

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
 Data File : BF088265.D
 Acq On : 22 Jun 2016 22:43
 Operator : UM/SJ
 Sample : H3660-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2(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-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	1.724	11	12	38	rVB	341006	647295	28.88%	3.370%
2	4.730	272	275	289	rBV	281583	478764	21.36%	2.493%
3	5.187	313	315	337	rVB	1621719	1702876	75.98%	8.867%
4	5.599	348	351	355	rVB	22156	31653	1.41%	0.165%
5	6.262	406	409	411	rBV	1591019	1712523	76.41%	8.917%
6	6.376	417	419	421	rBV	1547116	1912853	85.35%	9.960%
7	6.605	437	439	441	rBV	405750	424630	18.95%	2.211%
8	6.753	450	452	455	rBV	1455651	1422912	63.49%	7.409%
9	7.176	487	489	491	rBV	1216914	1221051	54.48%	6.358%
10	7.885	549	551	554	rBV	627135	604649	26.98%	3.148%
11	8.971	643	646	648	rBV	2309018	2241295	100.00%	11.670%
12	9.371	679	681	683	rBV	368783	320726	14.31%	1.670%
13	9.633	702	704	707	rBV	724875	665710	29.70%	3.466%
14	10.422	771	773	776	rBV	1158210	1111287	49.58%	5.786%
15	10.548	782	784	791	rVB	30701	39246	1.75%	0.204%
16	10.994	821	823	825	rBV	40262	38359	1.71%	0.200%
17	11.108	832	833	835	rBV	452602	588879	26.27%	3.066%
18	11.142	835	836	838	rVB	32909	27195	1.21%	0.142%
19	11.416	859	860	863	rVB	30401	35410	1.58%	0.184%
20	11.668	879	882	885	rBV	26535	50510	2.25%	0.263%
21	12.319	937	939	942	rBV2	52887	62114	2.77%	0.323%
