

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
 Data File : BF094246.D
 Acq On : 7 Apr 2017 1:52
 Operator : SJ/MA
 Sample : I2527-01
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DSN001

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-BF032217.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	3.993	351	358	361	rBV	1894515	2415094	49.75%	7.373%
2	4.375	419	423	433	rBV	1049698	1022717	21.07%	3.122%
3	5.446	601	605	613	rBV	1107023	1102895	22.72%	3.367%
4	5.593	625	630	633	rBV	2478490	2401333	49.47%	7.331%
5	5.851	669	674	678	rBV	1033556	959884	19.77%	2.930%
6	6.028	699	704	708	rBV	2954300	3018821	62.19%	9.216%
7	6.498	778	784	787	rBV	2143486	2592036	53.40%	7.913%
8	7.351	924	929	933	rBV	1387191	1337128	27.55%	4.082%
9	8.681	1148	1155	1158	rBV	4341404	4854318	100.00%	14.819%
10	9.169	1235	1238	1243	rBV	56468	56843	1.17%	0.174%
11	9.492	1285	1293	1303	rVB2	1412951	1485135	30.59%	4.534%
12	10.463	1453	1458	1469	rBV	1324302	1322488	27.24%	4.037%
13	10.610	1479	1483	1488	rBV	64879	64973	1.34%	0.198%
14	10.669	1488	1493	1496	rBV	68697	76500	1.58%	0.234%
15	11.316	1598	1603	1607	rBV	1412851	1373818	28.30%	4.194%
16	12.980	1881	1886	1892	rBV	1788290	1826998	37.64%	5.577%
17	13.298	1934	1940	1944	rBV2	3562962	4279151	88.15%	13.063%
18	14.463	2133	2138	2147	rBV6	30790	71580	1.47%	0.219%
19	14.563	2151	2155	2159	rBV	932298	972433	20.03%	2.969%
20	15.957	2389	2392	2397	rVB	43074	49672	1.02%	0.152%
21	16.192	2427	2432	2439	rBV	674614	785127	16.17%	2.397%
22	16.315	2448	2453	2459	rBV2	76051	129740	2.67%	0.396%
23	16.709	2515	2520	2525	rBV	75648	112394	2.32%	0.343%
24	17.162	2592	2597	2603	rBV	71845	122406	2.52%	0.374%
25	17.686	2680	2686	2695	rBV3	56756	124647	2.57%	0.381%
26	18.298	2784	2790	2800	rVB5	48454	118342	2.44%	0.361%
27	19.027	2907	2914	2923	rVB4	28985	81180	1.67%	0.248%

