

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
 Data File : BF086881.D
 Acq On : 11 May 2016 5:12
 Operator : UM/SJ
 Sample : H2916-02
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VITALE-FILL-CSPH3-2K

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-BF050916.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	4.841	239	241	249	rBV	352225	620419	14.77%	1.768%
2	5.287	277	280	282	rBV	3308458	3965351	94.43%	11.302%
3	5.687	309	315	320	rVB2	46726	91511	2.18%	0.261%
4	6.350	370	373	375	rBV	3339899	4199160	100.00%	11.968%
5	6.453	380	382	385	rBV	3265656	3775754	89.92%	10.761%
6	6.682	400	402	409	rVB	1095482	985879	23.48%	2.810%
7	6.842	413	416	418	rBV	3313719	3291743	78.39%	9.382%
8	7.253	450	452	455	rBV	2335474	2455123	58.47%	6.997%
9	7.973	512	515	517	rBV	1042079	1126032	26.82%	3.209%
10	9.047	607	609	612	rBV	4004479	3604214	85.83%	10.272%
11	9.448	642	644	646	rBV	487314	421519	10.04%	1.201%
12	9.665	661	663	665	rBV	117636	126737	3.02%	0.361%
13	9.722	665	668	670	rBV	1044526	1079700	25.71%	3.077%
14	9.893	679	683	684	rBV	29624	45824	1.09%	0.131%
15	10.156	704	706	708	rVB	257392	205017	4.88%	0.584%
16	10.373	722	725	728	rBV	81229	130213	3.10%	0.371%
17	10.510	734	737	739	rBV	1582428	1976405	47.07%	5.633%
18	10.625	746	747	752	rBV	228146	298572	7.11%	0.851%
