

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
 Data File : BF099994.D
 Acq On : 31 Oct 2017 7:09
 Operator : SJ/JU
 Sample : I6201-04
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CF-1B(4-5)

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-BF102317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	493	496	523	rVB	155186	267881	13.97%	1.539%
2	5.410	562	565	584	rBV	1581070	1728631	90.13%	9.933%
3	6.434	735	739	757	rBV	1616465	1820159	94.90%	10.459%
4	6.557	757	760	769	rVB	1892935	1812147	94.48%	10.413%
5	6.786	796	799	809	rBV	493445	435490	22.71%	2.502%
6	6.939	822	825	839	rVB	1539612	1367693	71.31%	7.859%
7	7.357	892	896	910	rBV	1144994	1066267	55.59%	6.127%
8	8.069	1014	1017	1023	rBV	690927	598917	31.23%	3.442%
9	8.475	1083	1086	1088	rBV	34761	24811	1.29%	0.143%
10	8.633	1109	1113	1119	rBV	25042	33309	1.74%	0.191%
11	9.075	1185	1188	1191	rBV	50623	41809	2.18%	0.240%
12	9.145	1195	1200	1203	rVV	2091561	1917997	100.00%	11.021%
13	9.210	1207	1211	1216	rVB4	28590	37915	1.98%	0.218%
14	9.539	1261	1267	1275	rBV	316942	320765	16.72%	1.843%
15	9.680	1285	1291	1293	rBV5	17308	24823	1.29%	0.143%
16	9.822	1312	1315	1321	rBV	724456	662678	34.55%	3.808%
17	10.069	1354	1357	1360	rBV3	22496	24581	1.28%	0.141%
18	10.139	1365	1369	1373	rBV4	20004	25791	1.34%	0.148%
19	10.463	1419	1424	1426	rBV2	55528	56655	2.95%	0.326%
