

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081817\
 Data File : BF097842.D
 Acq On : 18 Aug 2017 19:37
 Operator : SJ/JU
 Sample : PB101580BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB101580BL

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-BF081517.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	4.340	378	383	391	rBV	78492	92430	2.57%	0.293%
2	4.975	486	491	505	rBV	578223	782924	21.79%	2.479%
3	5.387	555	561	564	rBV	3159649	3338577	92.92%	10.570%
4	6.404	728	734	737	rBV	3212259	3399042	94.60%	10.762%
5	6.540	752	757	760	rBV	3267077	3281675	91.34%	10.390%
6	6.769	793	796	800	rBV	985640	780632	21.73%	2.472%
7	6.928	818	823	826	rBV	2852656	2522561	70.21%	7.987%
8	7.334	887	892	895	rBV	2140294	2121422	59.05%	6.717%
9	8.051	1010	1014	1018	rBV	1112581	1025526	28.54%	3.247%
10	9.133	1192	1198	1201	rBV	3273709	3592885	100.00%	11.376%
11	9.804	1307	1312	1316	rBV	1116074	1082874	30.14%	3.429%
12	10.592	1440	1446	1450	rBV	2021829	2160564	60.13%	6.841%
13	11.286	1559	1564	1568	rBV	1170786	1134134	31.57%	3.591%
14	12.880	1829	1835	1838	rBV	3511836	3508159	97.64%	11.107%
15	13.921	2008	2012	2016	rBV	1292020	1154286	32.13%	3.655%
16	15.033	2198	2201	2205	rBV2	46607	48729	1.36%	0.154%
17	15.351	2250	2255	2260	rBV	785741	997462	27.76%	3.158%
18	15.398	2260	2263	2269	rVB	73819	94934	2.64%	0.301%
19	15.821	2330	2335	2342	rVB2	75030	110658	3.08%	0.350%
20	16.304	2411	2417	2428	rVB	71326	126324	3.52%	0.400%
21	16.874	2508	2514	2521	rBV2	48935	96401	2.68%	0.305%
22	17.545	2622	2628	2640	rVB4	37512	88451	2.46%	0.280%
23	18.339	2760	2763	2774	rVB8	18108	43521	1.21%	0.138%