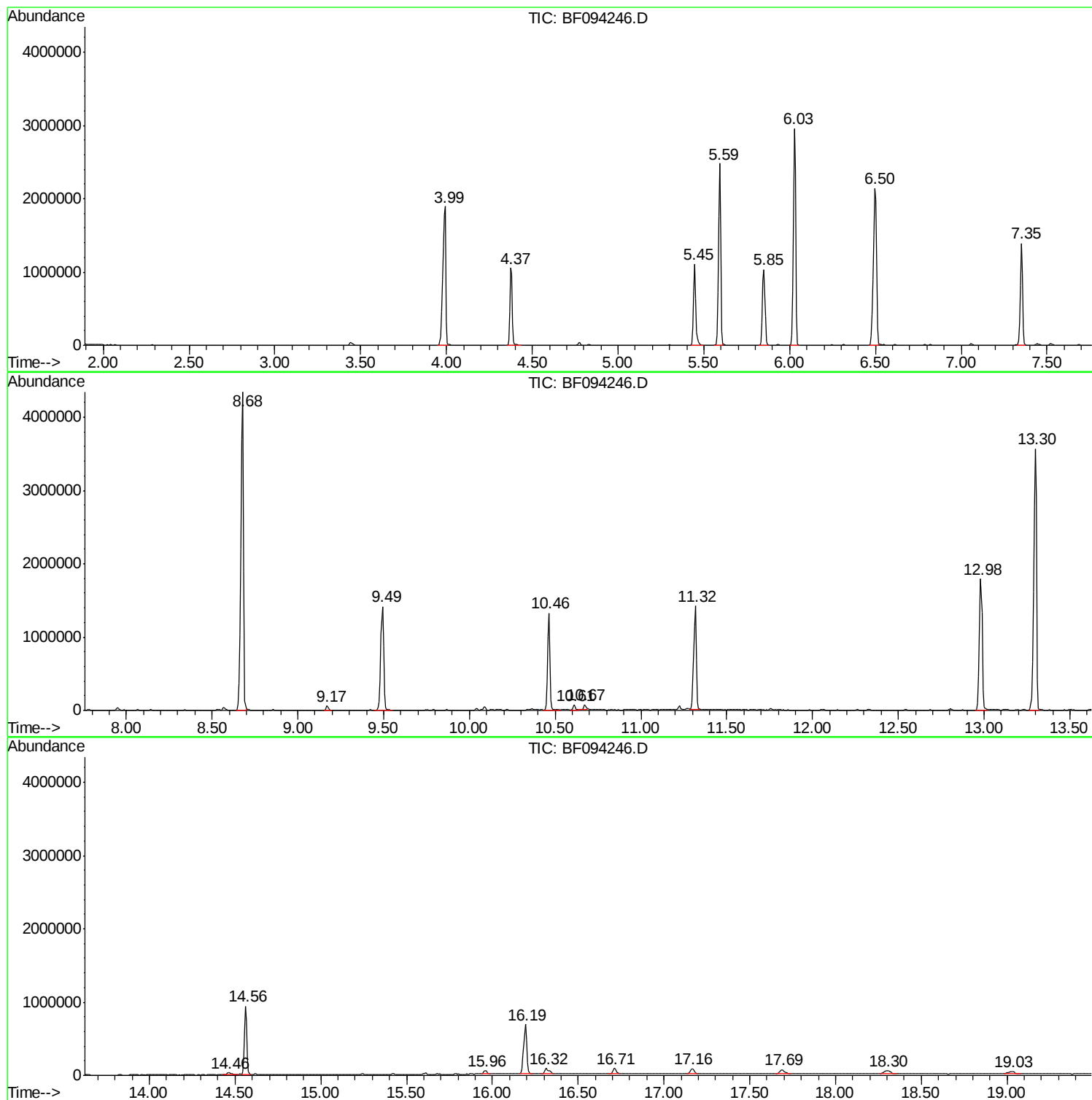
Sum of corrected areas: 32757653

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

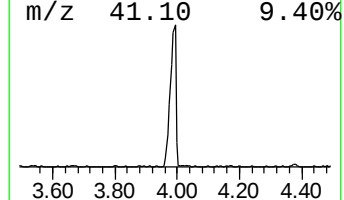
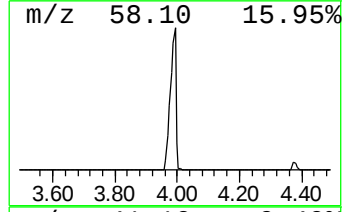
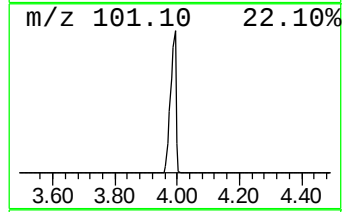
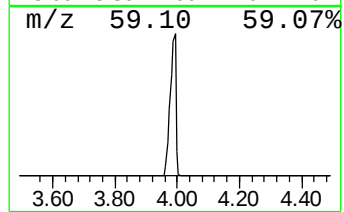
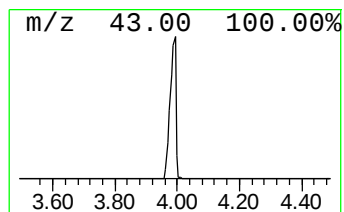
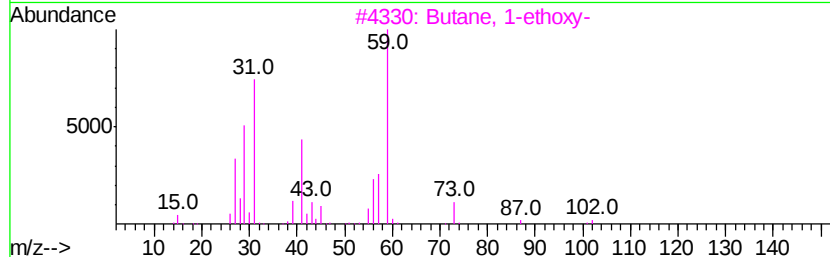
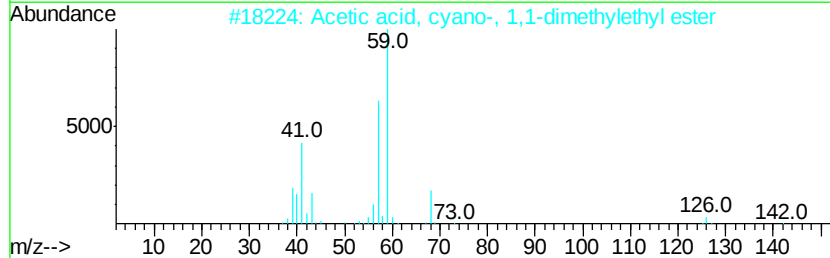
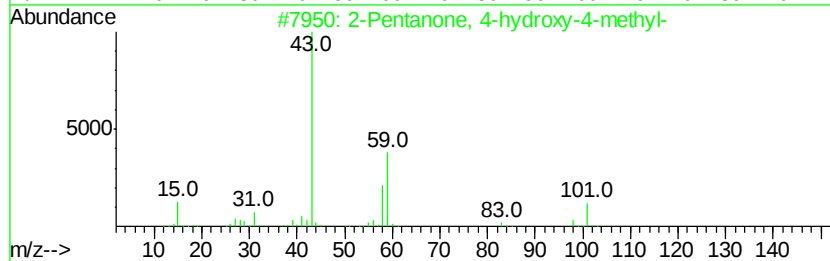
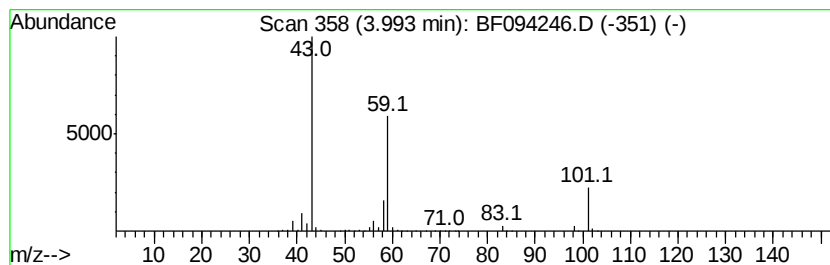
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	50.32 ng	2415090	1,4-Dichlorobenzene-d4	5.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25		
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

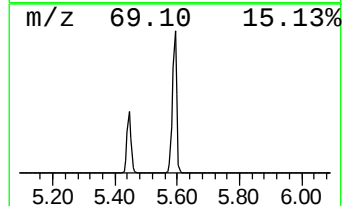
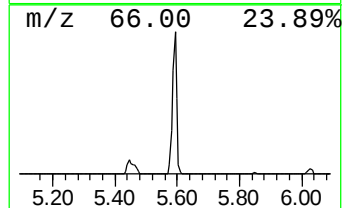
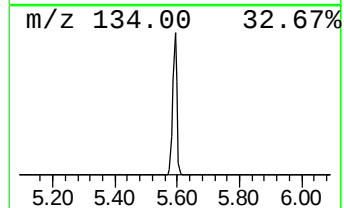
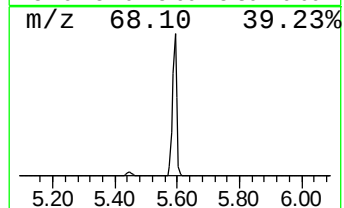