20	10.539	1435	1437	1441	rBV	90387	71099	3.71%	0.409%
21	10.621	1447	1451	1465	rBV	1161331	1121655	58.48%	6.445%
22	10.727	1465	1469	1477	rVB	114796	110913	5.78%	0.637%
23	11.192	1544	1548	1555	rVB	55387	62940	3.28%	0.362%
24	11.321	1566	1570	1579	rBV	666101	655557	34.18%	3.767%
25	11.833	1654	1657	1662	rBV2	30468	32390	1.69%	0.186%
26	12.710	1803	1806	1809	rVB	36094	25869	1.35%	0.149%
27	12.904	1835	1839	1842	rBV	1770286	1640679	85.54%	9.428%
28	13.786	1985	1989	2003	rBV	84167	106830	5.57%	0.614%
29	13.974	2018	2021	2032	rBV	452637	452028	23.57%	2.597%
30	14.109	2040	2044	2051	rBV	20908	20415	1.06%	0.117%
31	14.421	2094	2097	2102	rBV2	21586	25279	1.32%	0.145%
32	14.733	2146	2150	2153	rVB2	22060	23023	1.20%	0.132%
33	14.874	2170	2174	2180	rBV	88604	88432	4.61%	0.508%
34	15.056	2202	2205	2212	rBV	19914	23446	1.22%	0.135%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.468	2271	2275	2286	rVB	284763	390829	20.38%	2.246%
36	15.633	2297	2303	2307	rBV	52325	68319	3.56%	0.393%
37	16.633	2465	2473	2481	rBV6	19048	41539	2.17%	0.239%
38	16.992	2528	2534	2542	rBV2	90799	173003	9.02%	0.994%

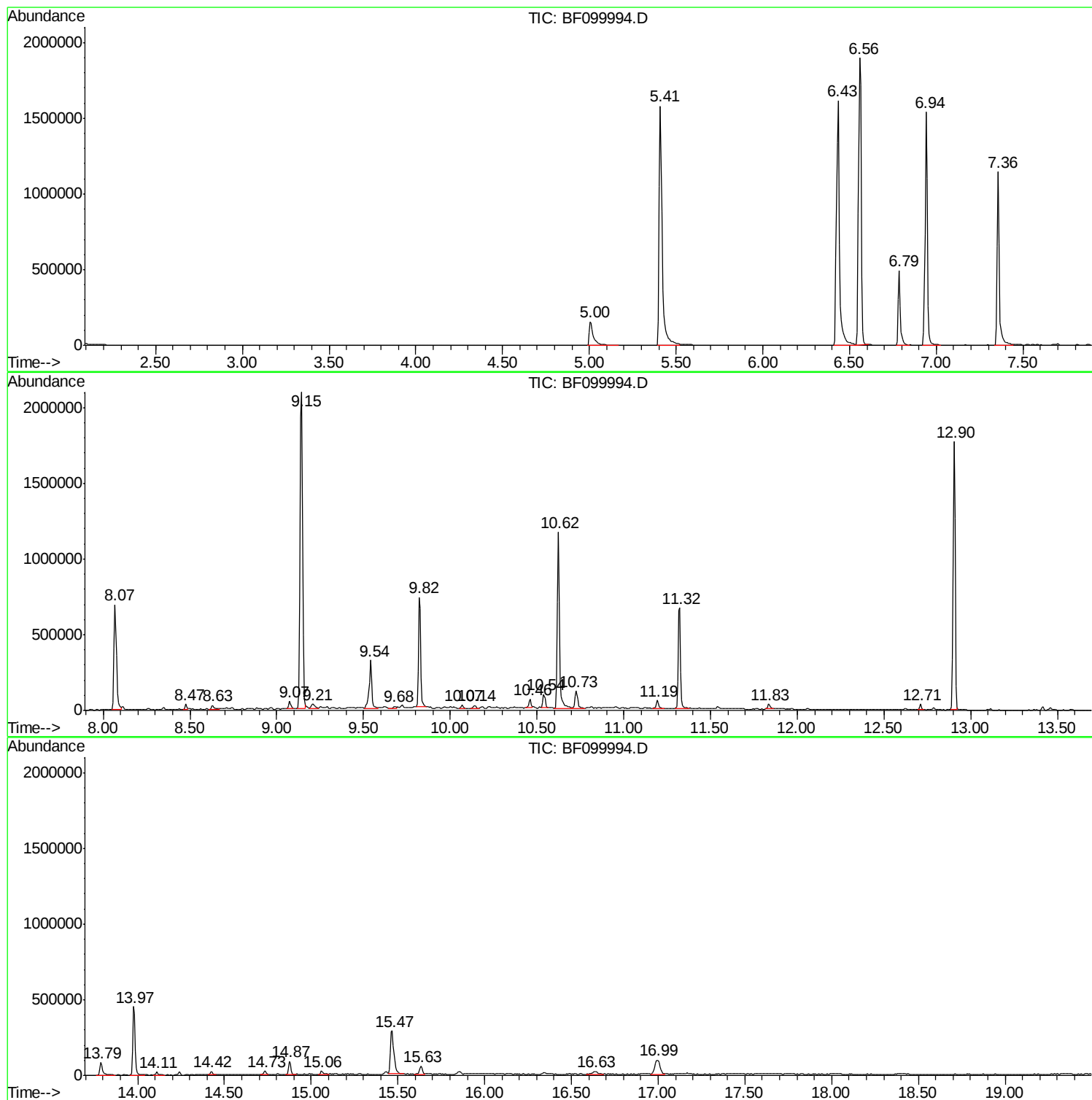
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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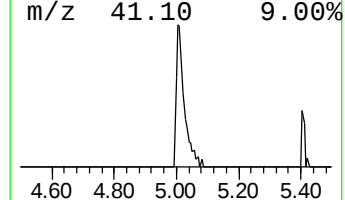
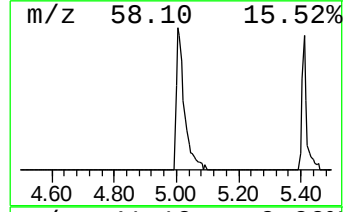