22	12.525	954	957	958	rBV	69534	71563	3.19%	0.373%
23	12.548	958	959	961	rVB	56199	49911	2.23%	0.260%
24	12.697	969	972	974	rBV	1712694	1613286	71.98%	8.400%
25	13.611	1050	1052	1059	rBV	69472	172866	7.71%	0.900%
26	13.737	1061	1063	1066	rBV	338361	519110	23.16%	2.703%
27	14.251	1103	1108	1113	rBV3	40946	158352	7.07%	0.825%
28	14.640	1140	1142	1145	rVB	118323	121537	5.42%	0.633%
29	14.811	1155	1157	1158	rVB	45226	48328	2.16%	0.252%
30	14.845	1158	1160	1168	rVB3	58631	176685	7.88%	0.920%
31	15.017	1172	1175	1177	rBV	18785	32724	1.46%	0.170%
32	15.108	1181	1183	1189	rVB	358665	474785	21.18%	2.472%
33	15.303	1197	1200	1203	rVB2	35067	65250	2.91%	0.340%
34	15.497	1214	1217	1219	rBV	72030	114948	5.13%	0.599%

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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

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35	16.148	1272	1274	1278	rVB3	22254	41318	1.84%	0.215%
36	16.388	1293	1295	1303	rVB2	27775	82461	3.68%	0.429%
37	16.926	1339	1342	1345	rBV4	11414	28253	1.26%	0.147%
38	17.634	1401	1404	1411	rVB3	19712	58084	2.59%	0.302%
39	18.491	1476	1479	1484	rVB5	14637	36141	1.61%	0.188%

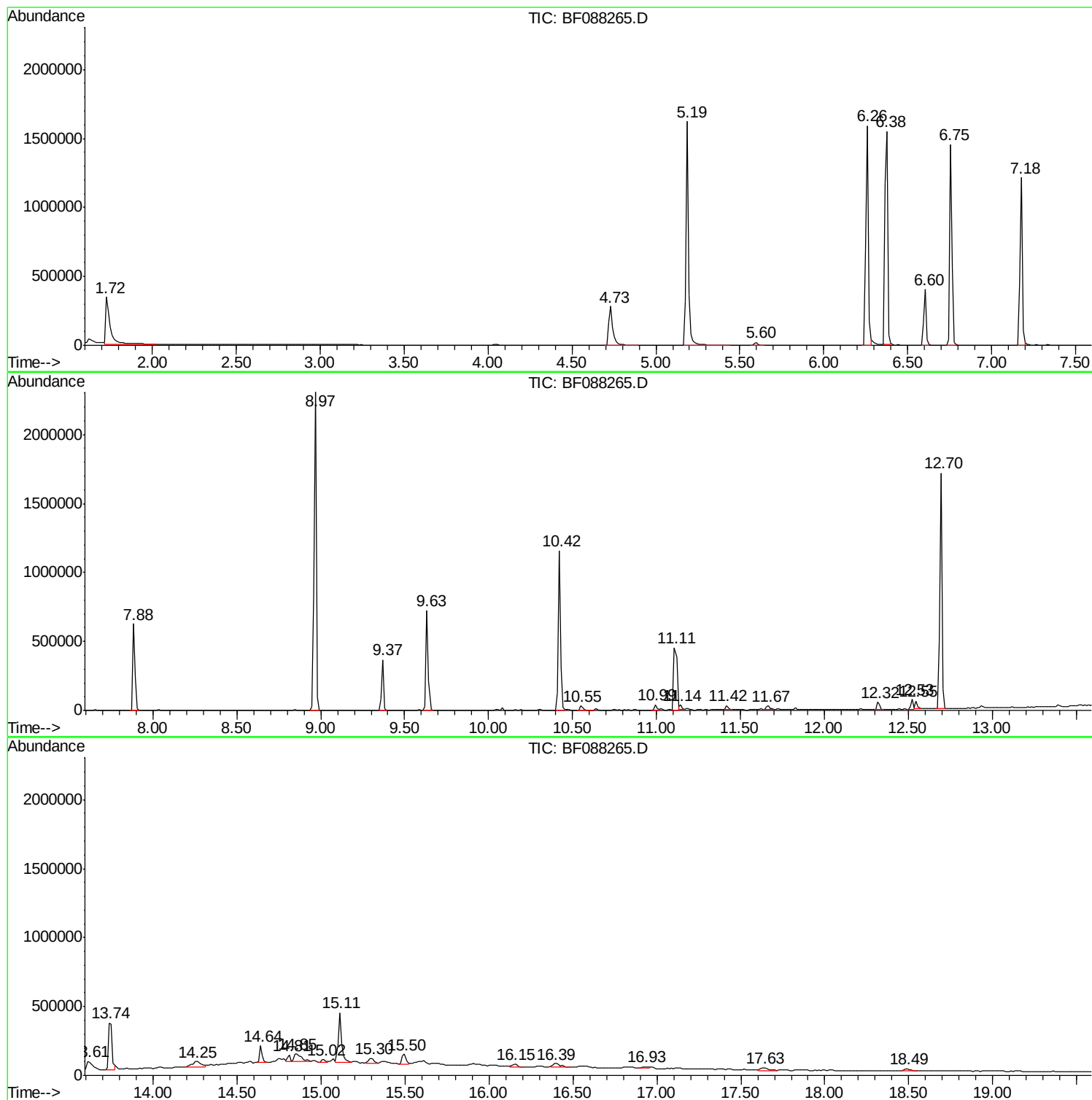
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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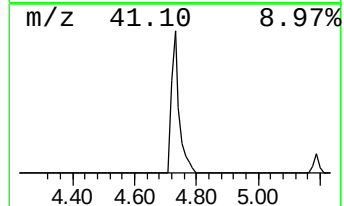
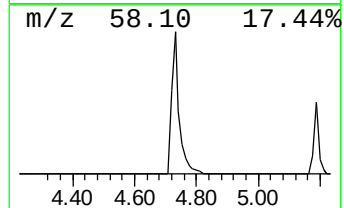