19	10.819	762	764	766	rBV	35525	49543	1.18%	0.141%
20	11.071	785	786	788	rBV	111274	116049	2.76%	0.331%
21	11.196	795	797	799	rBV	1016702	942166	22.44%	2.685%
22	11.745	842	845	849	rBV2	66071	113117	2.69%	0.322%
23	12.396	900	902	904	rBV	35715	52590	1.25%	0.150%
24	12.522	909	913	919	rBV2	19440	44824	1.07%	0.128%
25	12.625	919	922	926	rBV2	73057	129783	3.09%	0.370%
26	12.785	933	936	938	rBV	2008743	2847895	67.82%	8.117%
27	13.711	1013	1017	1024	rBV	127390	436882	10.40%	1.245%
28	13.825	1024	1027	1029	rBV	695645	803468	19.13%	2.290%
29	13.997	1040	1042	1046	rBV	28002	44378	1.06%	0.126%
30	14.305	1067	1069	1070	rBV	44460	42830	1.02%	0.122%
31	14.899	1119	1121	1124	rBV2	47880	70799	1.69%	0.202%
32	15.197	1145	1147	1154	rVB	548680	663208	15.79%	1.890%
33	15.402	1163	1165	1168	rVB	31760	45272	1.08%	0.129%
34	15.608	1180	1183	1186	rVB	42689	72714	1.73%	0.207%

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VITALE-FILL-CSPH3-2K

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-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.700	1189	1191	1197	rBV5	22483	84392	2.01%	0.241%
36	16.545	1262	1265	1270	rVB2	23911	48452	1.15%	0.138%
37	17.848	1375	1379	1387	rVB4	22397	78806	1.88%	0.225%

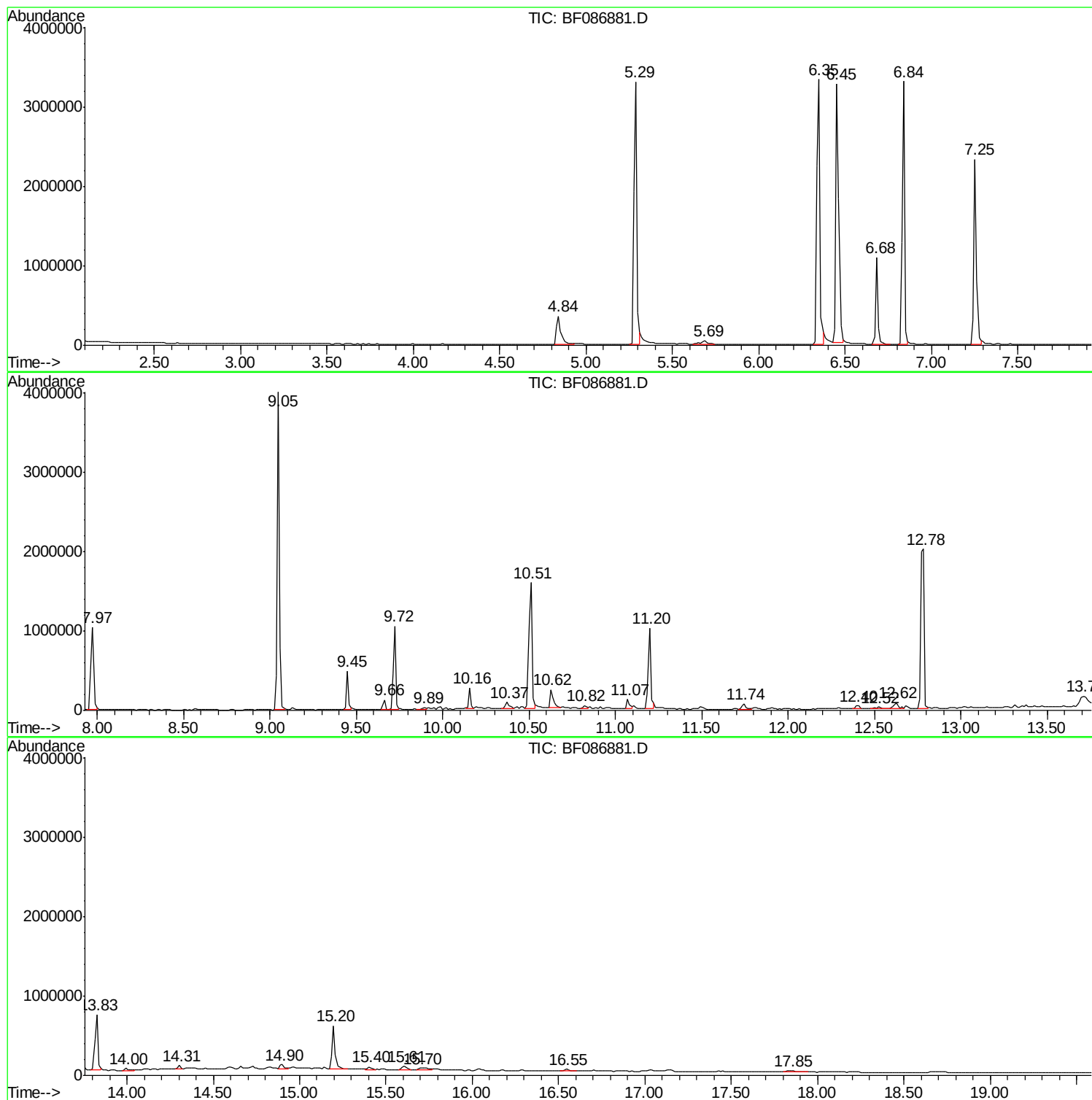
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TIC Library : C:\DATABASE\NIST02.L