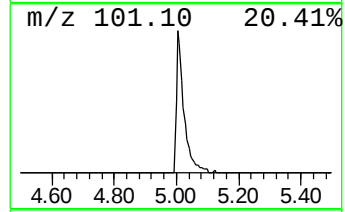
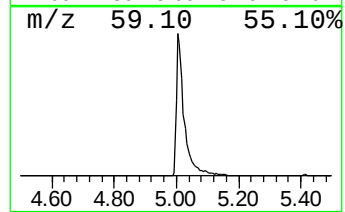
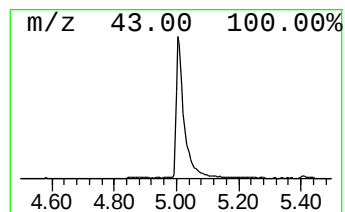
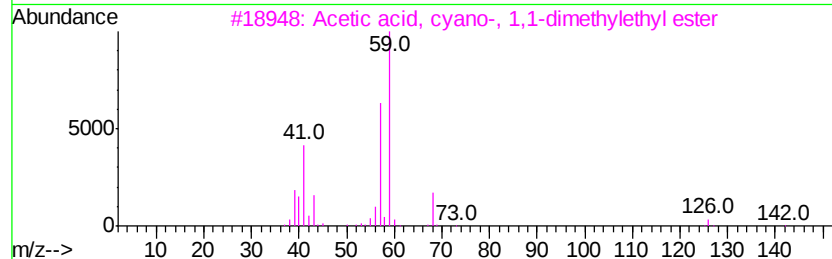
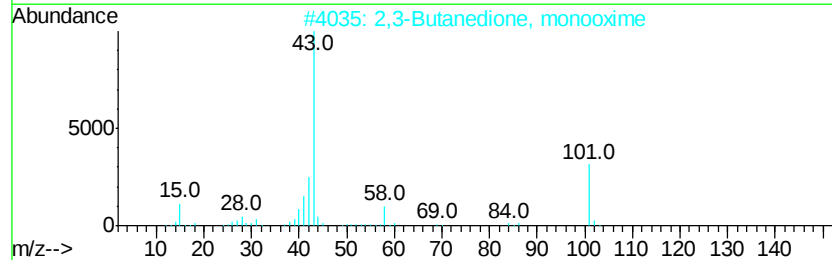
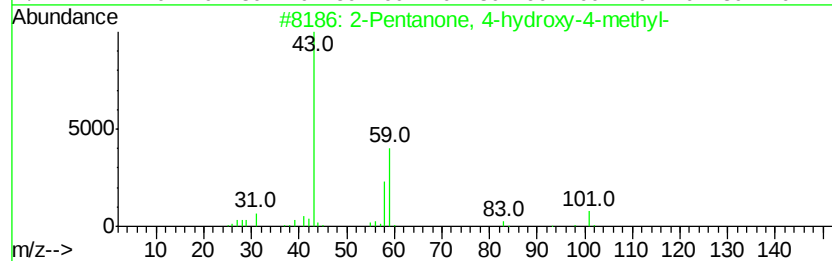
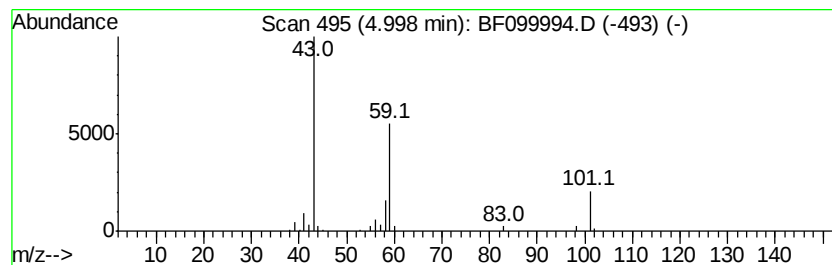
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	12.30 ng	267881	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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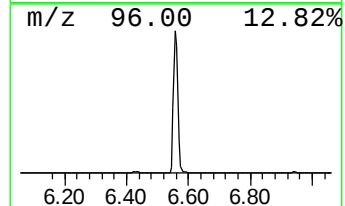
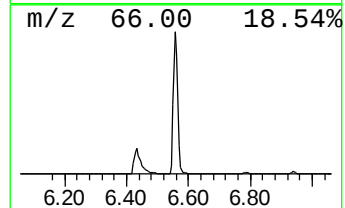
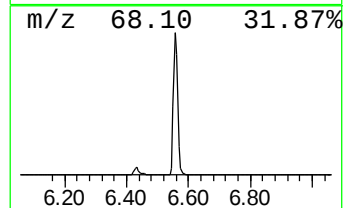
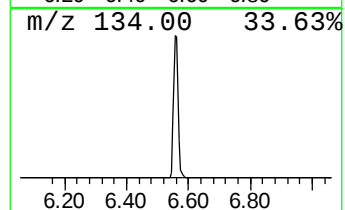
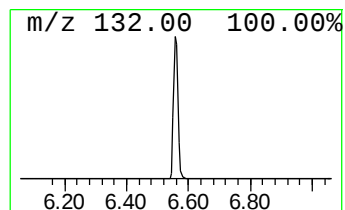
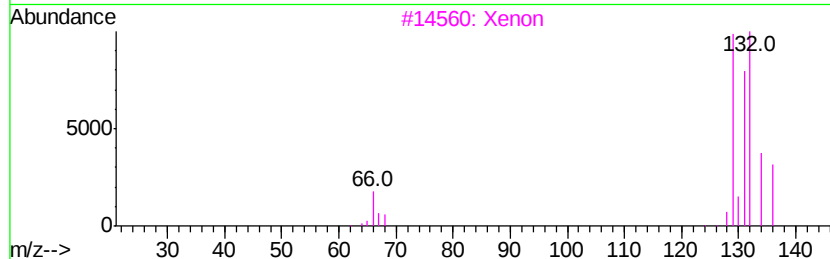
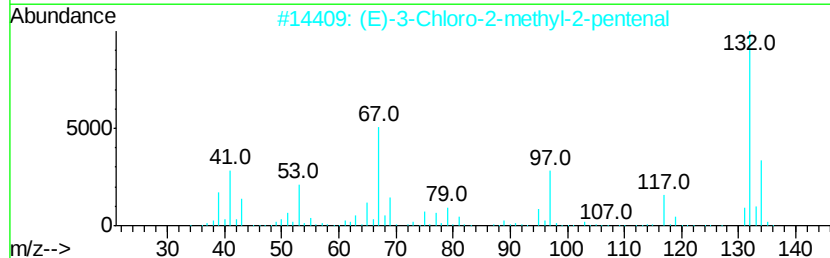
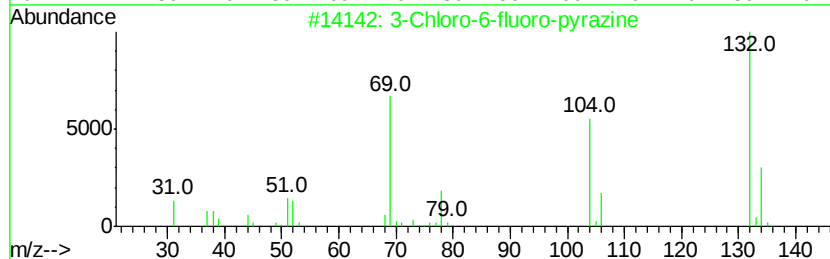
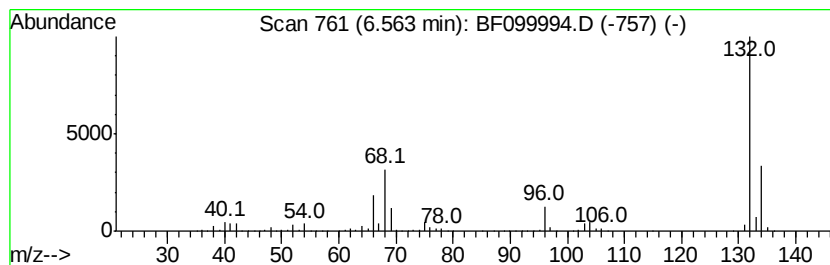
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	83.22 ng	1812150	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Xenon	132	Xe	007440-63-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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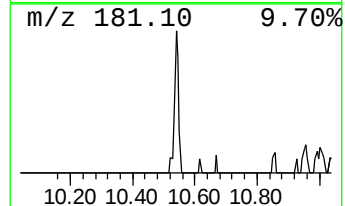
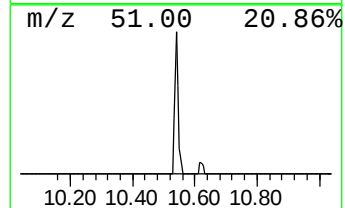
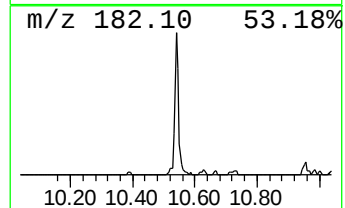
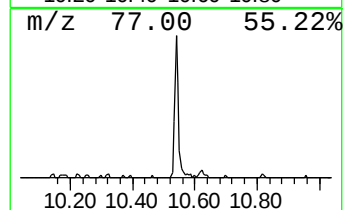
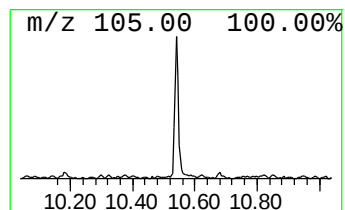
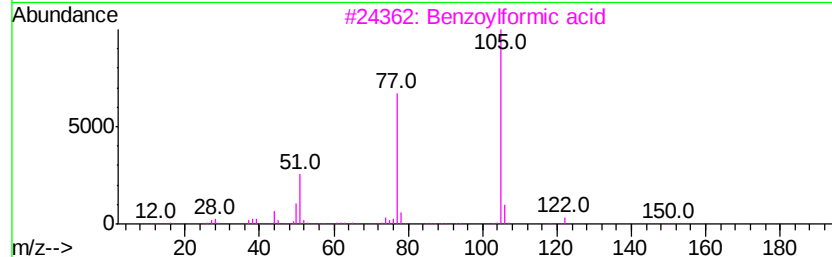
