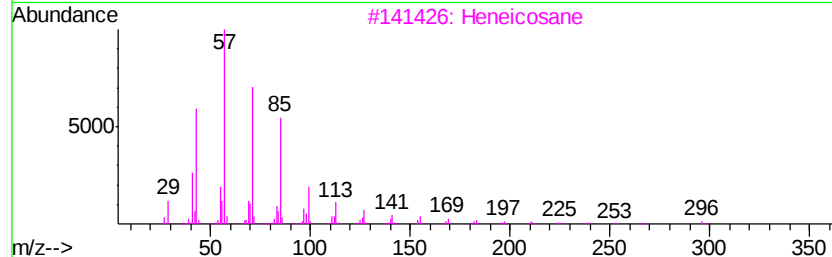
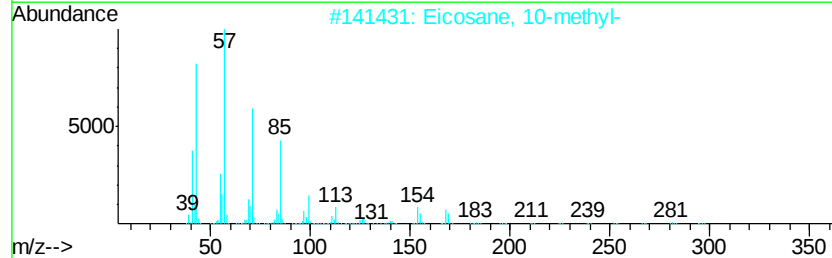
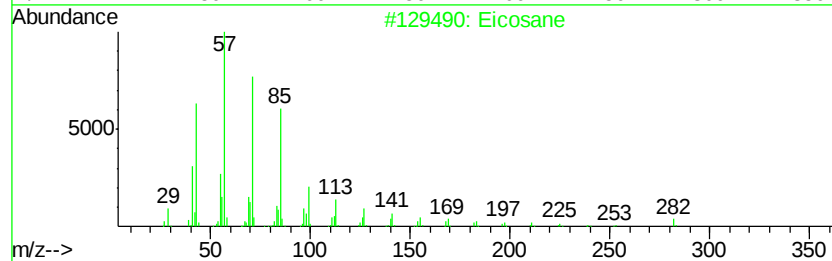
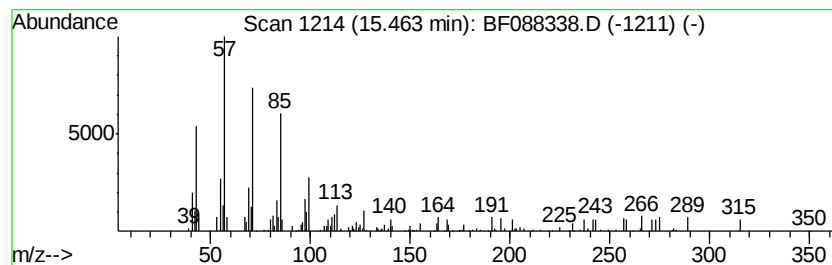
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Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	2.16 ng	58808	Perylene-d12	15.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	89
2	Eicosane, 10-methyl-	296 C21H44	054833-23-7	72
3	Heneicosane	296 C21H44	000629-94-7	72
4	Eicosane, 2-methyl-	296 C21H44	001560-84-5	72
5	Nonadecane, 9-methyl-	282 C20H42	013287-24-6	64



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NCHC-011

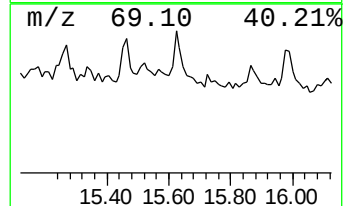
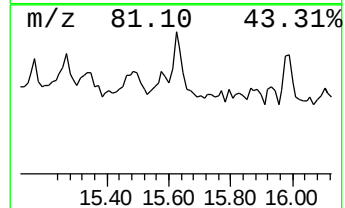
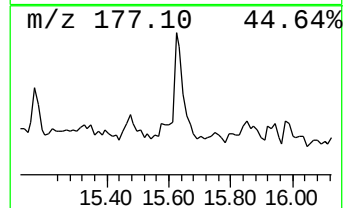
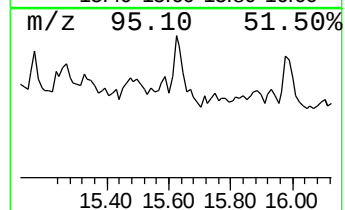
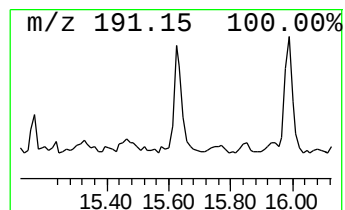
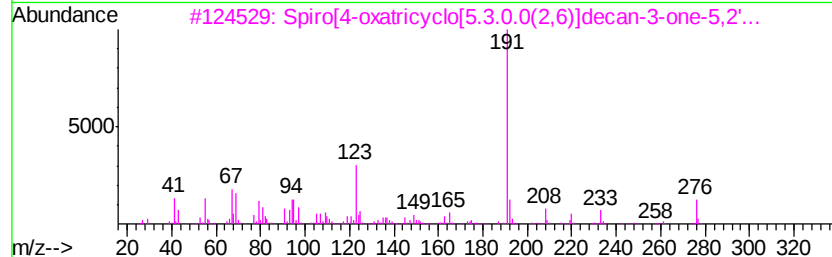
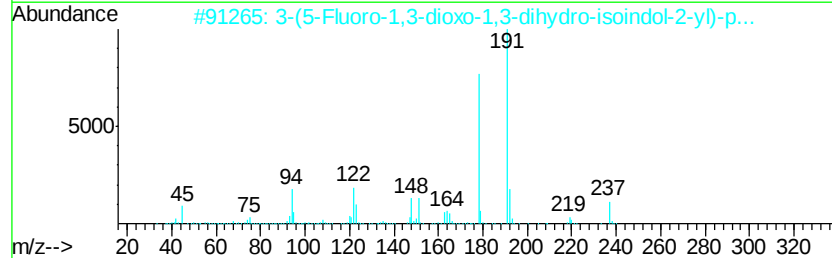
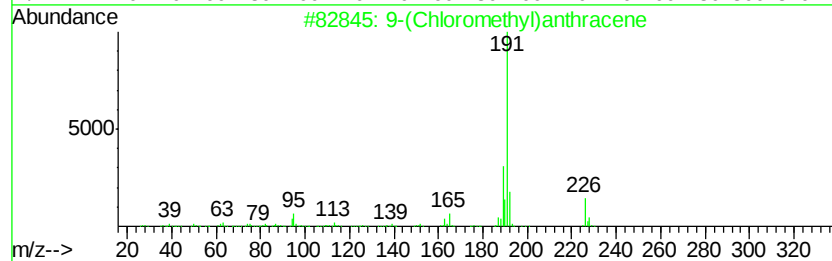
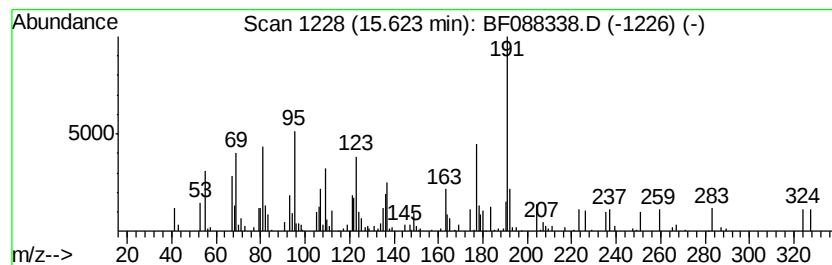