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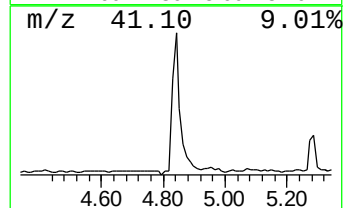
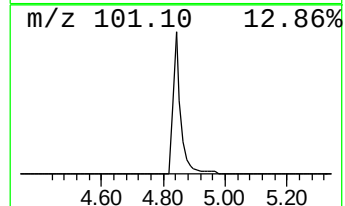
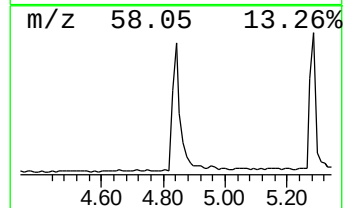
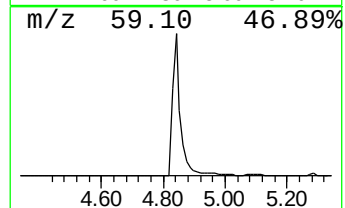
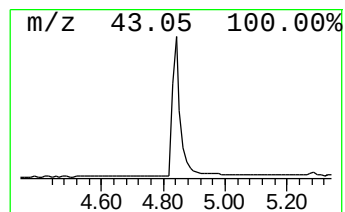
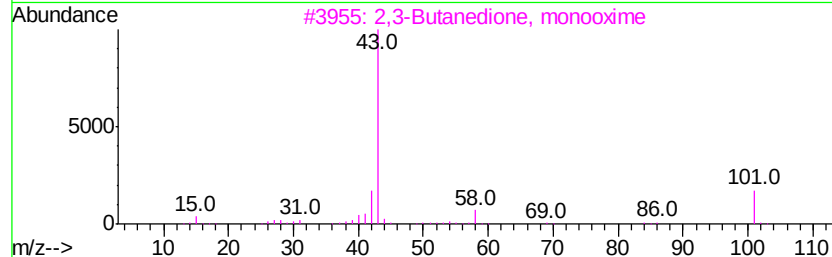
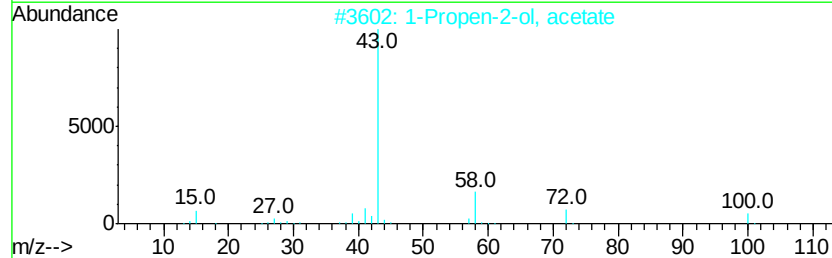
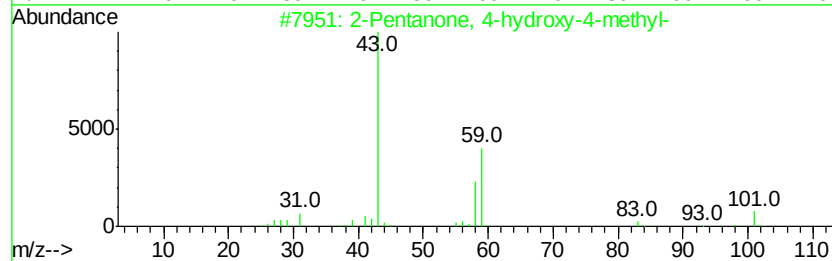
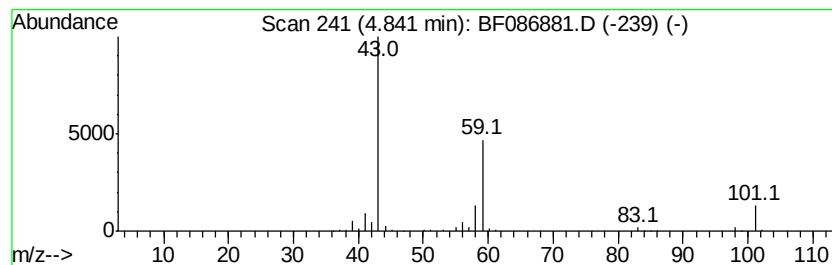
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	12.59 ng	620419	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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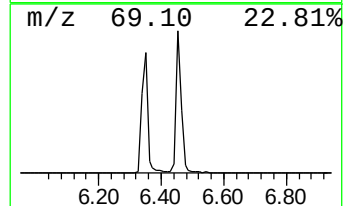
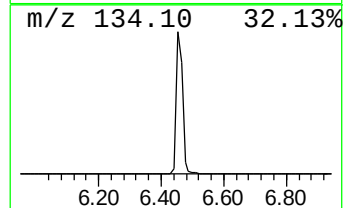
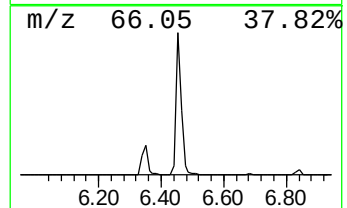
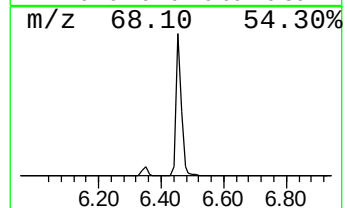
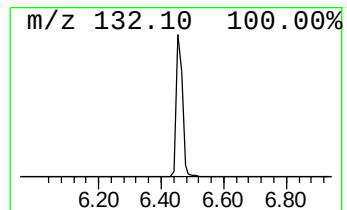
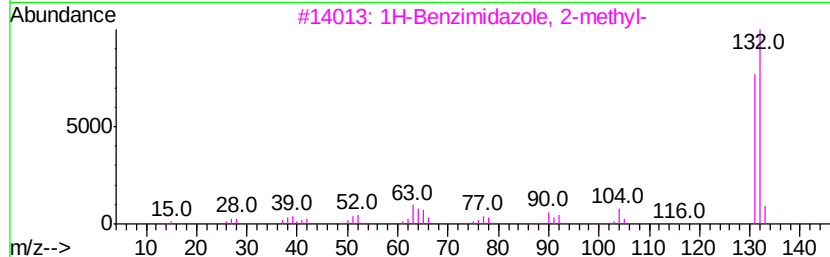
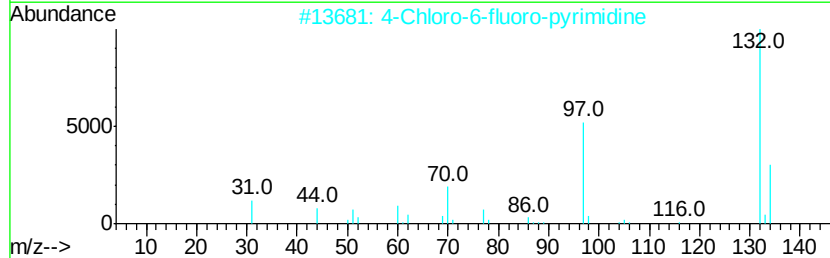
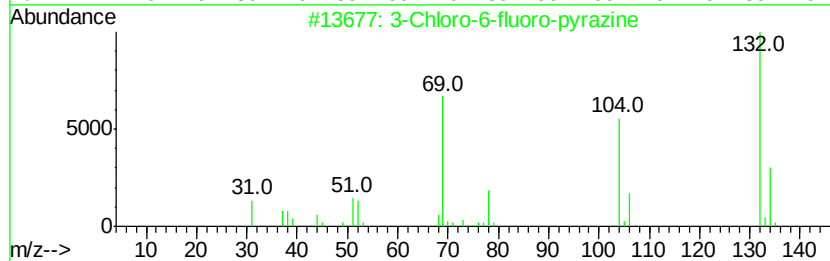
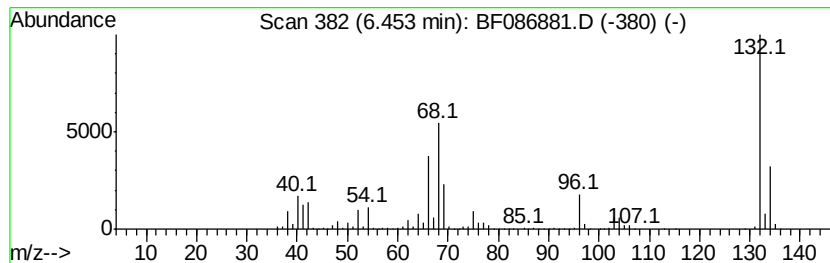
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Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	76.60 ng	3775750	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine			132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	22
4	Pyrazolo(2,3-a)pyridine, 7-methyl-			132	C8H8N2	034760-58-2	22