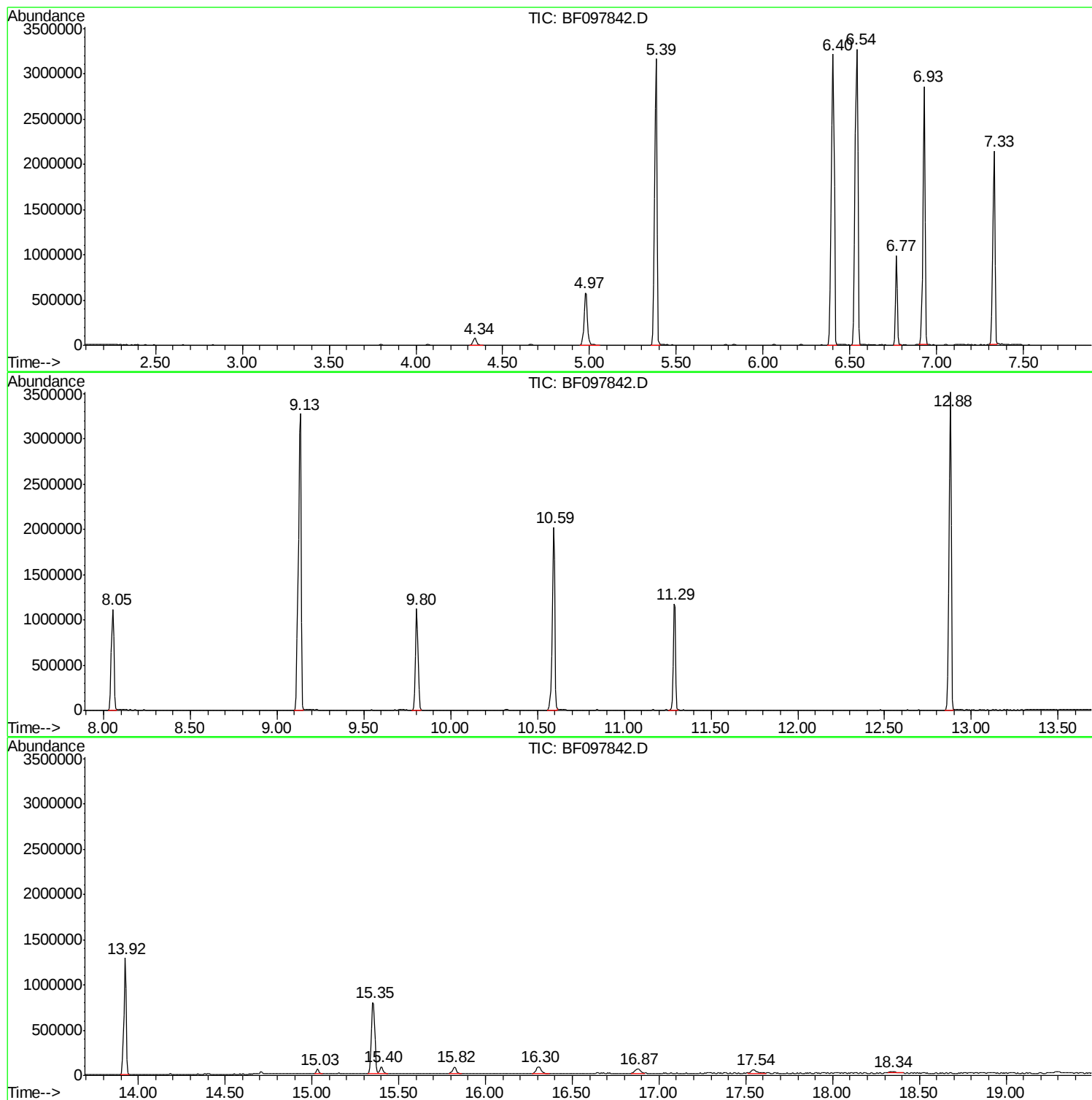
Sum of corrected areas: 31584171

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081817\
Data File : BF097842.D
Acq On : 18 Aug 2017 19:37
Operator : SJ/JU
Sample : PB101580BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB101580BL

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081817\
Data File : BF097842.D
Acq On : 18 Aug 2017 19:37
Operator : SJ/JU
Sample : PB101580BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB101580BL

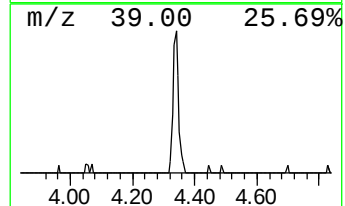
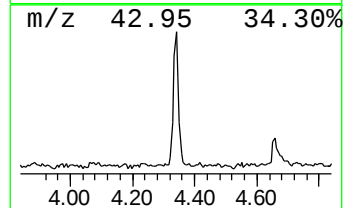
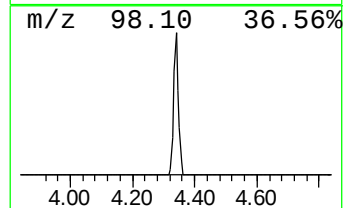
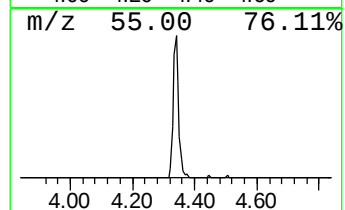
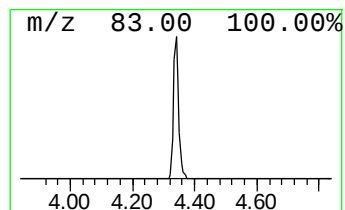
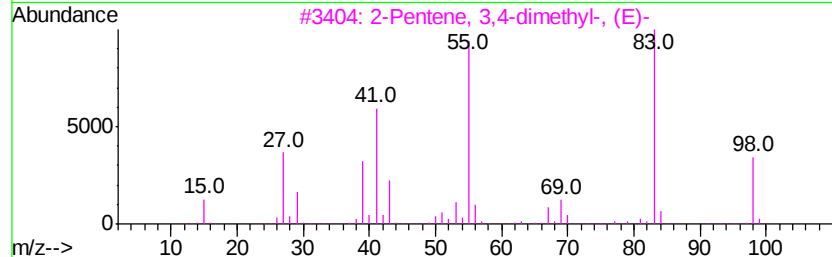
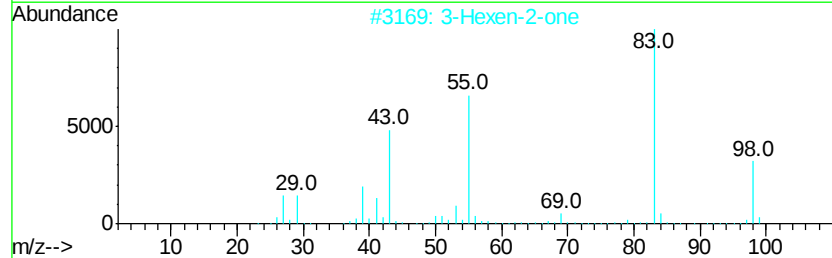
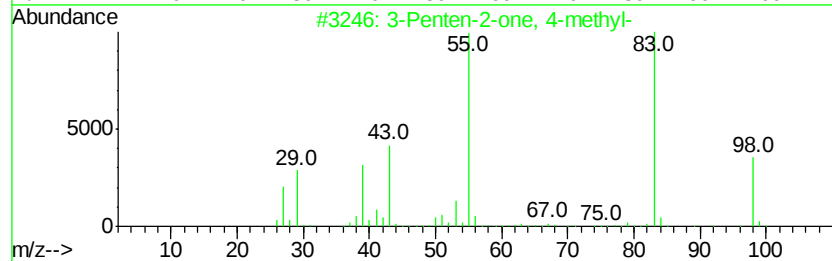
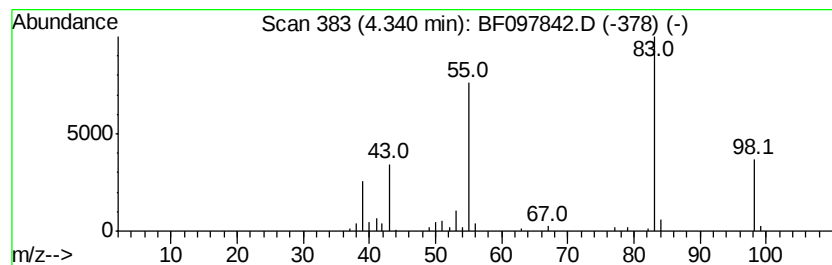
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.34	2.37 ng	92430	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081817\
Data File : BF097842.D
Acq On : 18 Aug 2017 19:37
Operator : SJ/JU
Sample : PB101580BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB101580BL