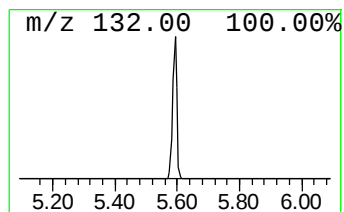
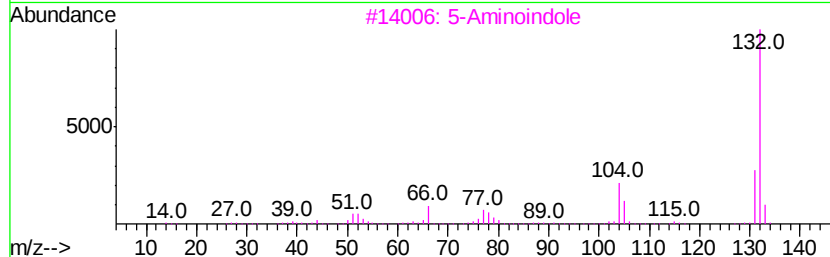
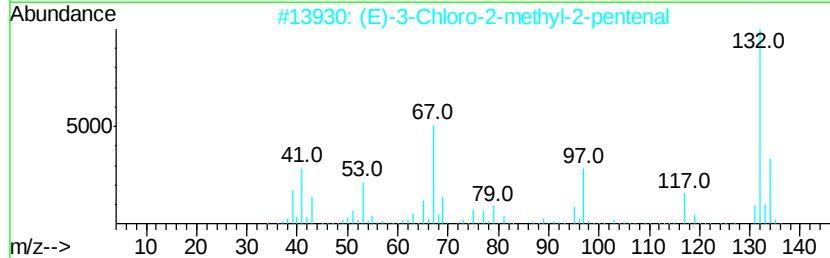
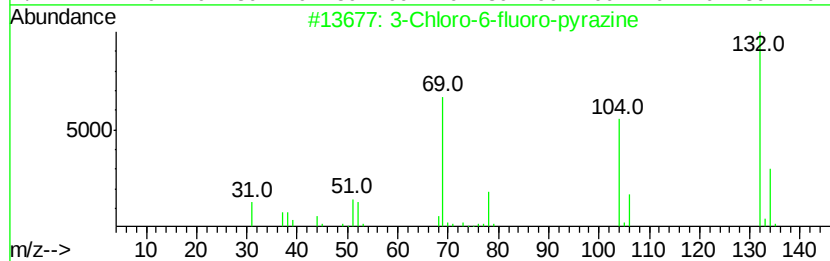
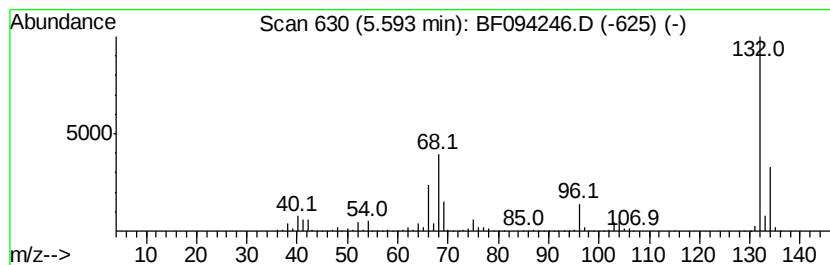
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.59 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	50.03 ng	2401330	1,4-Dichlorobenzene-d4	5.85

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	16
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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

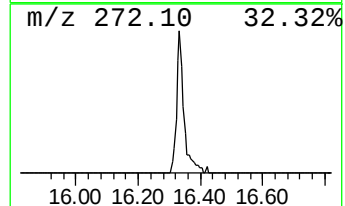
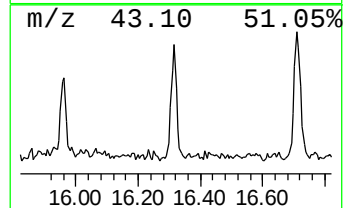
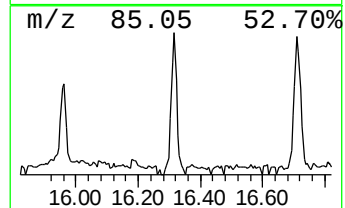
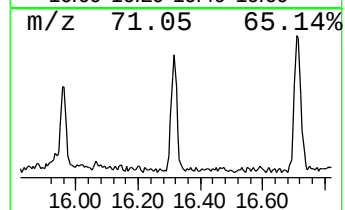
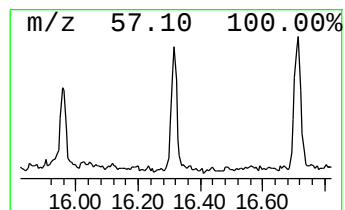
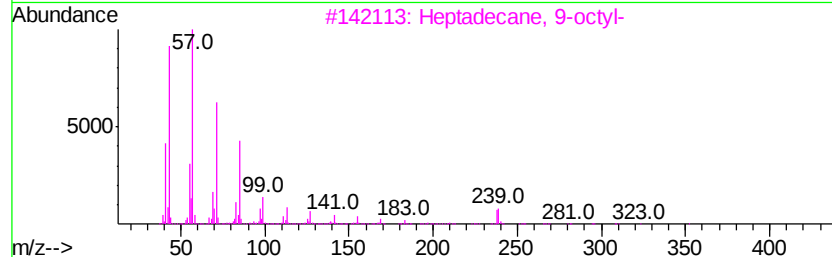
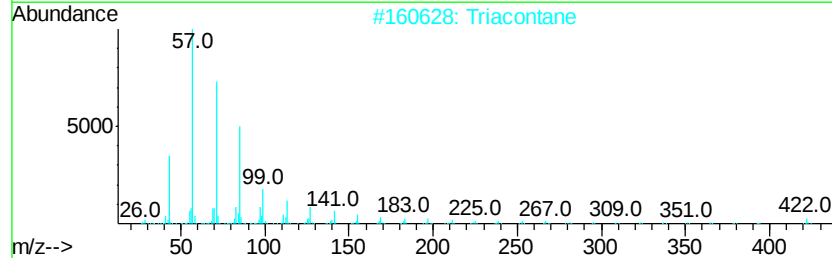
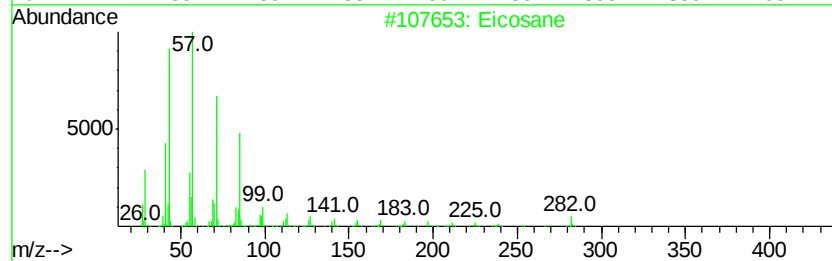
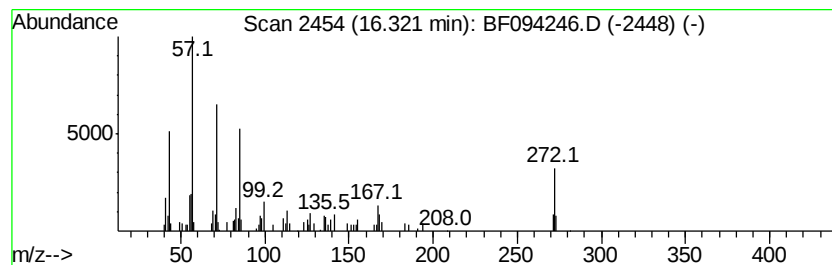