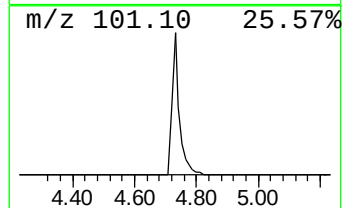
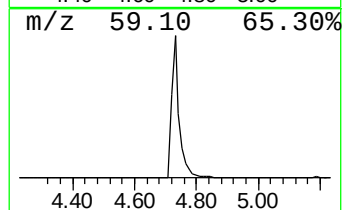
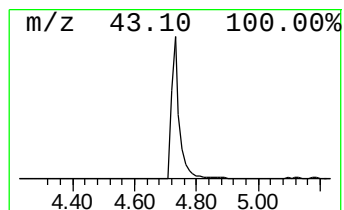
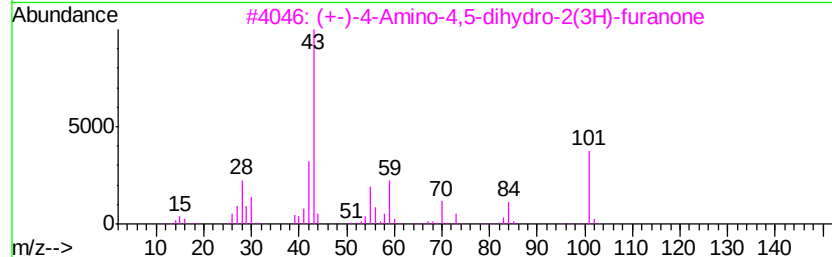
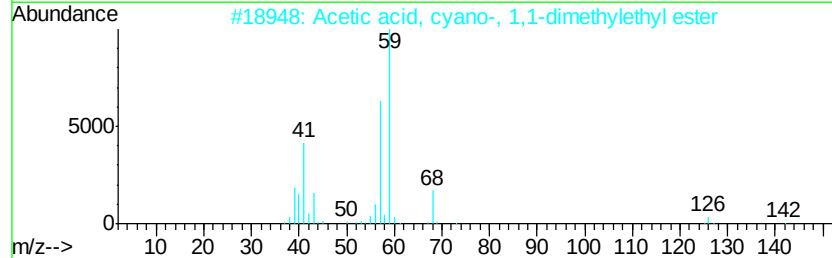
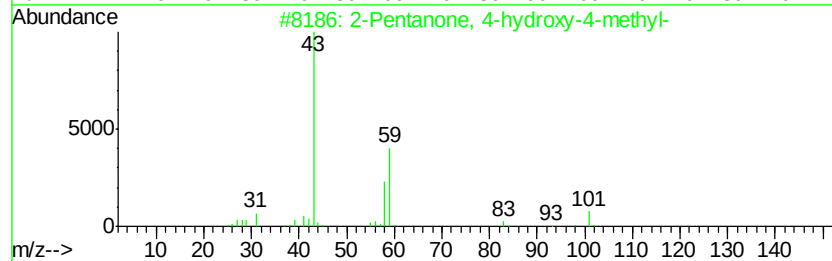
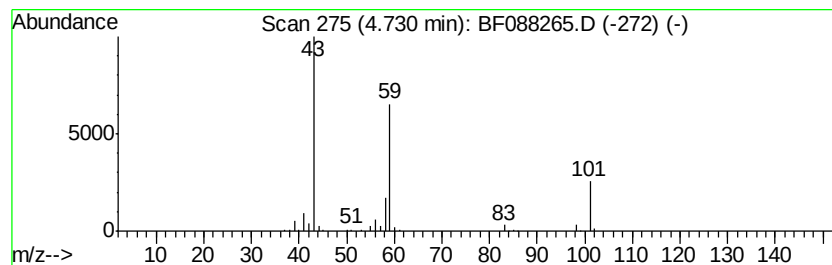
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	22.55 ng	478764	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Guanidine	59	CH5N3	000113-00-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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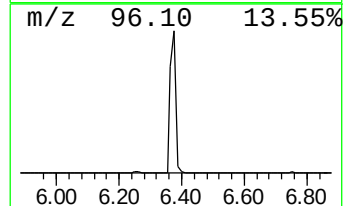
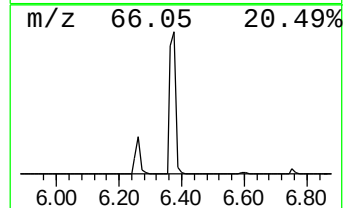
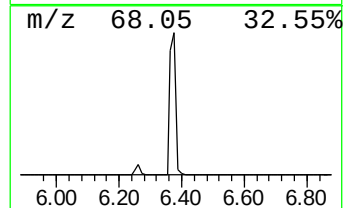
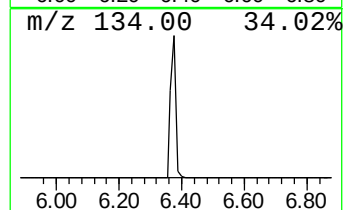
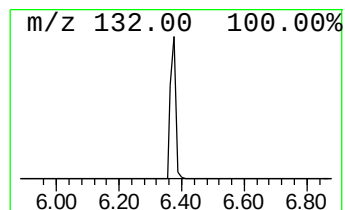
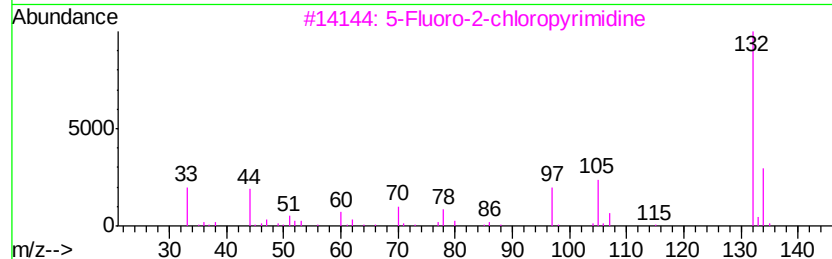
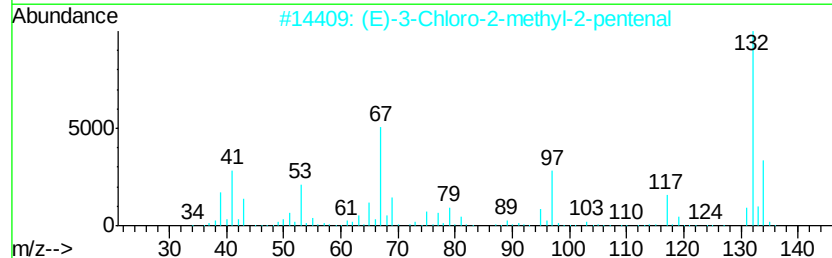
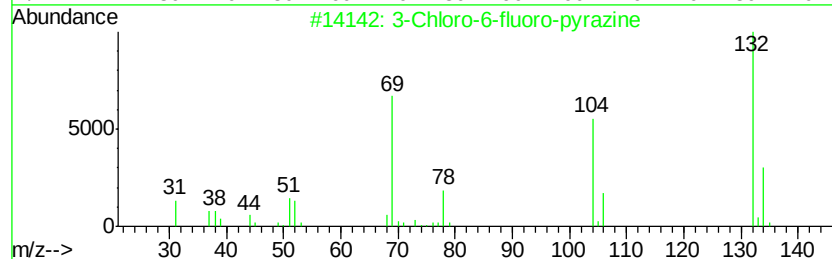
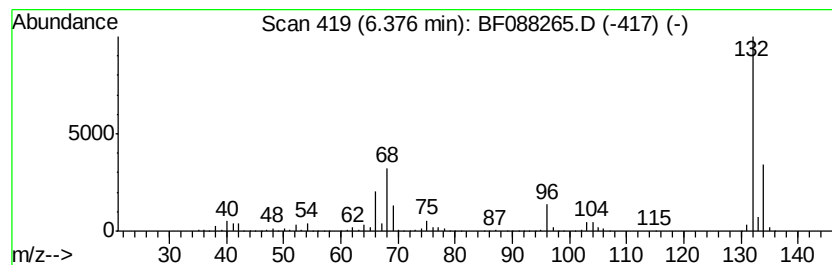
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown6.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	90.10 ng	1912850	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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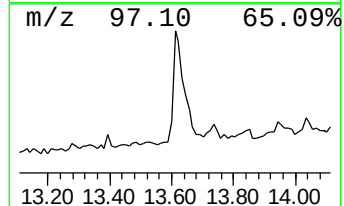
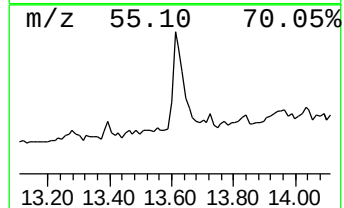
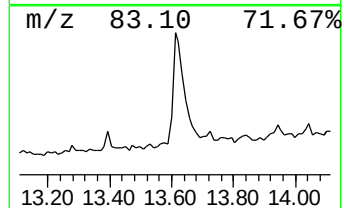
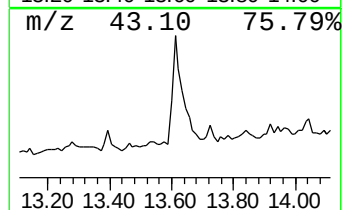
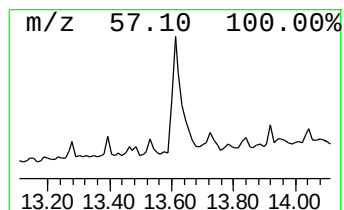
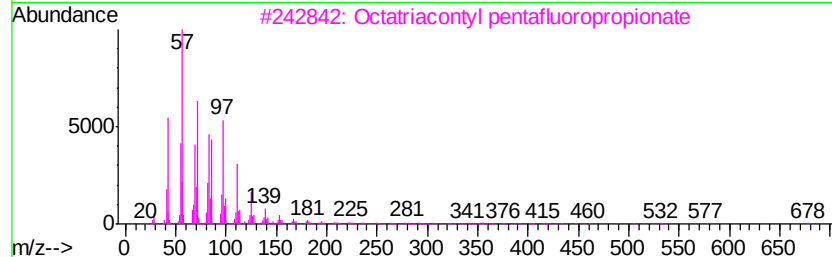