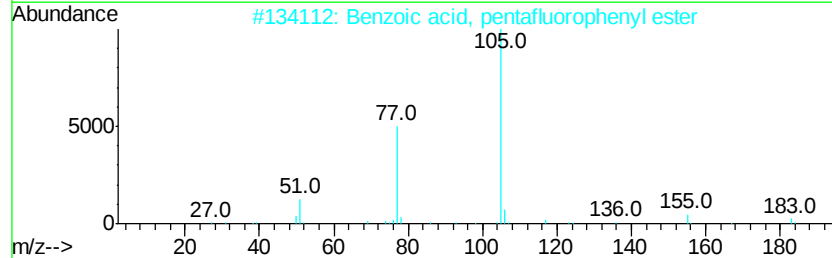
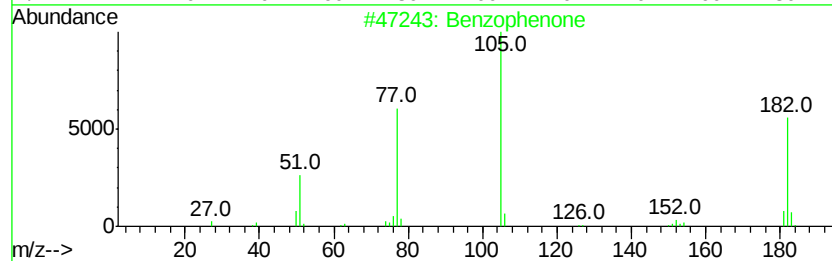
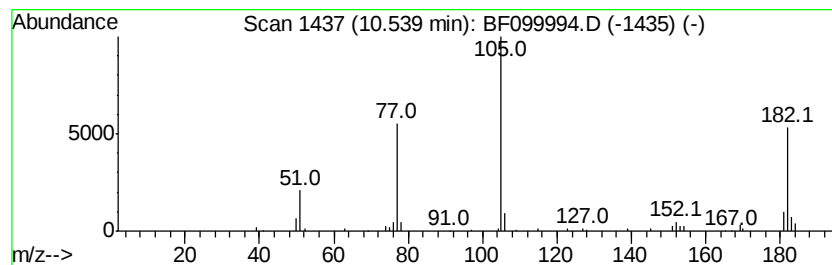
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	2.15 ng	71099	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
3		Benzovlformic acid	150	C8H6O3	000611-73-4	43
4		Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43
5		S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	43



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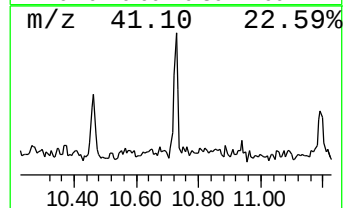
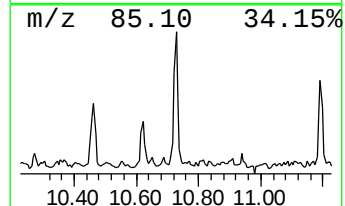
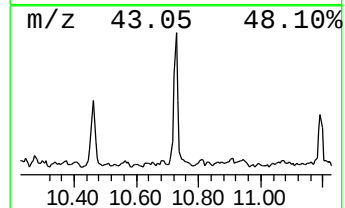
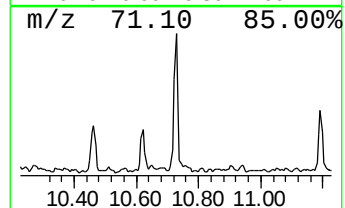
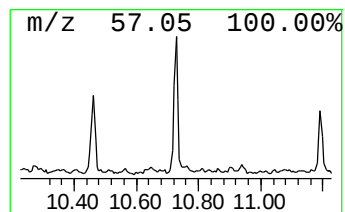
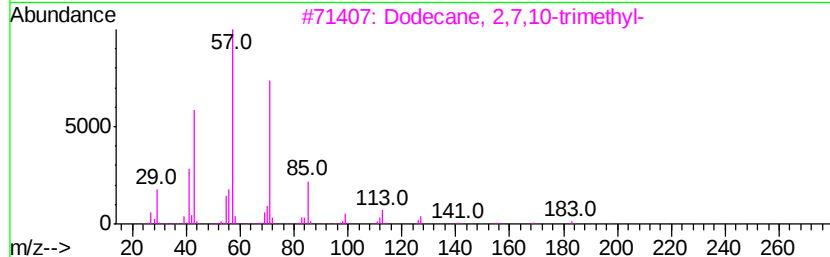
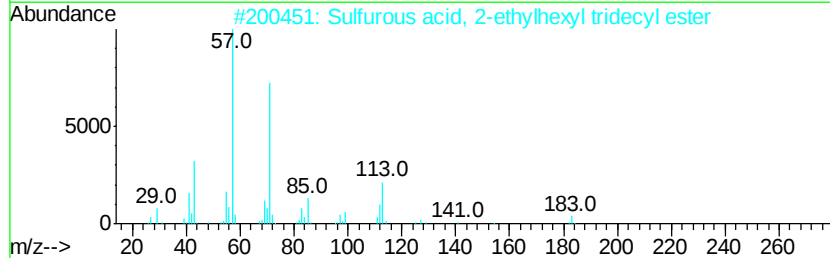
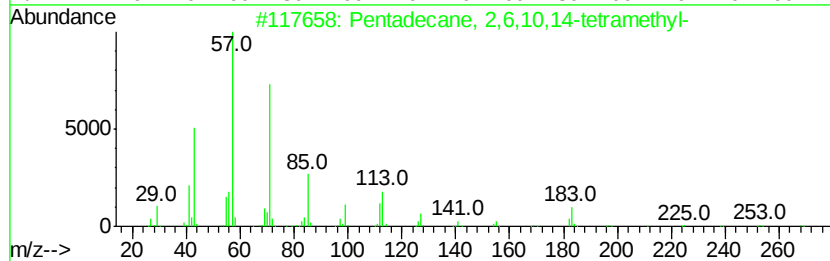
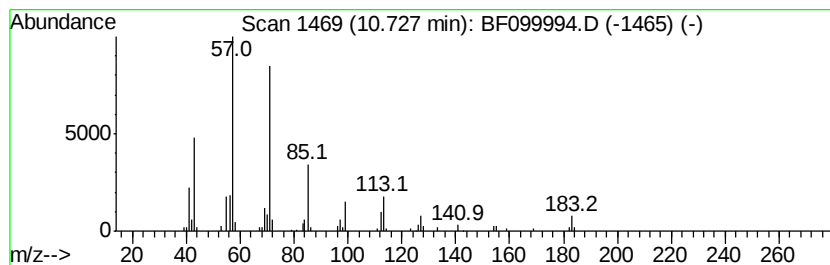
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecane, 2,6,10,14-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	3.38 ng	110913	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
2		Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	80
3		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
5		Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	80



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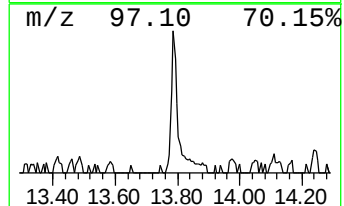