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	3.30 ng	129740	Perylene-d12	16.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	93
2	Triacontane		422	C30H62	000638-68-6	83
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	83
4	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	83
5	Heneicosane		296	C21H44	000629-94-7	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

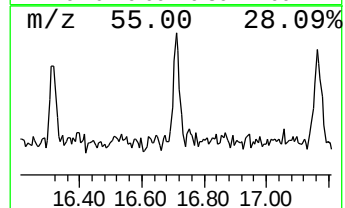
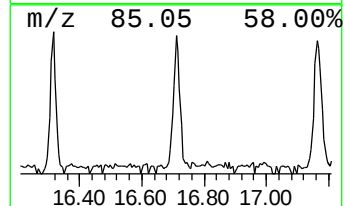
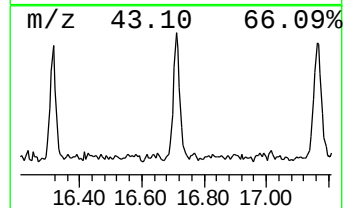
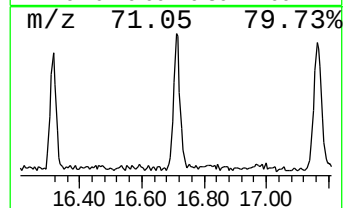
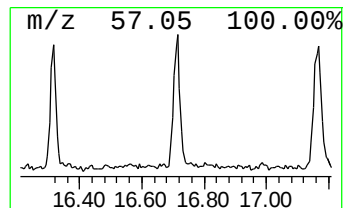
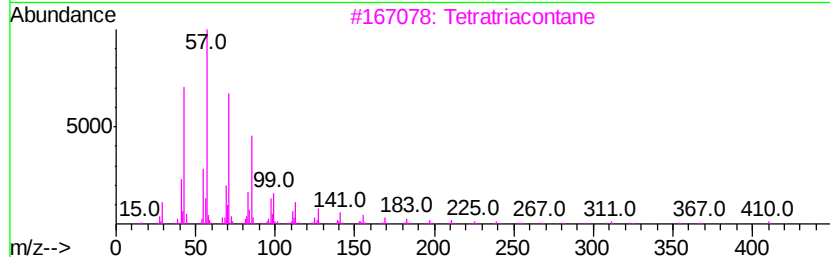
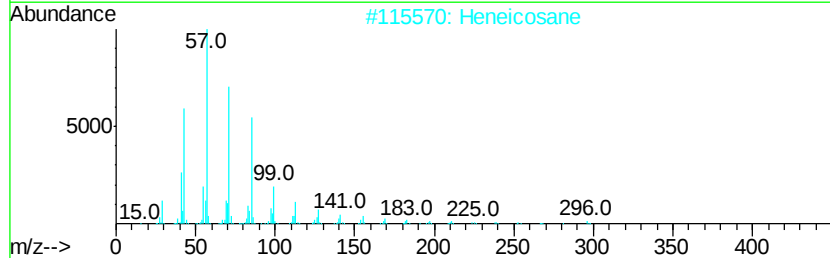
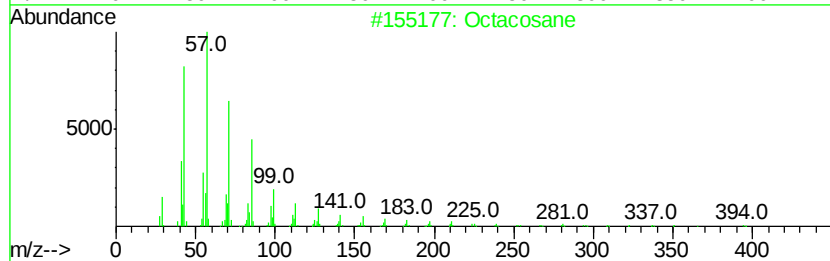
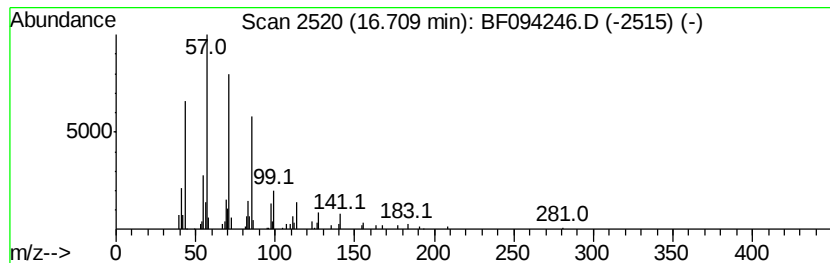
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	2.86 ng	112394	Perylene-d12	16.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Tetratriacontane		479	C34H70	014167-59-0	91