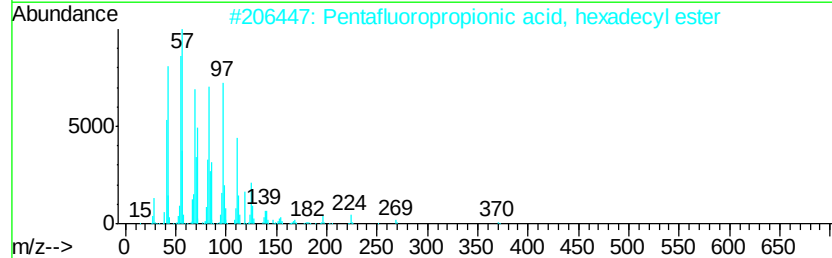
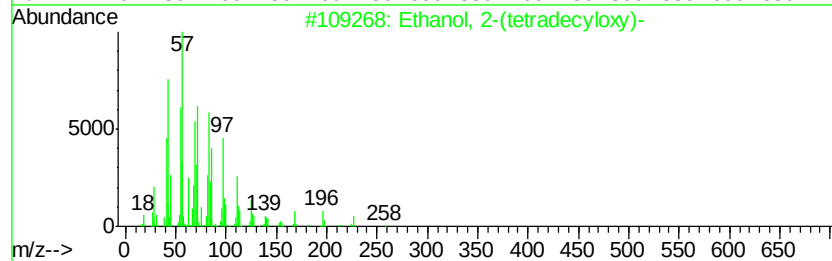
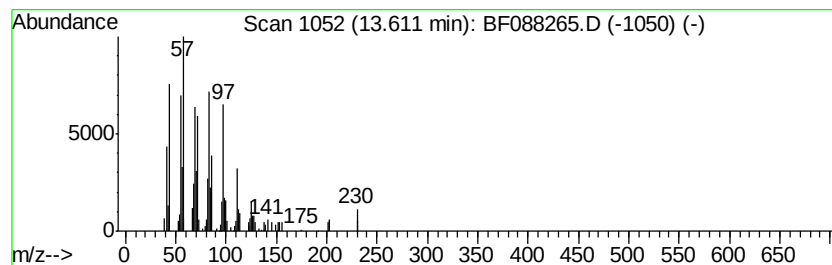
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Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	6.66 ng	172866	Chrysene-d12	13.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		Pentafluoropropionic acid, hexadecyl ester	388	C19H33F5O2	006222-07-7	90
3		Octatriacontyl pentafluoropropionate	697	C41H77F5O2	1000351-89-1	90
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
5		Hexatriacontyl pentafluoropropionate	669	C39H73F5O2	1000351-89-0	87



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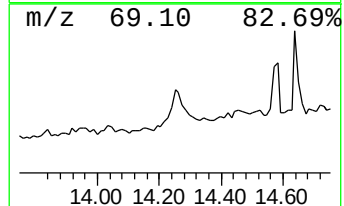
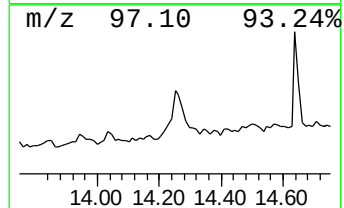
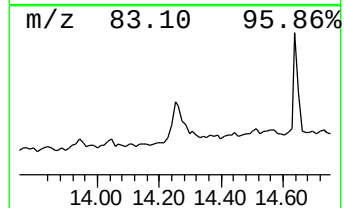
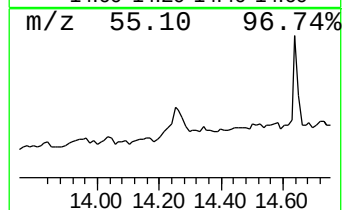
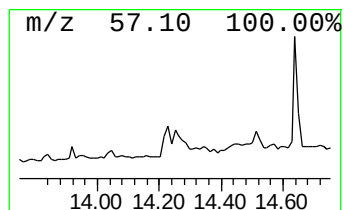
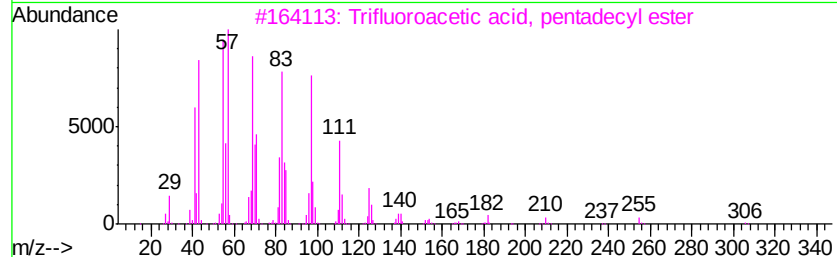
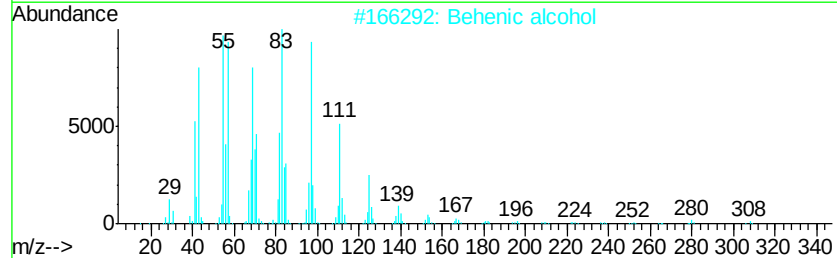
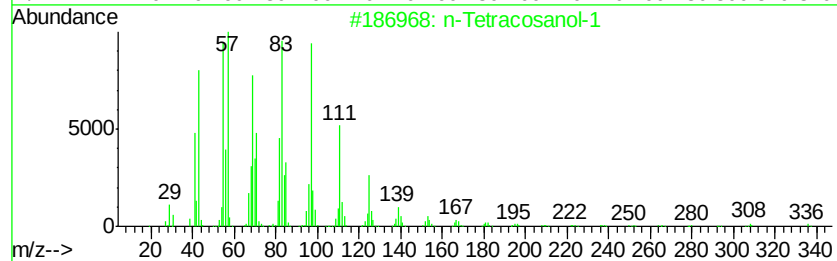
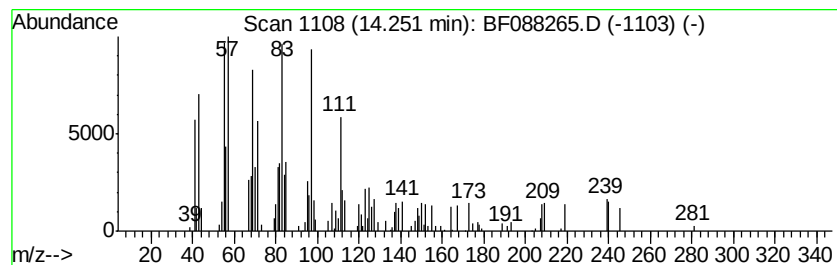
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.25	6.10 ng	158352	Chrysene-d12	13.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
2	Behenic alcohol	326	C22H46O	000661-19-8	81
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	74
4	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	74
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	74