5	Tranlycypromine-propionyl			189	C12H15NO	1000123-86-3	22



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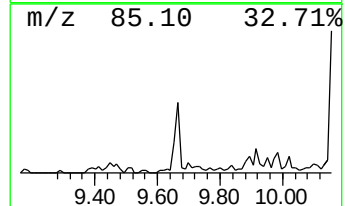
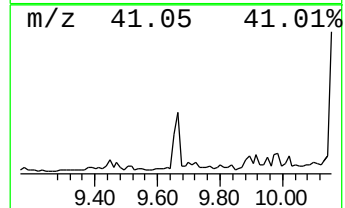
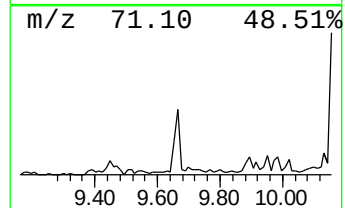
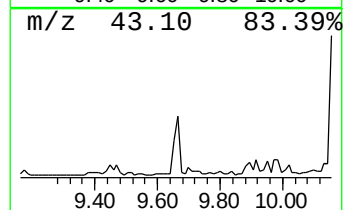
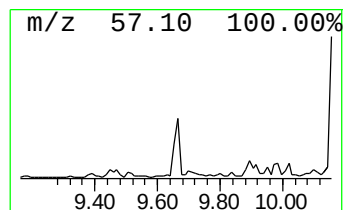
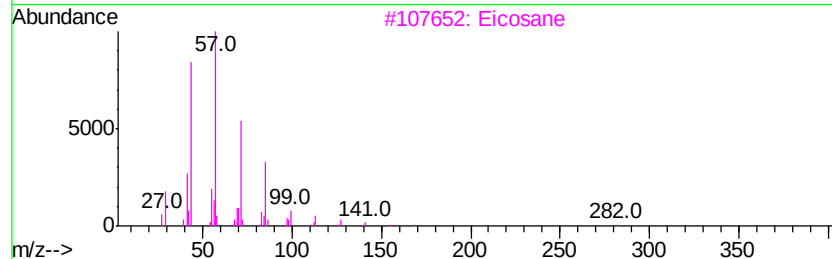
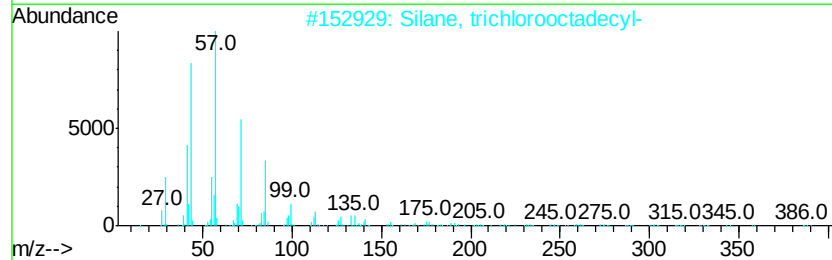
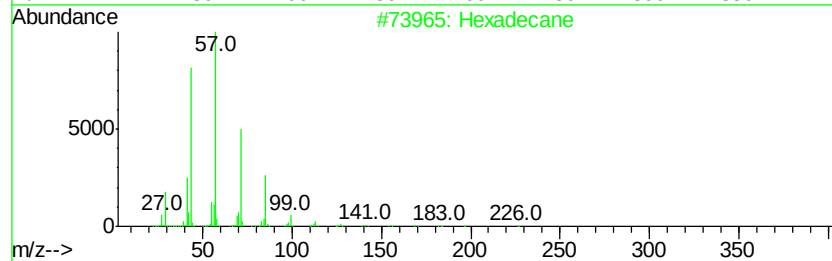
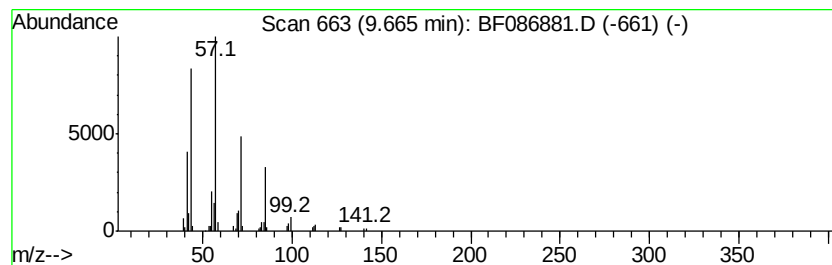
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	2.35 ng	126737	Acenaphthene-d10	9.72
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Silane, trichlorooctadecyl-	386 C18H37Cl3Si	000112-04-9	90
3	Eicosane	282 C20H42	000112-95-8	86
4	Tetradecane	198 C14H30	000629-59-4	86
5	Pentadecane	212 C15H32	000629-62-9	86



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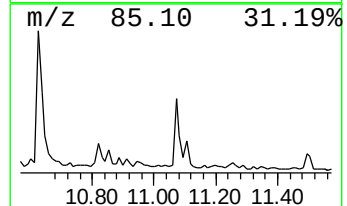
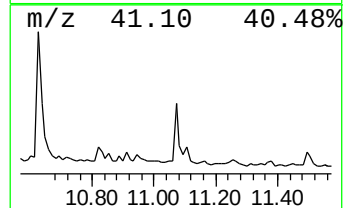
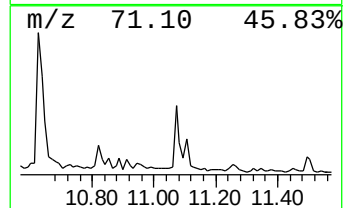
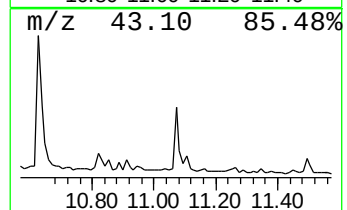
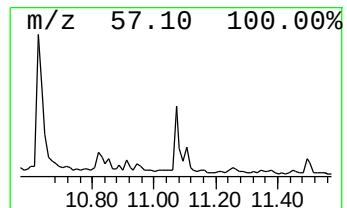
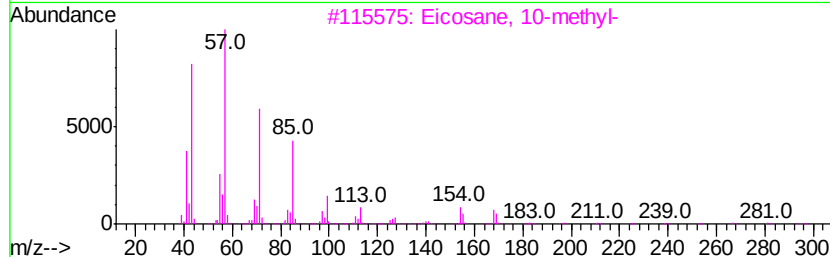
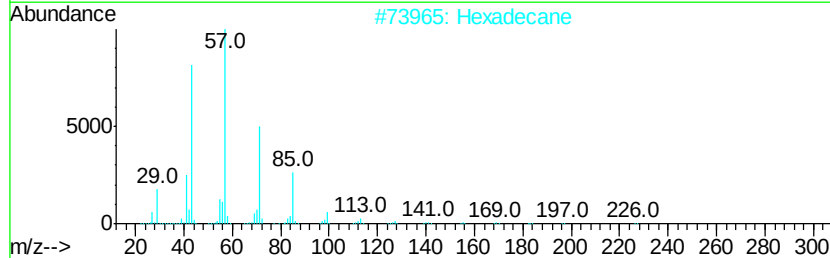
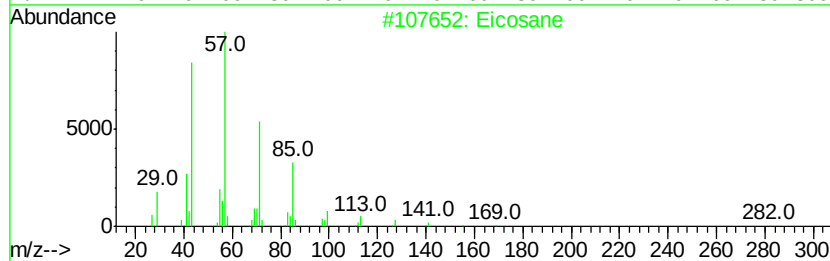
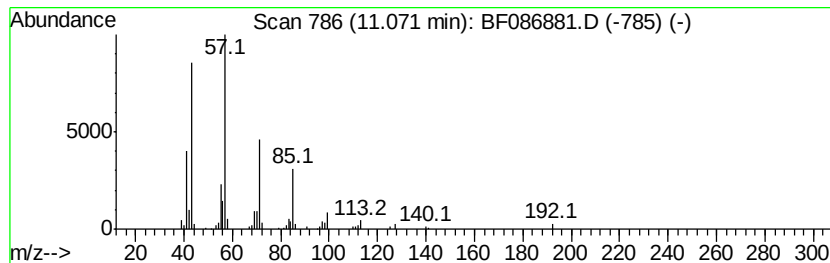
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.07	2.46 ng	116049	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Hexadecane		226	C16H34	000544-76-3	91