4	Pentacosane		352	C25H52	000629-99-2	91
5	Octadecane, 3-ethyl-5-(2-ethylbu...		366	C26H54	055282-12-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

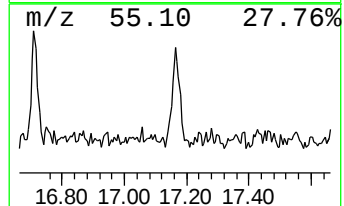
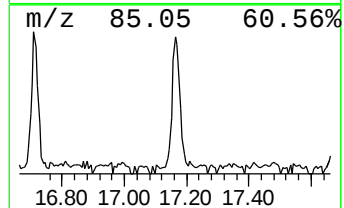
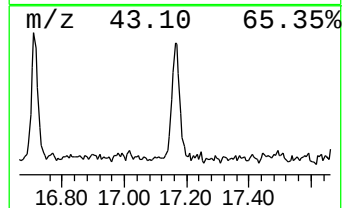
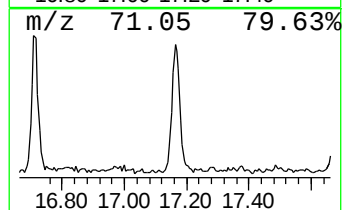
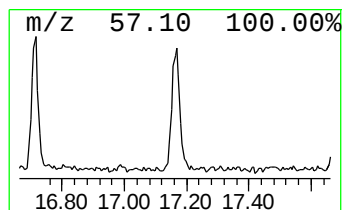
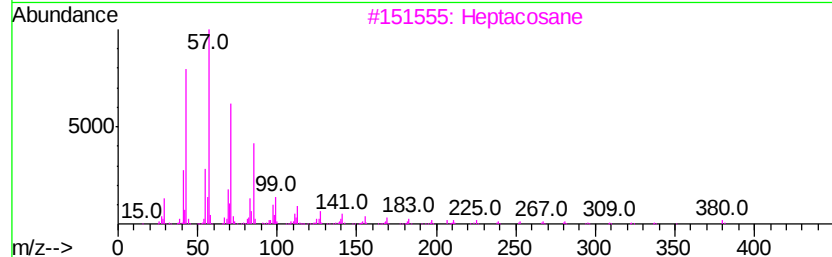
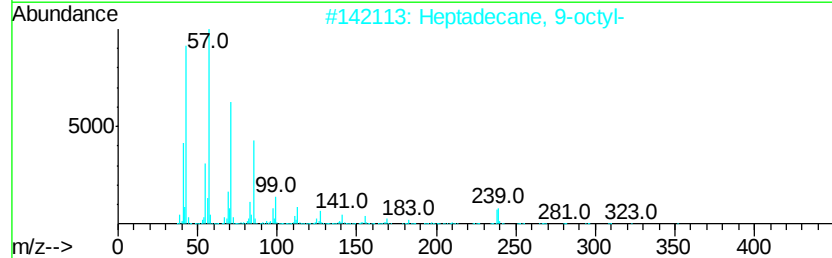
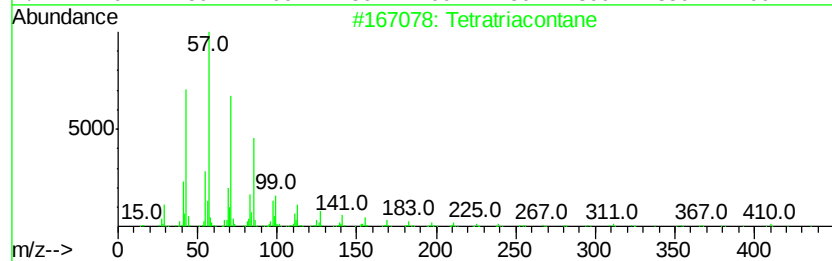
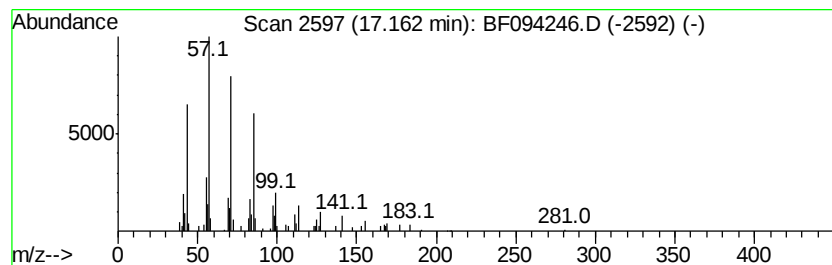
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetratriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	3.12 ng	122406	Perylene-d12	16.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

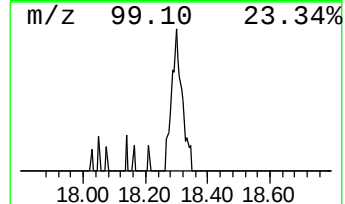
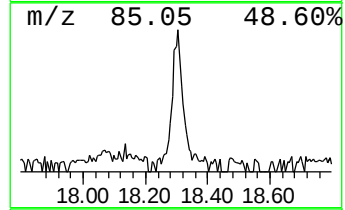
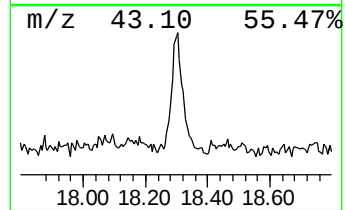
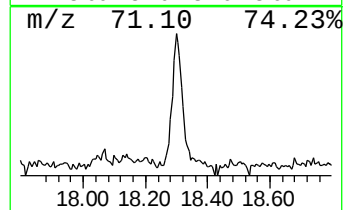