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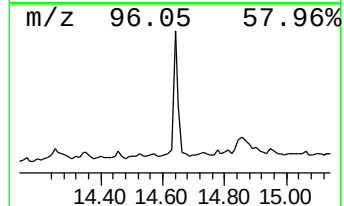
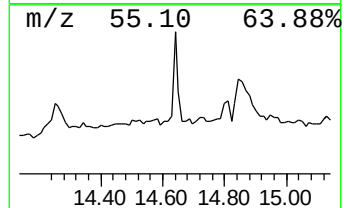
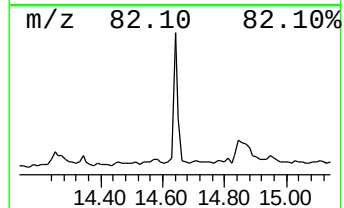
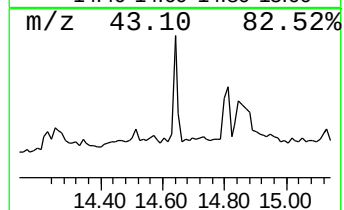
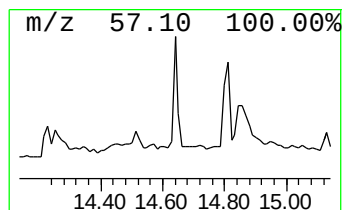
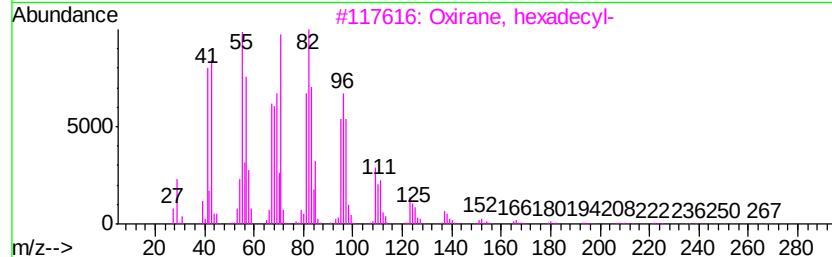
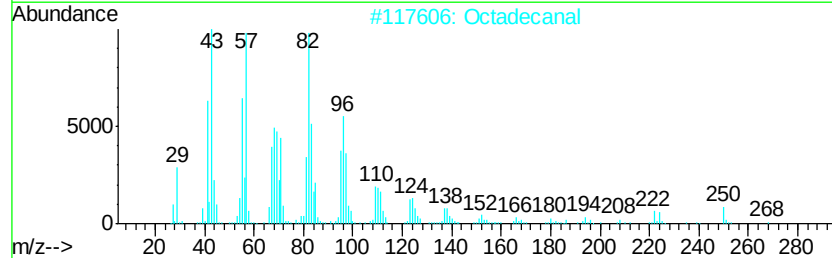
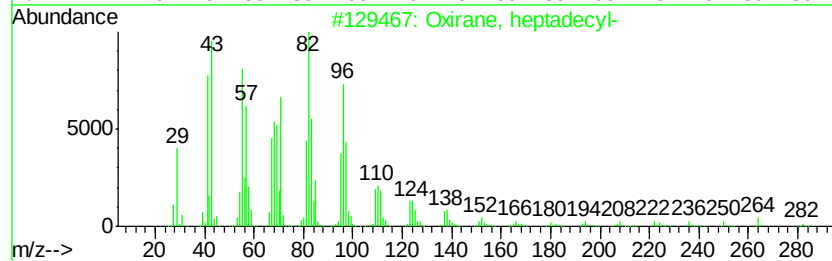
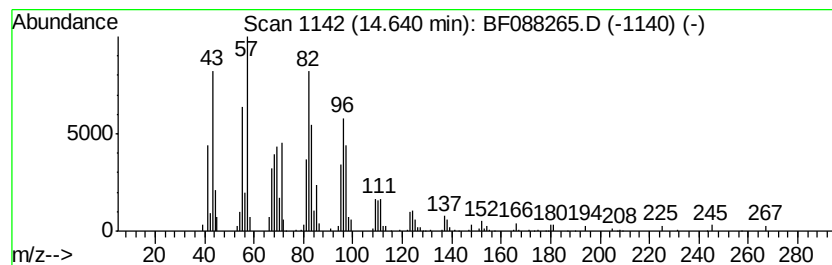
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Peak Number 7 Oxirane, heptadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.64	5.12 ng	121537	Perylene-d12		15.11
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2	Octadecanal	268	C18H36O	000638-66-4	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
4	17-Octadecenal	266	C18H34O	056554-86-0	90
5	1,19-Eicosadiene	278	C20H38	014811-95-1	81



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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(0-6)

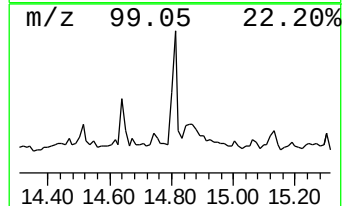
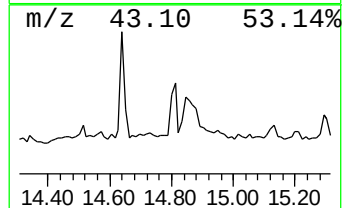
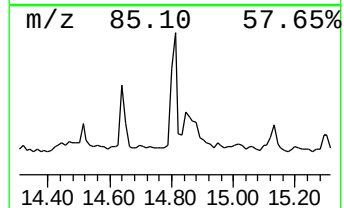
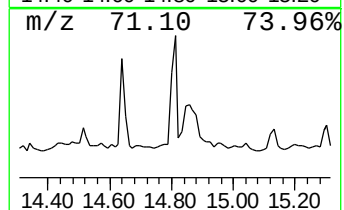
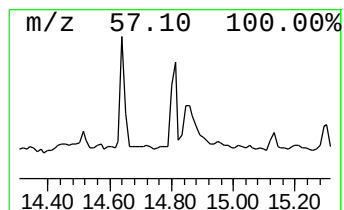
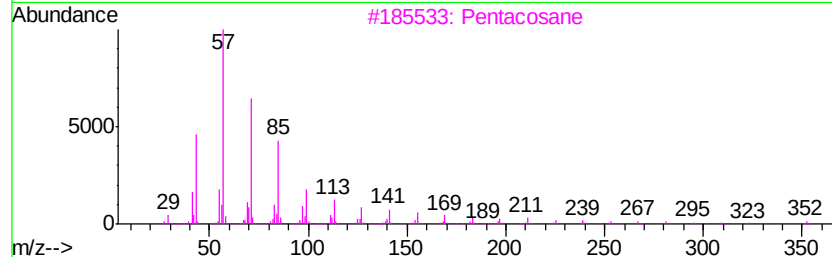
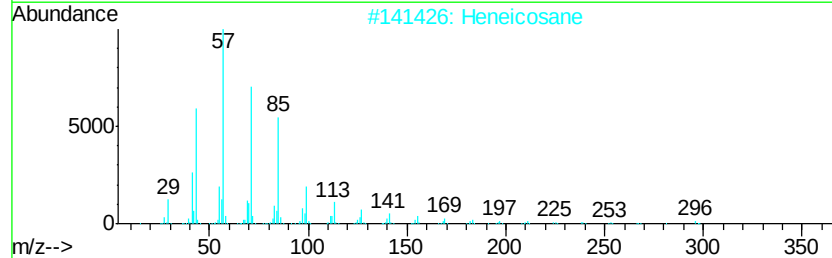
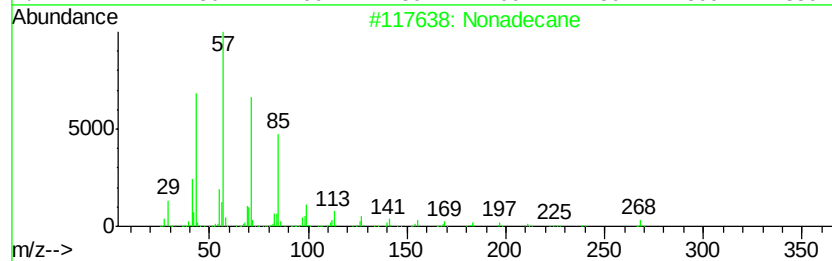
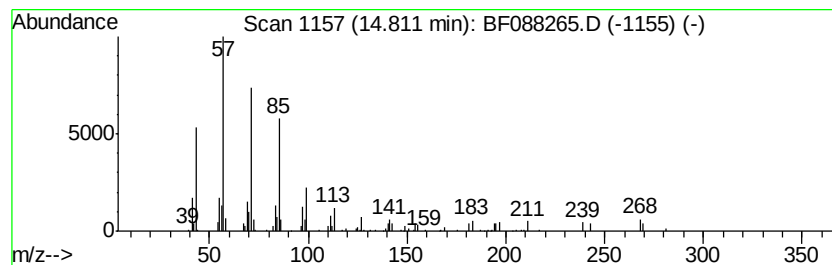
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.04 ng	48328	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86