3	Eicosane, 10-methyl-		296	C21H44	054833-23-7	90
4	Octadecane		254	C18H38	000593-45-3	90
5	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	90



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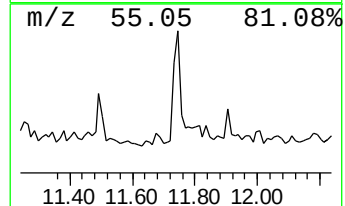
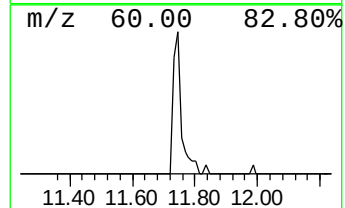
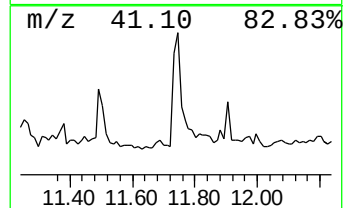
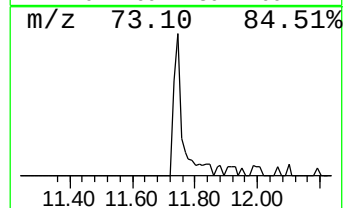
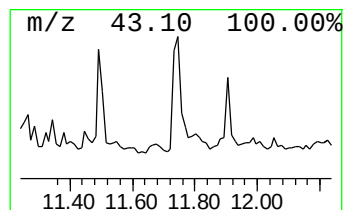
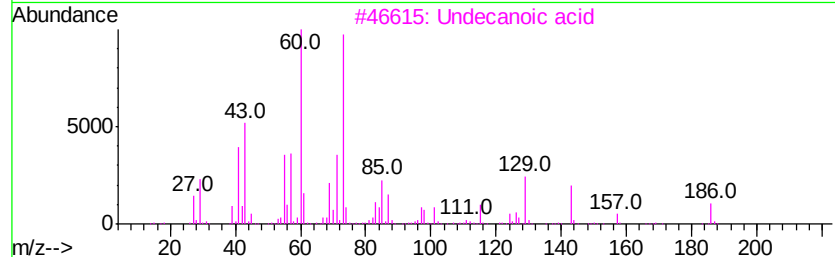
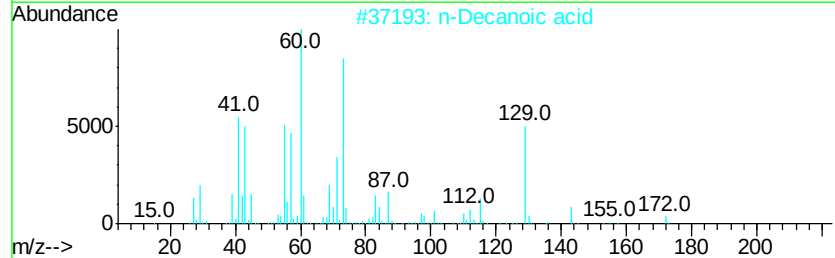
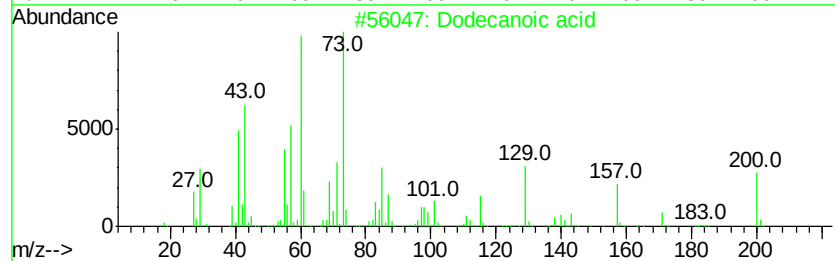
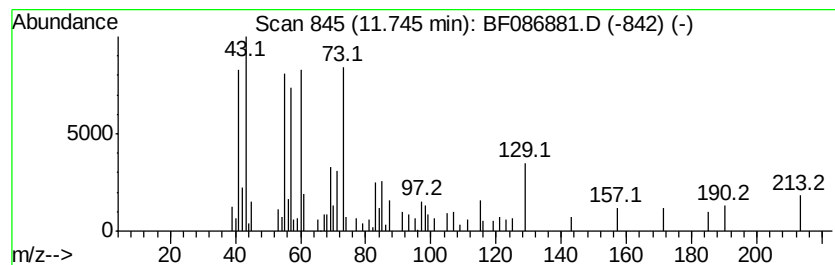
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Dodecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.40 ng	113117	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	59
2		n-Decanoic acid	172	C10H20O2	000334-48-5	47
3		Undecanoic acid	186	C11H22O2	000112-37-8	47
4		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47
5		n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	43



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VITALE-FILL-CSPH3-2K

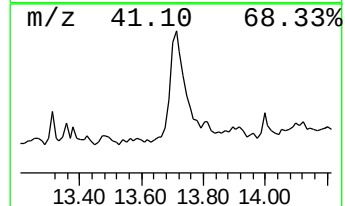
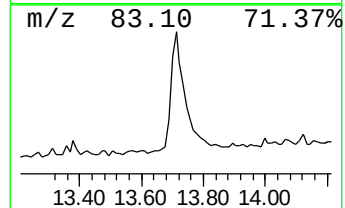
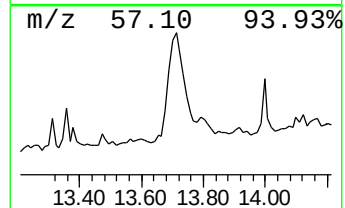
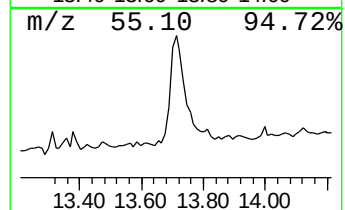
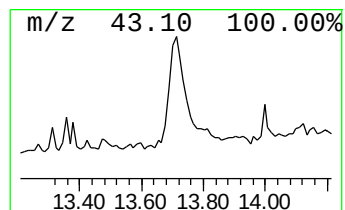