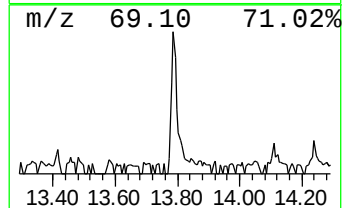
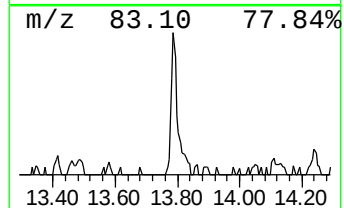
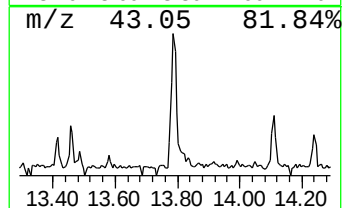
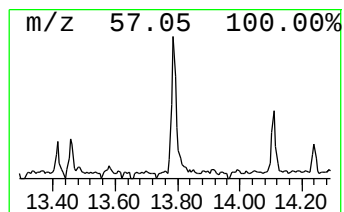
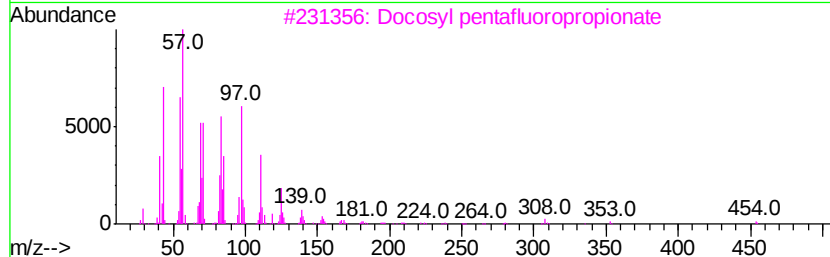
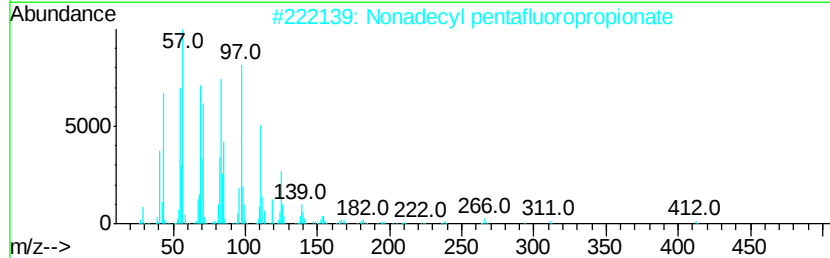
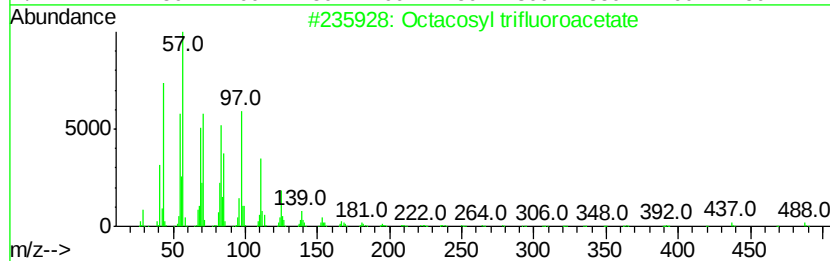
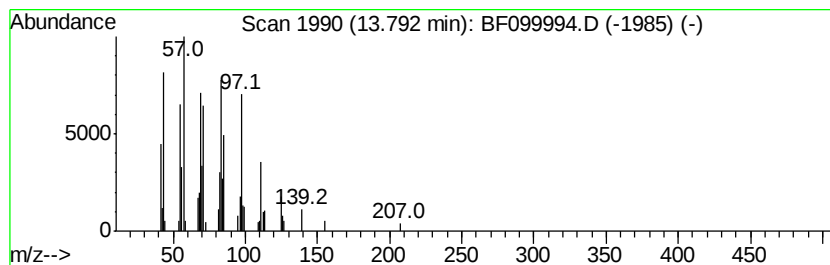
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Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	4.73 ng	106830	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	93
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
4		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
5		Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099994.D
Acq On : 31 Oct 2017 7:09
Operator : SJ/JU
Sample : I6201-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

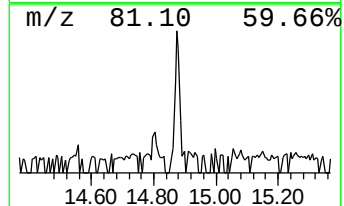
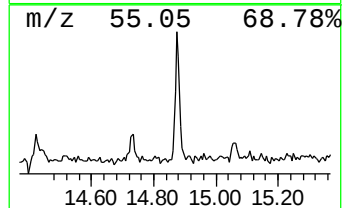
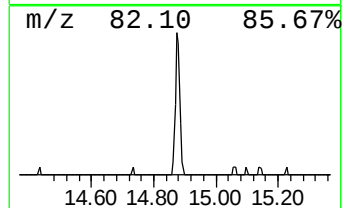
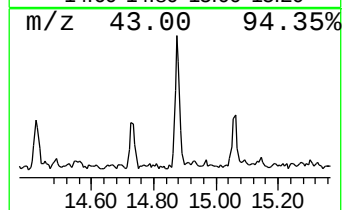
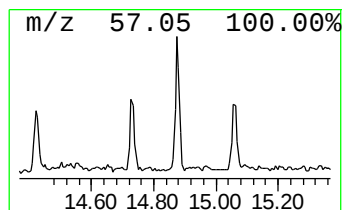
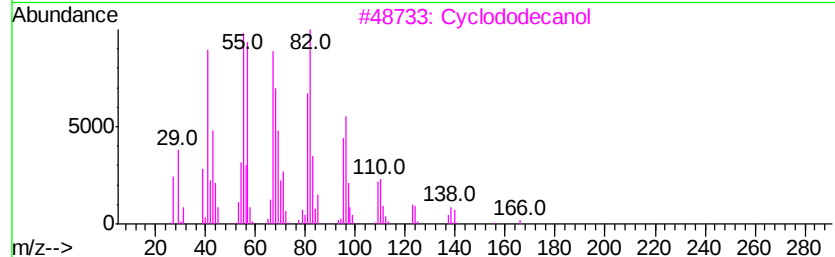
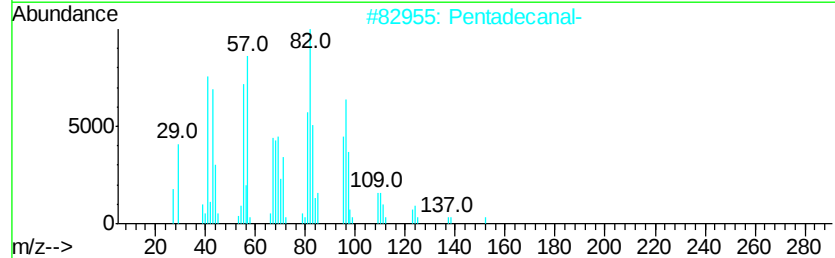
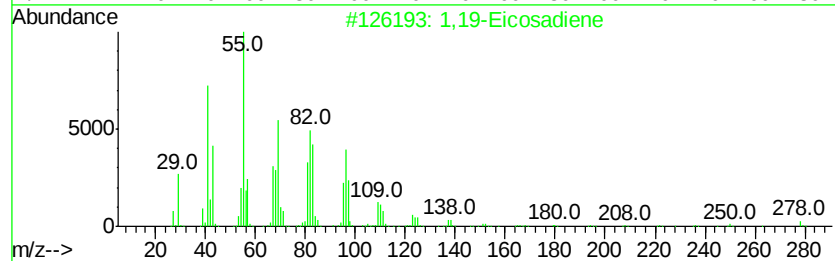
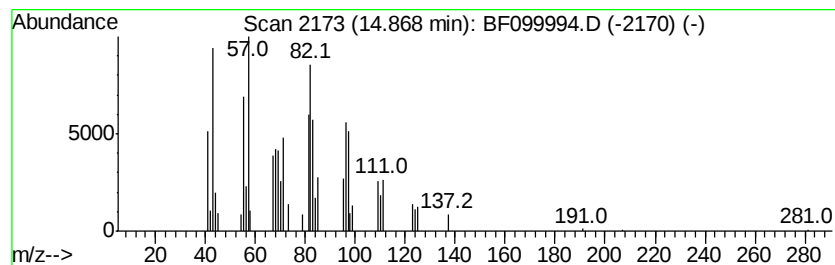
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ClientSampleId :
CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,19-Eicosadiene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.87	4.53 ng	88432	Perylene-d12		15.47