5		Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088265.D
Acq On : 22 Jun 2016 22:43
Operator : UM/SJ
Sample : H3660-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(0-6)

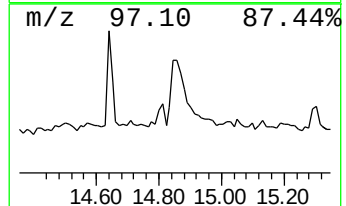
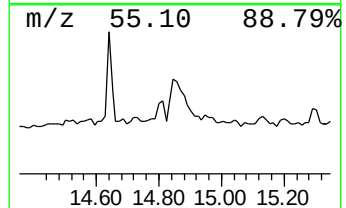
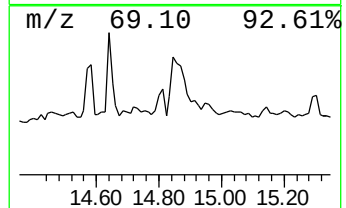
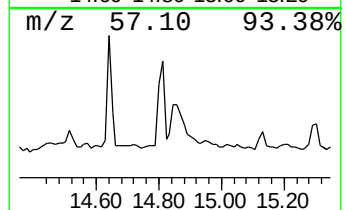
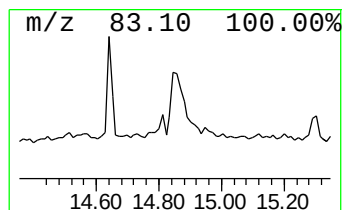
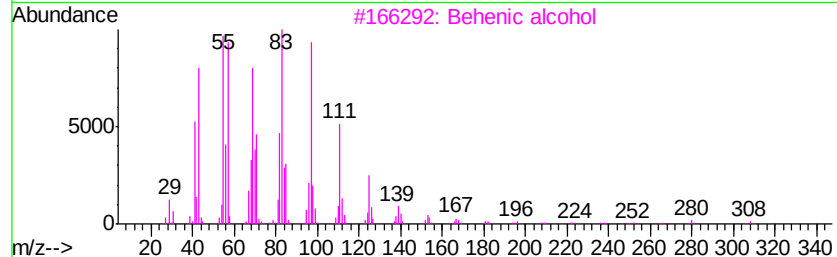
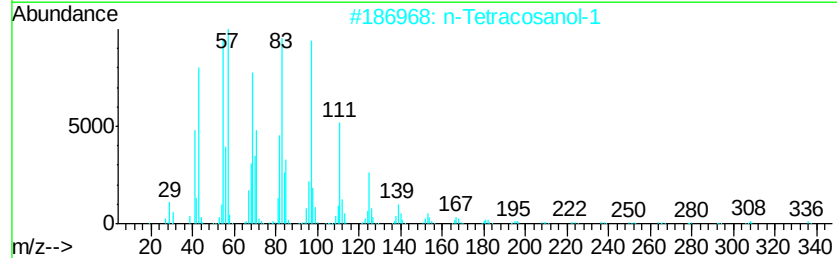
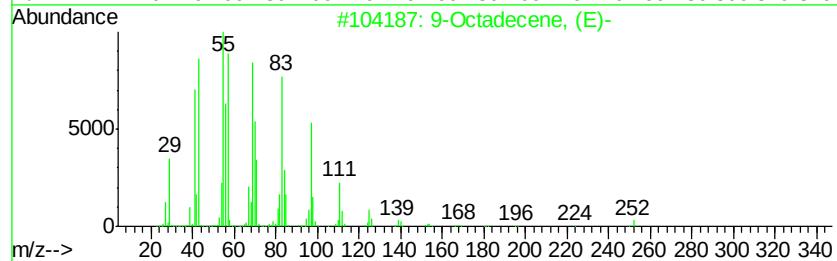
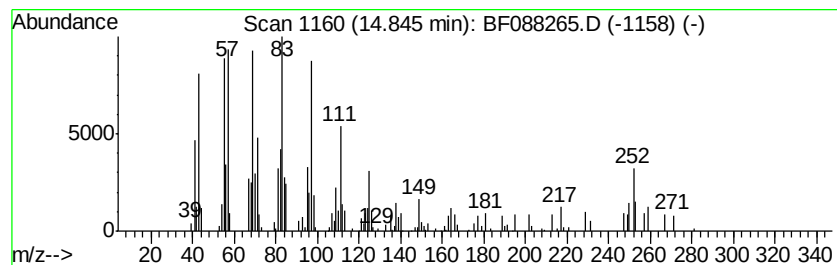
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	7.44 ng	176685	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecene, (E)-	252	C18H36	007206-25-9	93
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		Behenic alcohol	326	C22H46O	000661-19-8	90
4		5-Octadecene, (E)-	252	C18H36	007206-21-5	83
5		E-7-Octadecene	252	C18H36	1000130-92-0	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062216\
Data File : BF088265.D
Acq On : 22 Jun 2016 22:43
Operator : UM/SJ
Sample : H3660-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

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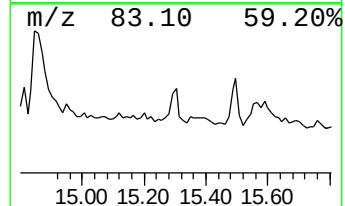
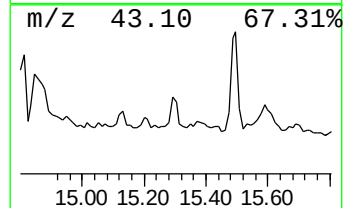
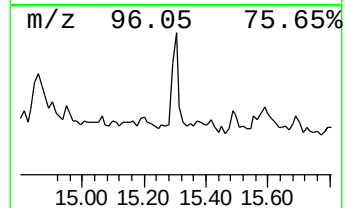
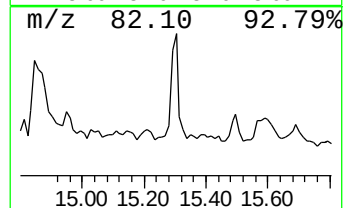
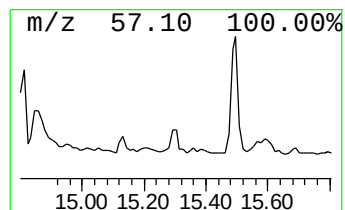