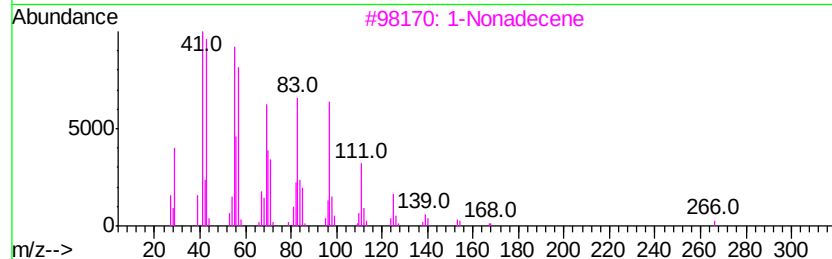
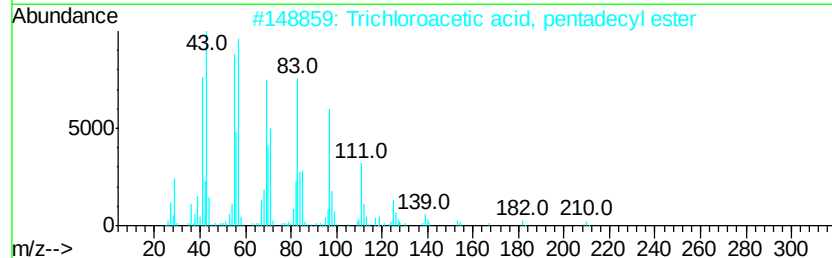
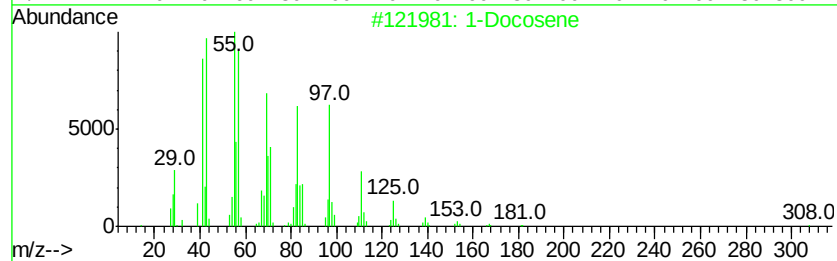
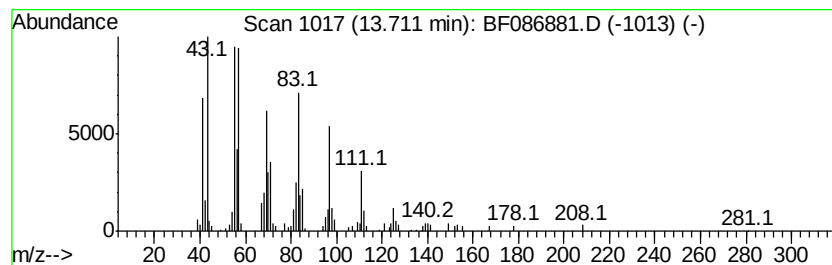
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	10.87 ng	436882	Chrysene-d12	13.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	95
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5			Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
Data File : BF086881.D
Acq On : 11 May 2016 5:12
Operator : UM/SJ
Sample : H2916-02
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-2K

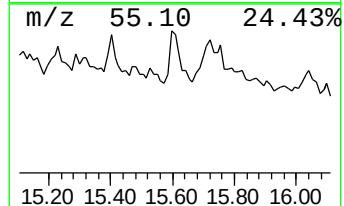
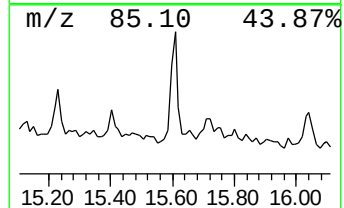
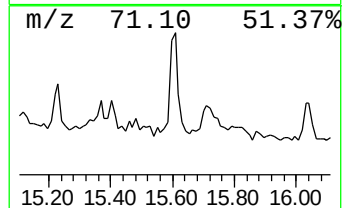
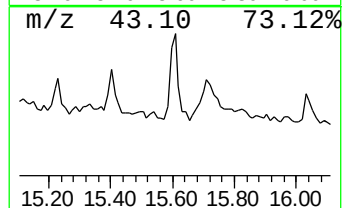
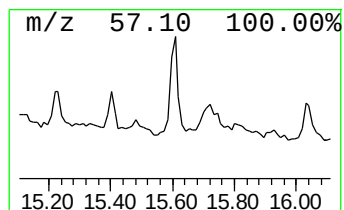
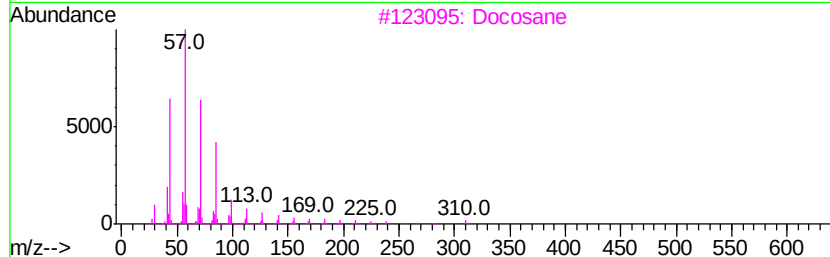
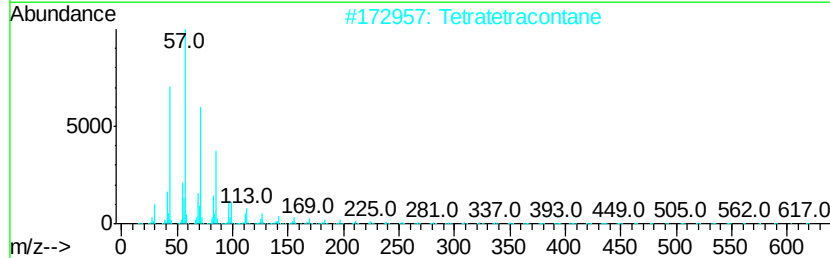
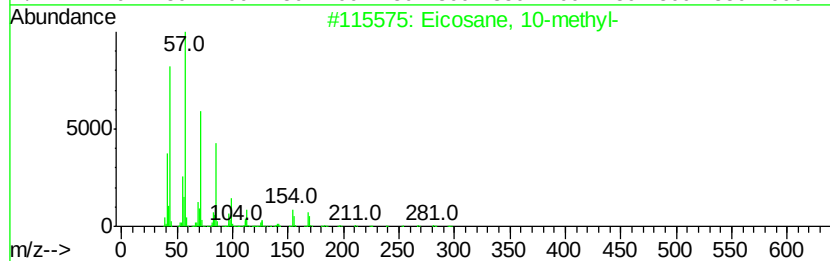
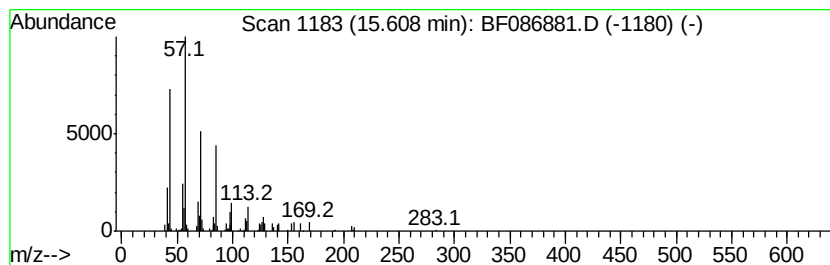
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Eicosane, 10-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	2.19 ng	72714	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	87
2		Tetratetracontane	619	C44H90	007098-22-8	86
3		Docosane	310	C22H46	000629-97-0	86
4		Nonacosane	408	C29H60	000630-03-5	86
5		Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