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	80
2	Pentadecanal-	226	C15H30O	002765-11-9	72
3	Cyclododecanol	184	C12H24O	001724-39-6	53
4	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	43
5	1-Heptacosanol	396	C27H56O	002004-39-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
Data File : BF099994.D
Acq On : 31 Oct 2017 7:09
Operator : SJ/JU
Sample : I6201-04
Misc :
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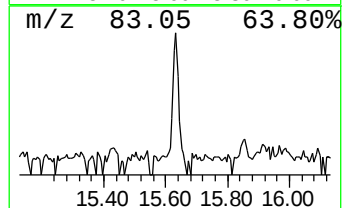
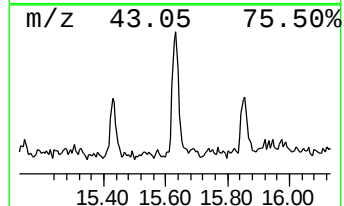
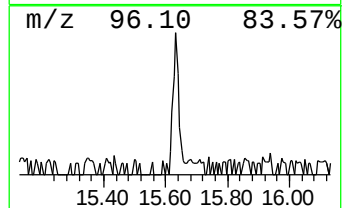
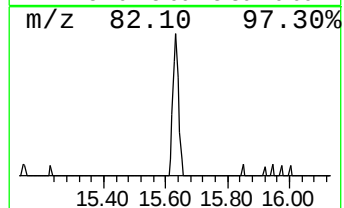
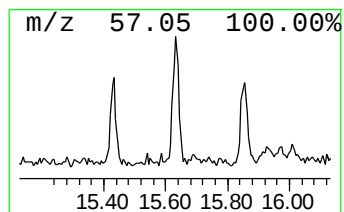
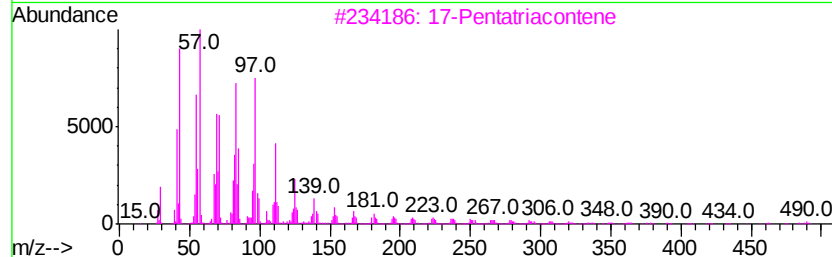
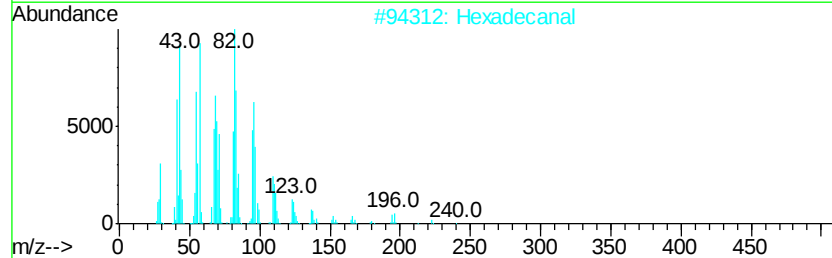
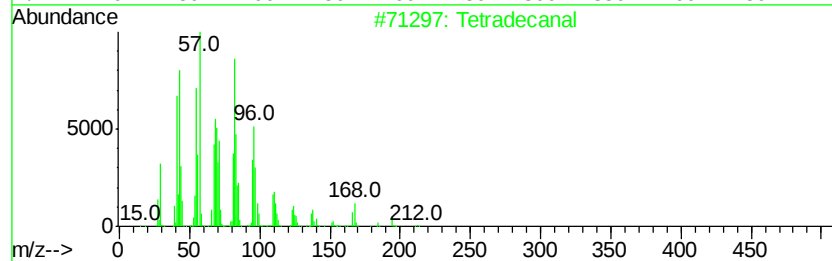
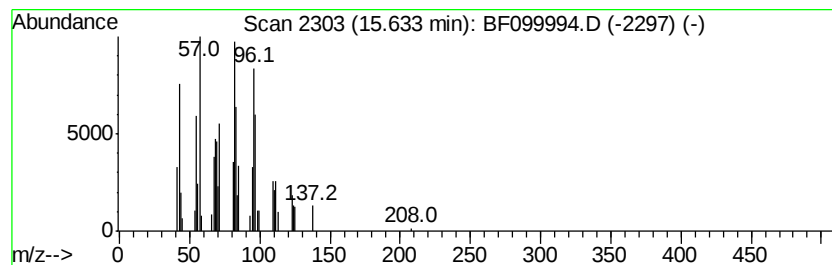
Instrument :
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ClientSampleId :
CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.63	3.50 ng	68319	Perylene-d12	15.47	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanal	212	C14H28O	000124-25-4	64
2	Hexadecanal	240	C16H32O	000629-80-1	52
3	17-Pentatriacontene	491	C35H70	006971-40-0	49
4	1-Hentetracontanol	593	C41H84O	040710-42-7	43
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
Data File : BF099994.D