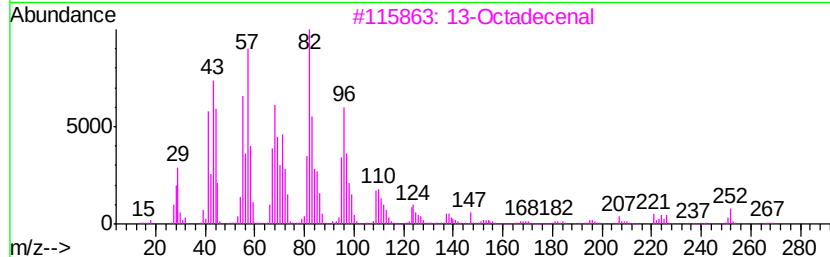
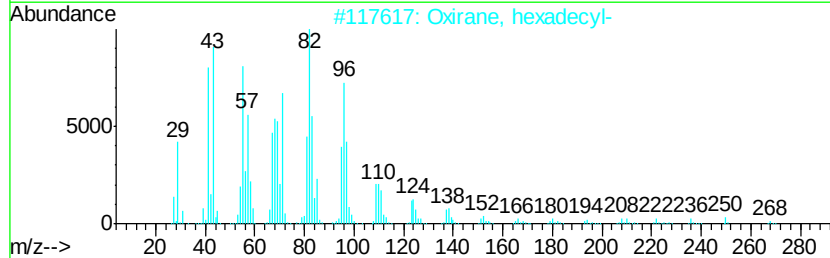
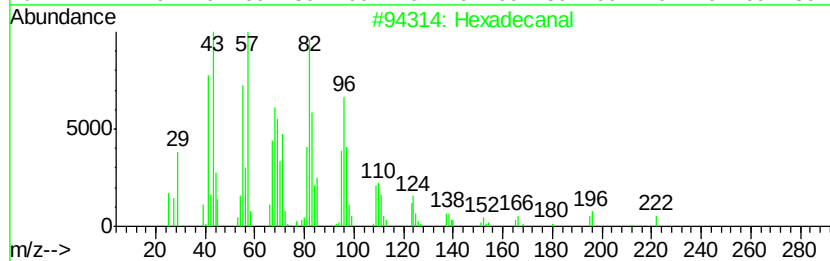
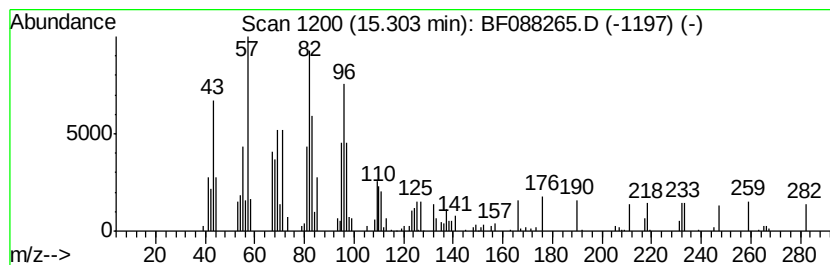
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.30	2.75 ng	65250	Perylene-d12	15.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanal	240	C16H32O	000629-80-1	87
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
3			13-Octadecenal	266	C18H34O	056554-90-6	80
4			Pentadecanal-	226	C15H30O	002765-11-9	80
5			Tetradecanal	212	C14H28O	000124-25-4	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062216\
Data File : BF088265.D
Acq On : 22 Jun 2016 22:43
Operator : UM/SJ
Sample : H3660-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-2(0-6)

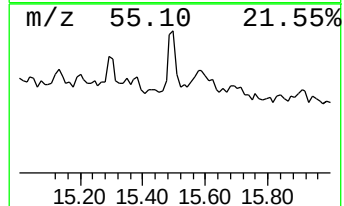
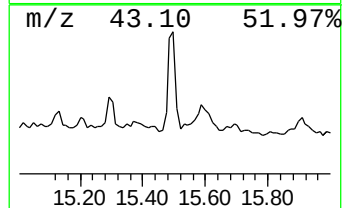
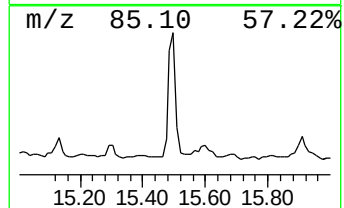
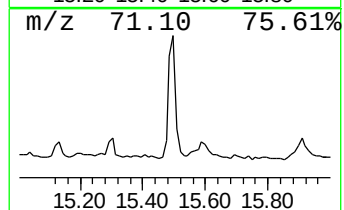
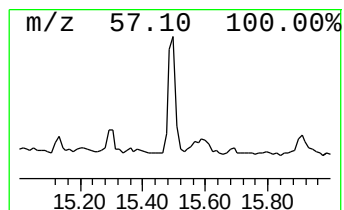
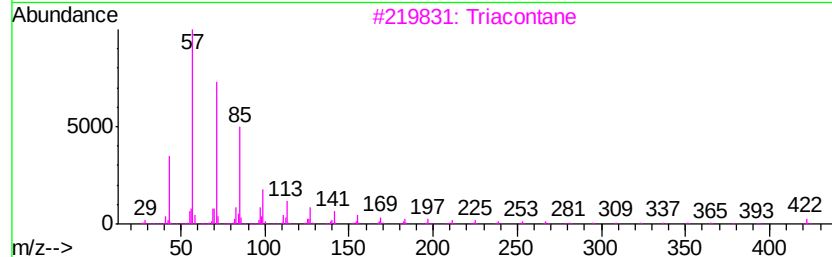
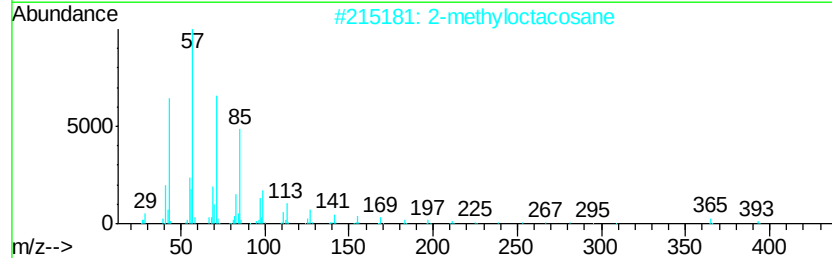
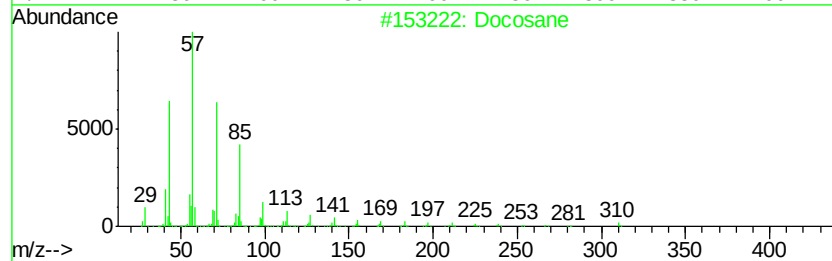
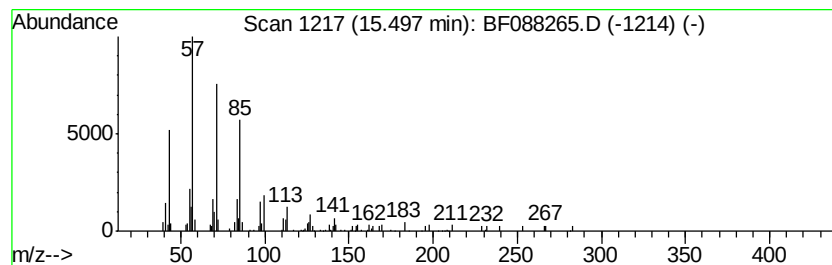
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.50	4.84 ng	114948	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062216\
Data File : BF088265.D
Acq On : 22 Jun 2016 22:43
Operator : UM/SJ
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Misc :