Data File : BF086881.D
Acq On : 11 May 2016 5:12
Operator : UM/SJ
Sample : H2916-02
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-2K

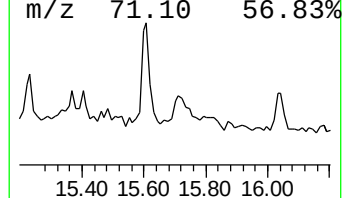
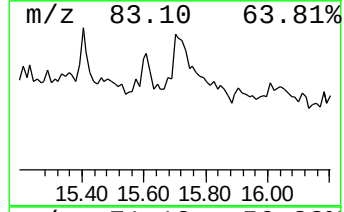
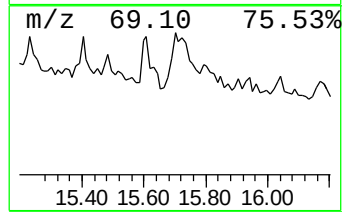
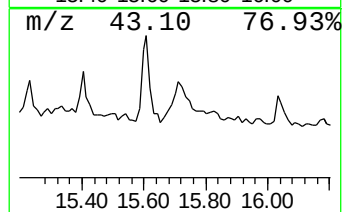
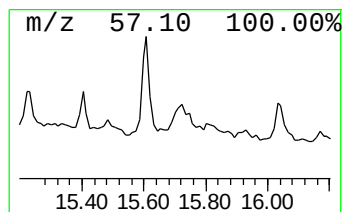
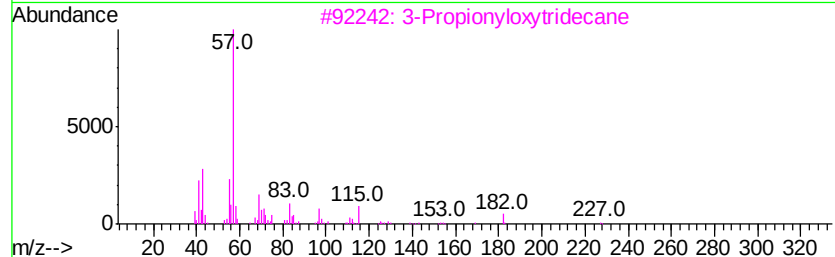
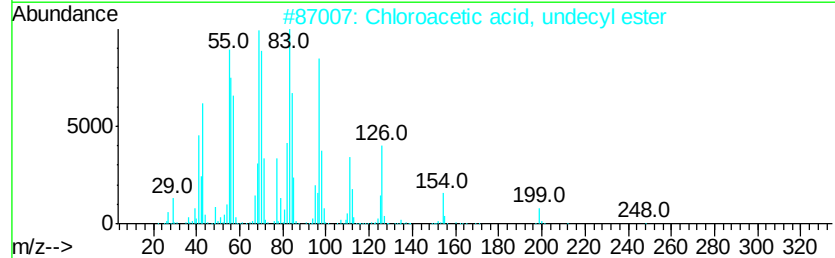
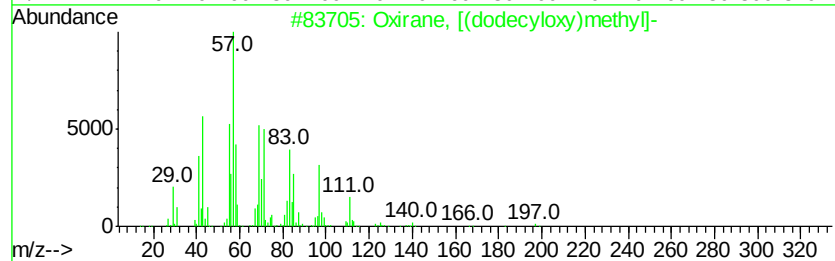
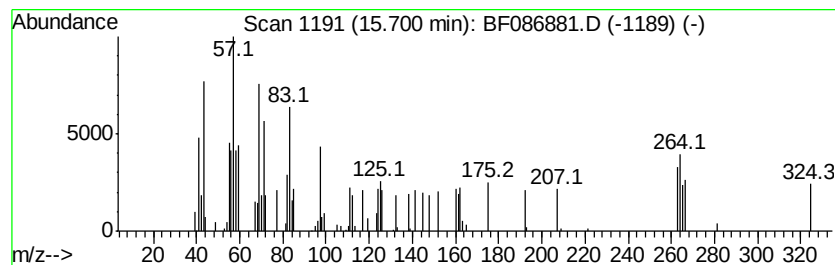
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown15.70 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	2.54 ng	84392	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	27
2		Chloroacetic acid, undecyl ester	248	C13H25ClO2	005458-29-7	25
3		3-Propionyloxytridecane	256	C16H32O2	1000245-62-5	22
4		5-Hexen-2-one, 5-methyl-	112	C7H12O	003240-09-3	22
5		Cyclopentanecarboxylic acid, 2-p...	324	C21H40O2	1000280-59-0	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
Data File : BF086881.D
Acq On : 11 May 2016 5:12
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Sample : H2916-02
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-2K

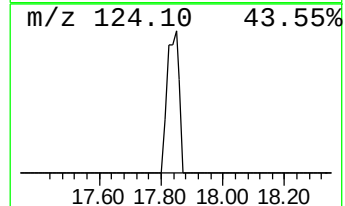
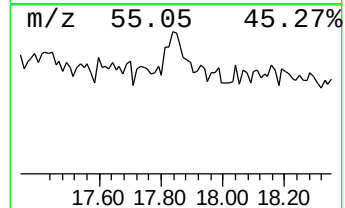
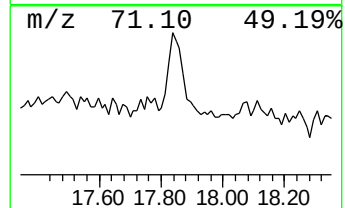
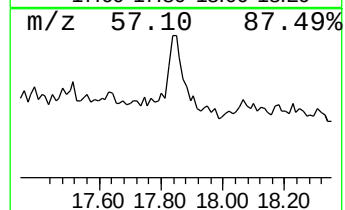