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.62 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	3.44 ng	93704	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	9-	(Chloromethyl)anthracene	226	C15H11Cl	024463-19-2	38
2	3-(5-Fluoro-1,3-dioxo-1,3-dihydr...		237	C11H8FN04	1000278-27-9	38
3	Spiro[4-oxatricyclo[5.3.0.0(2,6)...		276	C18H28O2	1000156-82-9	32
4	9H-Fluorene-9-carbonitrile		191	C14H9N	001529-40-4	25
5	4(1H)-Pteridinone, 2-amino-6,7-d...		191	C8H9N5O	000611-55-2	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088338.D
Acq On : 24 Jun 2016 18:24
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NCHC-011

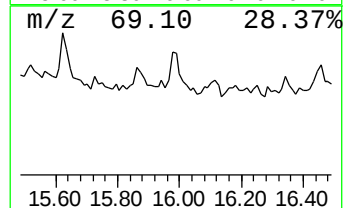
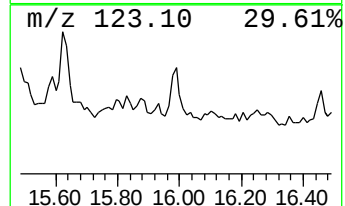
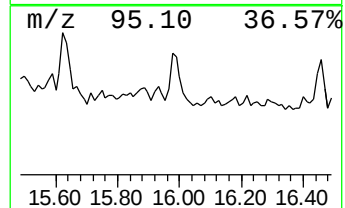
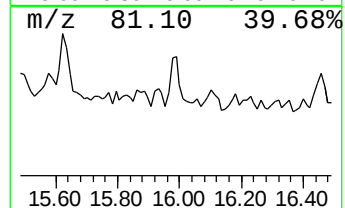
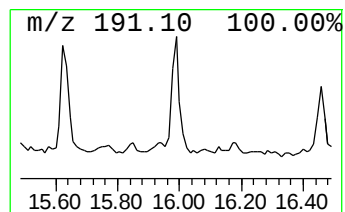
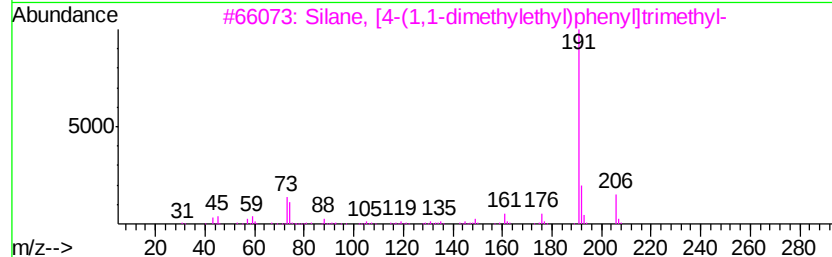
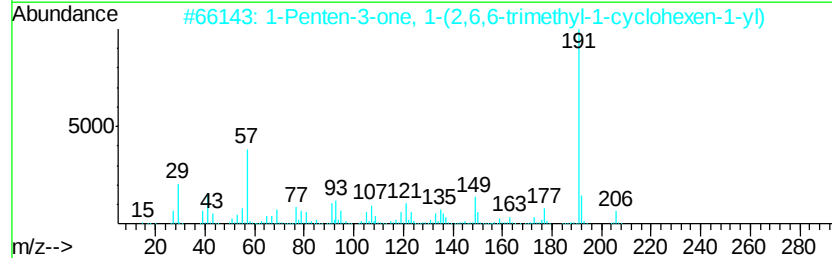
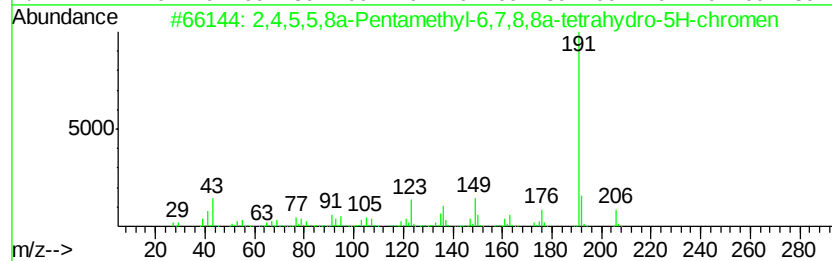
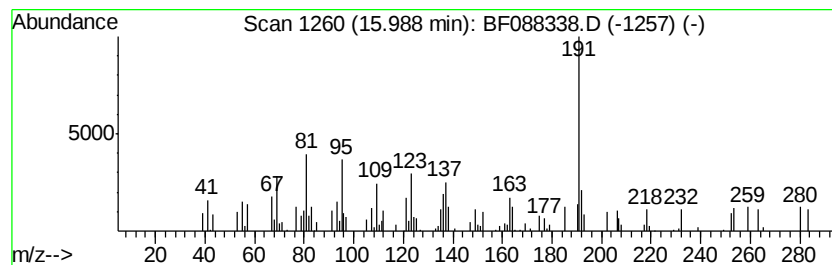
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,4,5,5,8a-Pentamethyl-6,7,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.27 ng	61744	Perylene-d12	15.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	62
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
3		Silane, [4-(1,1-dimethylethyl)ph...	206	C13H22Si	018412-68-5	38
4		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	38
5		Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062416\
Data File : BF088338.D
Acq On : 24 Jun 2016 18:24
Operator : UM/SJ
Sample : H3676-04
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NCHC-011

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.72	3.6	ng	84877	1	6.58	466106	20.0
unknown6.35	6.35	69.9	ng	1629690	1	6.58	466106	20.0
Heptacosane	10.97	2.0	ng	67328	4	11.10	661905	20.0
Ethanol, 2-(tetra...	13.58	3.0	ng	84251	5	13.71	563870	20.0
Eicosane	15.46	2.2	ng	58808	6	15.07	544797	20.0
unknown15.62	15.62	3.4	ng	93704	6	15.07	544797	20.0
2,4,5,5,8a-Pentam...	15.99	2.3	ng	61744	6	15.07	544797	20.0