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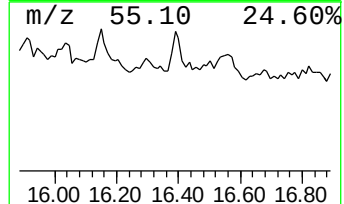
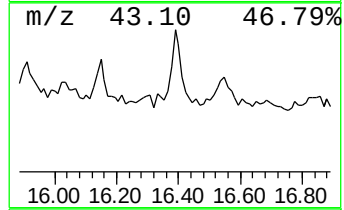
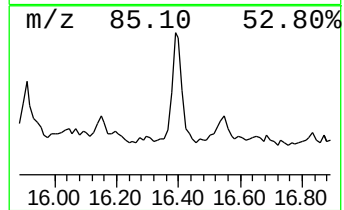
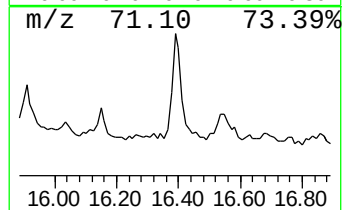
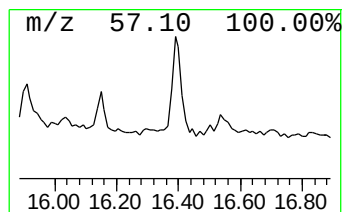
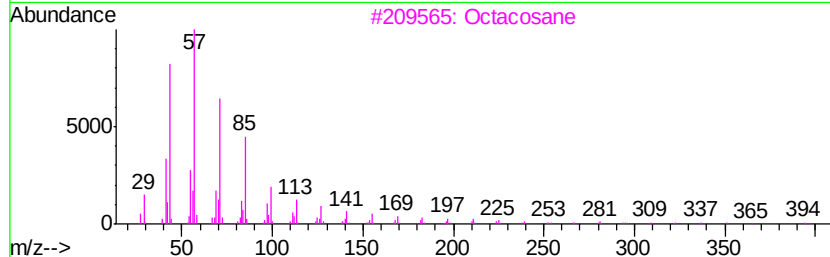
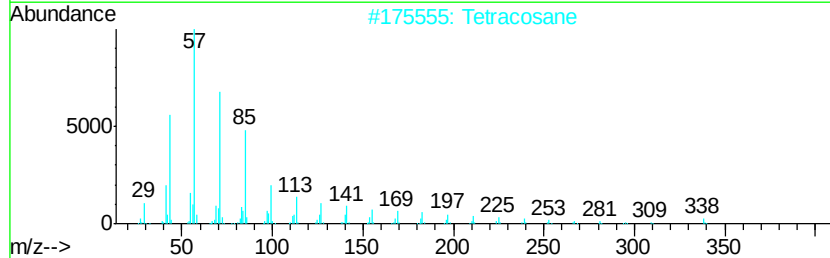
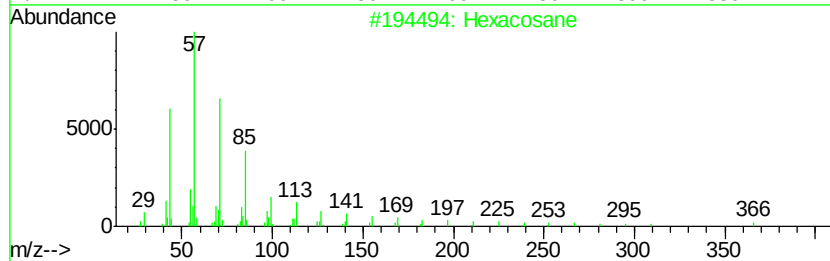
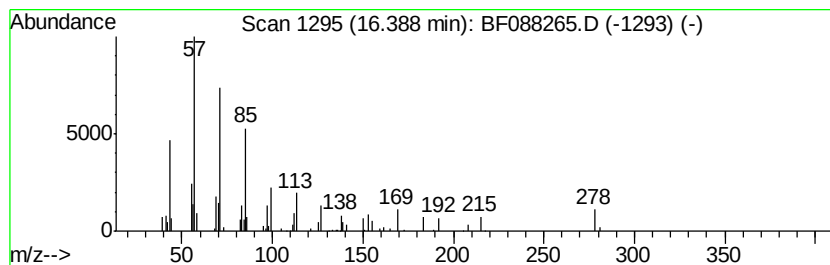
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.39	3.47 ng	82461	Perylene-d12	15.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	78
2		Tetracosane	338	C24H50	000646-31-1	72
3		Octacosane	394	C28H58	000630-02-4	72
4		Heneicosane	296	C21H44	000629-94-7	64
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062216\
Data File : BF088265.D
Acq On : 22 Jun 2016 22:43
Operator : UM/SJ
Sample : H3660-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.73	22.6	ng	478764	1	6.60	424630	20.0
unknown6.38	6.38	90.1	ng	1912850	1	6.60	424630	20.0
Ethanol, 2-(tetra...	13.61	6.7	ng	172866	5	13.75	519110	20.0
n-Tetracosanol-1	14.25	6.1	ng	158352	5	13.75	519110	20.0
Oxirane, heptadecyl-	14.64	5.1	ng	121537	6	15.11	474785	20.0
Nonadecane	14.81	2.0	ng	48328	6	15.11	474785	20.0
9-Octadecene, (E)-	14.85	7.4	ng	176685	6	15.11	474785	20.0
Hexadecanal	15.30	2.8	ng	65250	6	15.11	474785	20.0
Docosane	15.50	4.8	ng	114948	6	15.11	474785	20.0
Hexacosane	16.39	3.5	ng	82461	6	15.11	474785	20.0