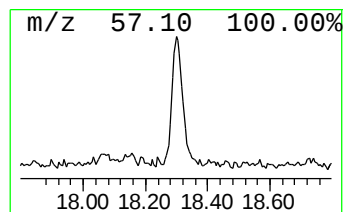
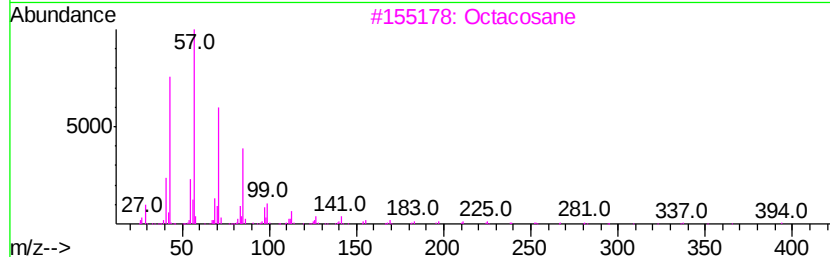
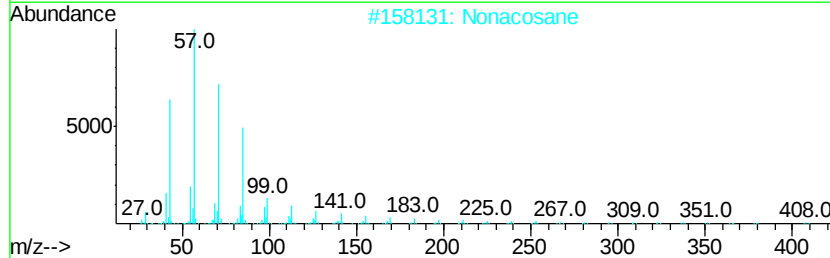
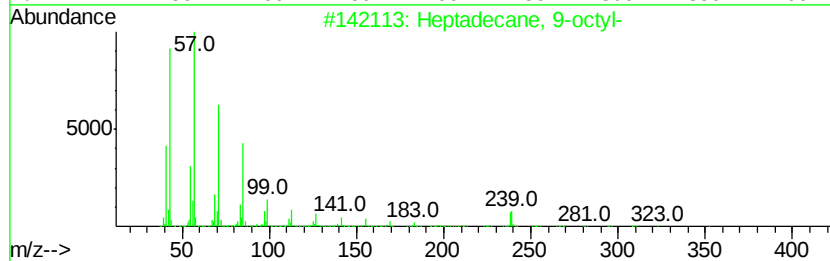
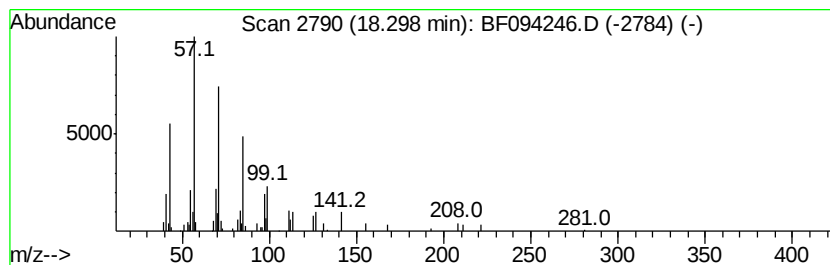
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.01 ng	118342	Perylene-d12	16.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
2		Nonacosane	408	C29H60	000630-03-5	72
3		Octacosane	394	C28H58	000630-02-4	72
4		triacontane	422	C30H62	000638-68-6	72
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

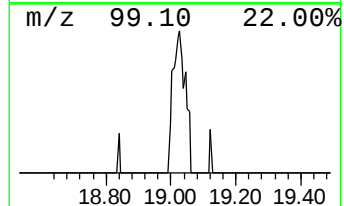
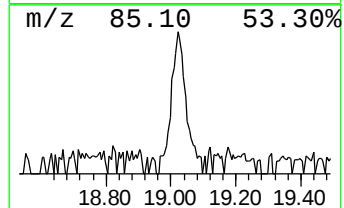
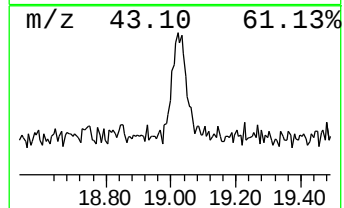
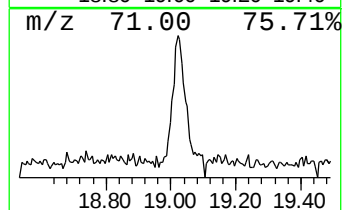
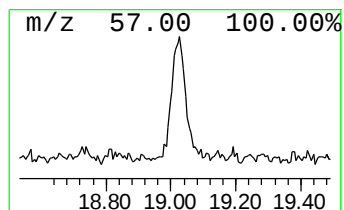
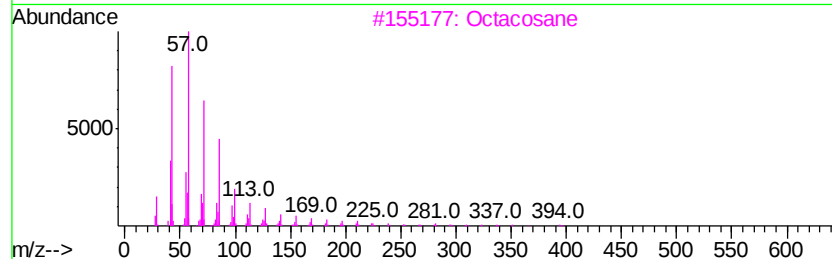
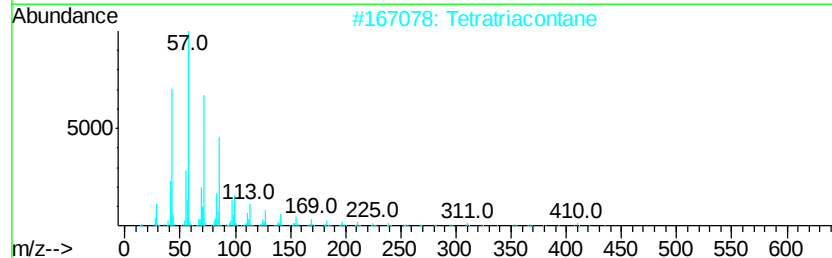
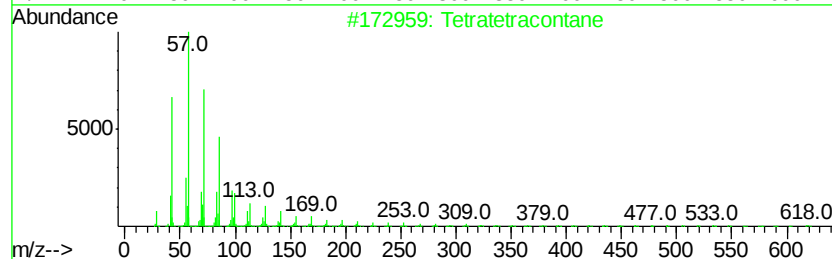
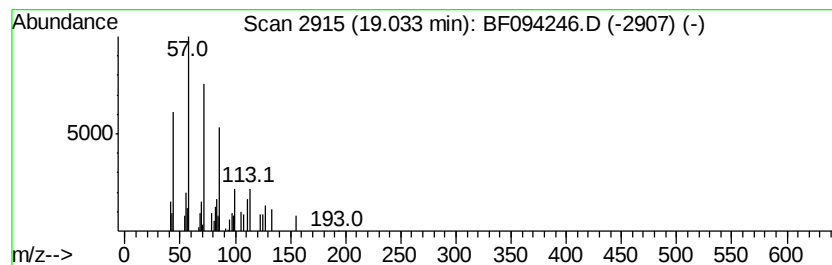
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	2.07 ng	81180	Perylene-d12	16.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	90
2		Tetratriacontane	479	C34H70	014167-59-0	86
3		Octacosane	394	C28H58	000630-02-4	86
4		Heneicosane	296	C21H44	000629-94-7	80
5		Pentacosane	352	C25H52	000629-99-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040617\
Data File : BF094246.D
Acq On : 7 Apr 2017 1:52
Operator : SJ/MA
Sample : I2527-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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...	3.99	50.3	ng	2415090	1	5.85	959884	20.0
unknown5.59	5.59	50.0	ng	2401330	1	5.85	959884	20.0
Eicosane	16.32	3.3	ng	129740	6	16.19	785127	20.0
Octacosane	16.71	2.9	ng	112394	6	16.19	785127	20.0
Tetratriacontane	17.16	3.1	ng	122406	6	16.19	785127	20.0
Heptadecane, 9-oc...	18.30	3.0	ng	118342	6	16.19	785127	20.0
Tetratetracontane	19.03	2.1	ng	81180	6	16.19	785127	20.0