Acq On : 31 Oct 2017 7:09
Operator : SJ/JU
Sample : I6201-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-1B(4-5)

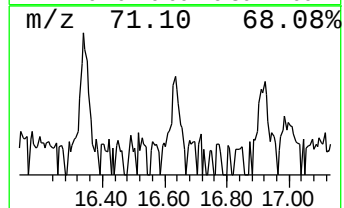
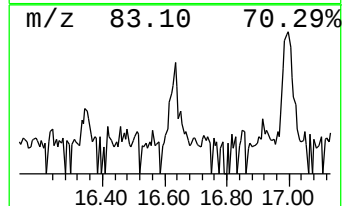
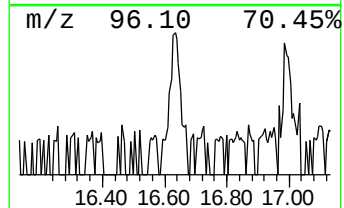
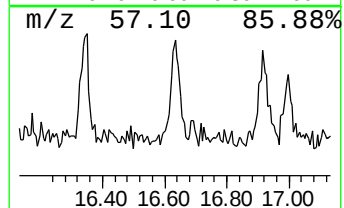
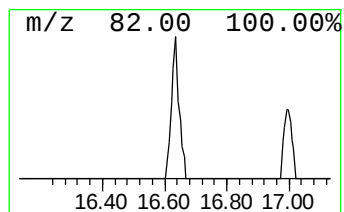
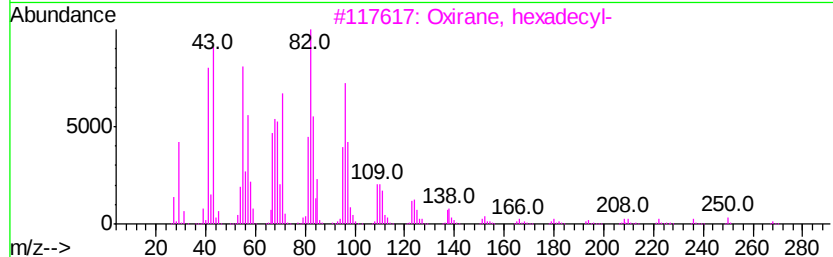
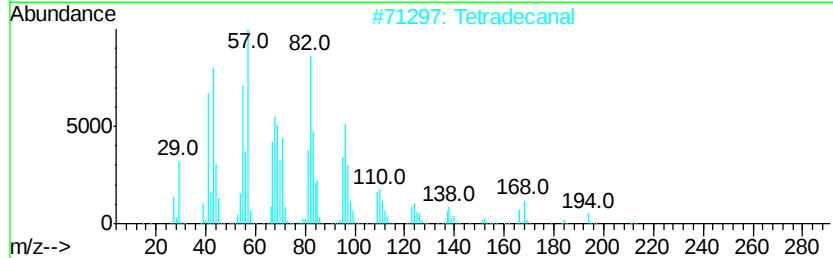
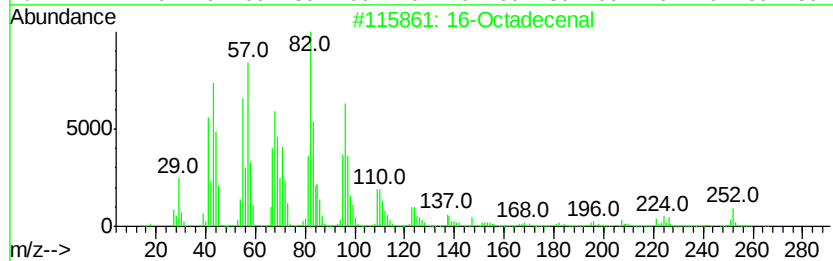
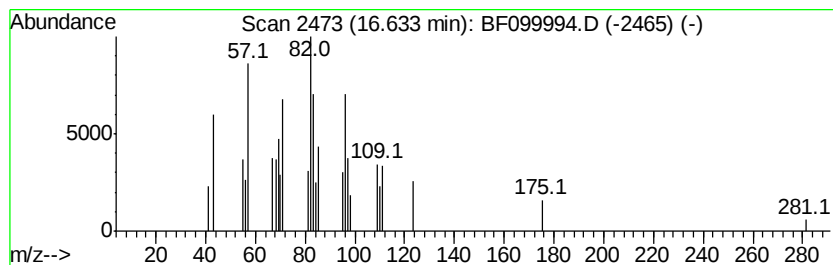
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 16-Octadecenal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.13 ng	41539	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	16-Octadecenal	266	C18H34O	056554-87-1	59
2		Tetradecanal	212	C14H28O	000124-25-4	53
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	53
4		17-Octadecenal	266	C18H34O	056554-86-0	53
5		12-Octadecenal	266	C18H34O	056554-91-7	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099994.D
Acq On : 31 Oct 2017 7:09
Operator : SJ/JU
Sample : I6201-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-1B(4-5)

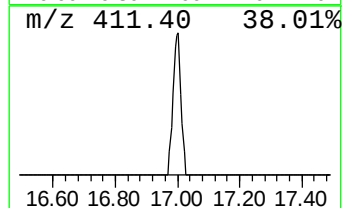
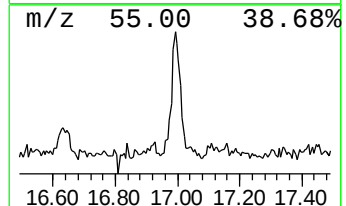
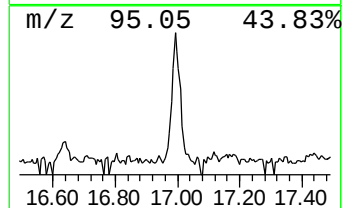
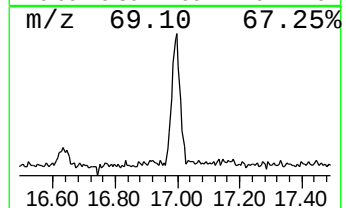
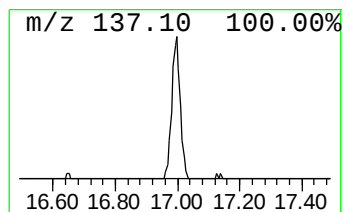
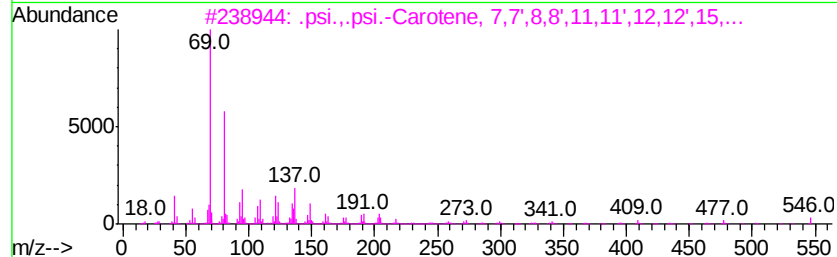