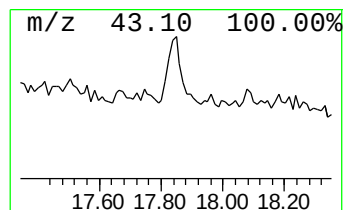
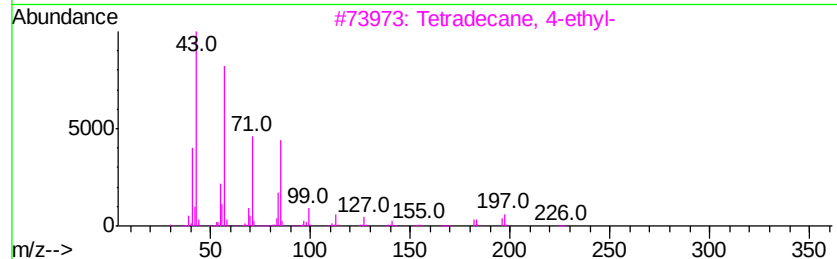
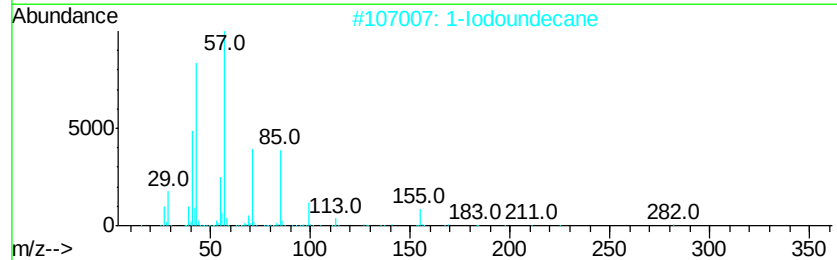
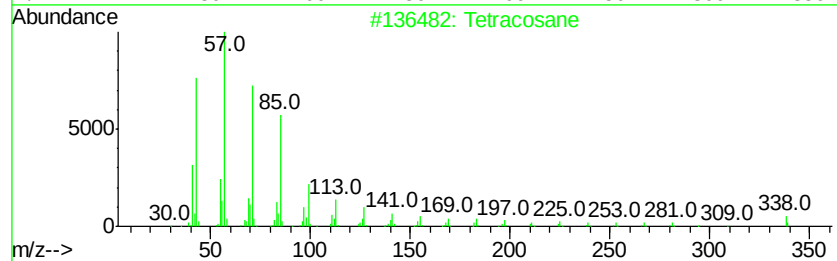
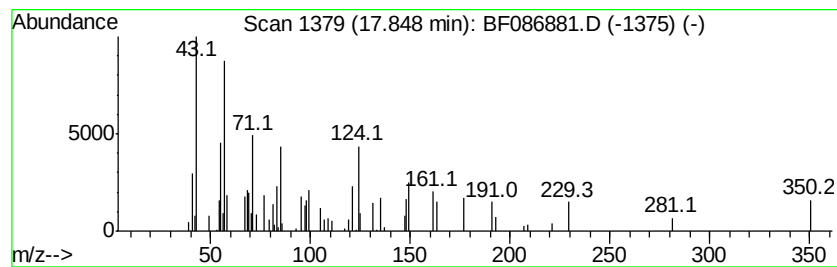
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown17.85 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	2.38 ng	78806	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	35
2		1-Iodoundecane	282	C11H23I	004282-44-4	27
3		Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	27
4		Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	25
5		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
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Acq On : 11 May 2016 5:12
Operator : UM/SJ
Sample : H2916-02
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-2K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.84	12.6	ng	620419	1	6.68	985879	20.0
unknown6.45	6.45	76.6	ng	3775750	1	6.68	985879	20.0
Hexadecane	9.66	2.4	ng	126737	3	9.72	1079700	20.0
Eicosane	11.07	2.5	ng	116049	4	11.20	942166	20.0
Dodecanoic acid	11.74	2.4	ng	113117	4	11.20	942166	20.0
1-Docosene	13.71	10.9	ng	436882	5	13.83	803468	20.0
Eicosane, 10-methyl-	15.61	2.2	ng	72714	6	15.20	663208	20.0
unknown15.70	15.70	2.5	ng	84392	6	15.20	663208	20.0
unknown17.85	17.85	2.4	ng	78806	6	15.20	663208	20.0