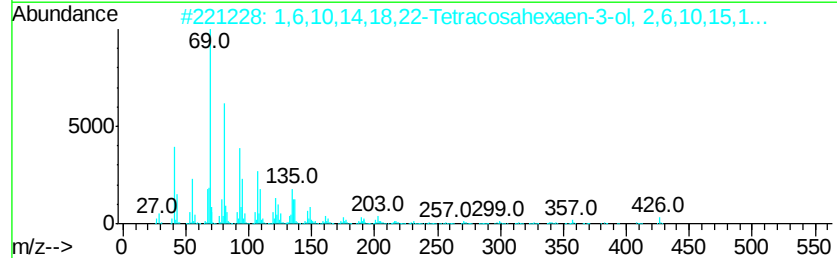
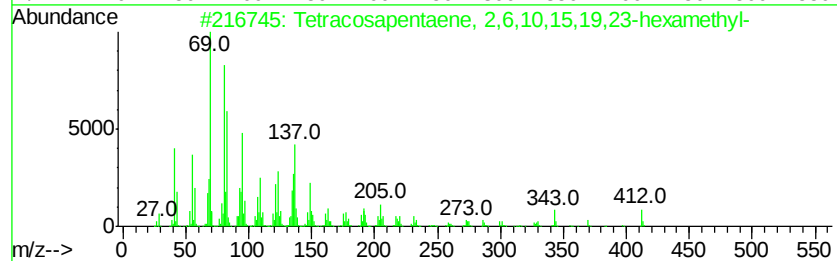
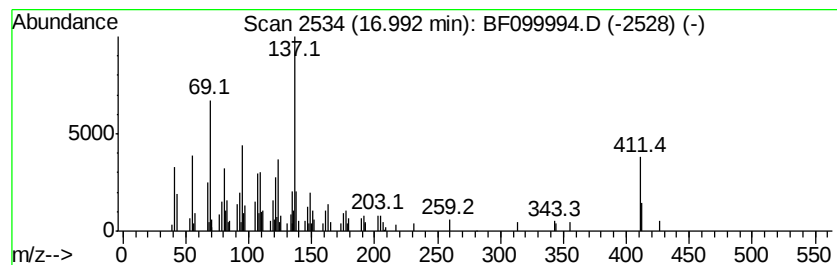
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosapentaene, 2,6,10,1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	8.85 ng	173003	Perylene-d12	15.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosapentaene, 2,6,10,15,19,...	412	C30H52	026266-08-0	60
2			1,6,10,14,18,22-Tetracosahexaen-...	426	C30H500	054159-46-5	53
3			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	43
4			Naphthalene, 1,1'-(1,2-ethanediv...	302	C22H38	054934-69-9	38
5			3,5-Octadiene, 2,2,4,5,7,7-hexam...	194	C14H26	055712-52-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
Data File : BF099994.D
Acq On : 31 Oct 2017 7:09
Operator : SJ/JU
Sample : I6201-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	12.3	ng	267881	1	6.79	435490	20.0
unknown6.56	6.56	83.2	ng	1812150	1	6.79	435490	20.0
Benzophenone	10.54	2.1	ng	71099	3	9.82	662678	20.0
Pentadecane, 2,6,...	10.73	3.4	ng	110913	4	11.32	655557	20.0
Octacosyl trifluo...	13.79	4.7	ng	106830	5	13.97	452028	20.0
1,19-Eicosadiene	14.87	4.5	ng	88432	6	15.47	390829	20.0
Tetradecanal	15.63	3.5	ng	68319	6	15.47	390829	20.0
16-Octadecenal	16.63	2.1	ng	41539	6	15.47	390829	20.0
Tetracosapentaene...	16.99	8.8	ng	173003	6	15.47	390829	20.0