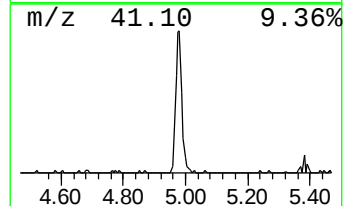
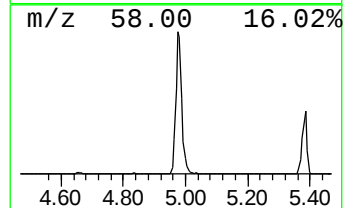
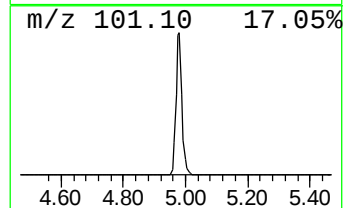
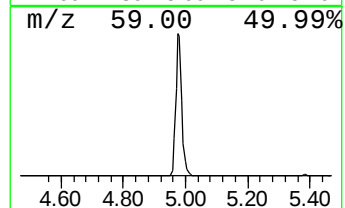
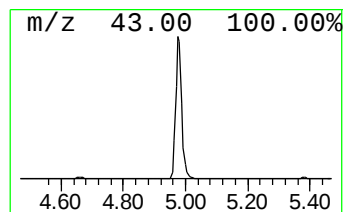
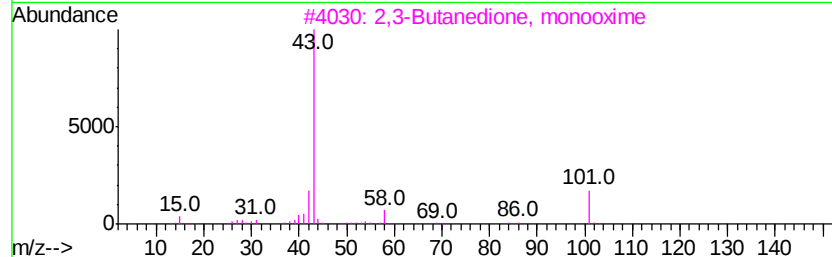
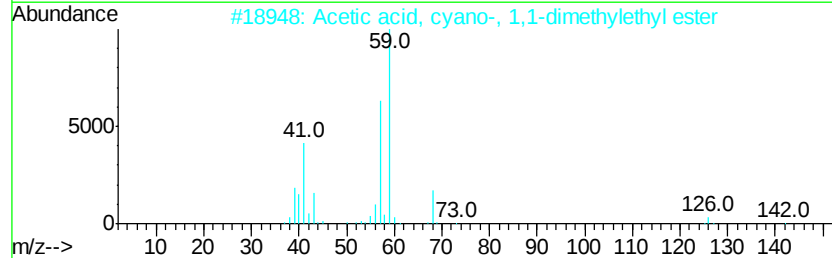
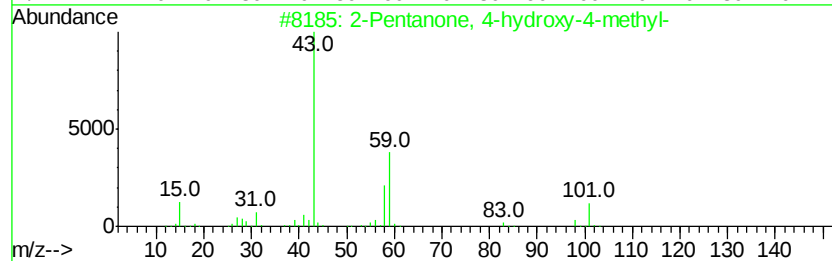
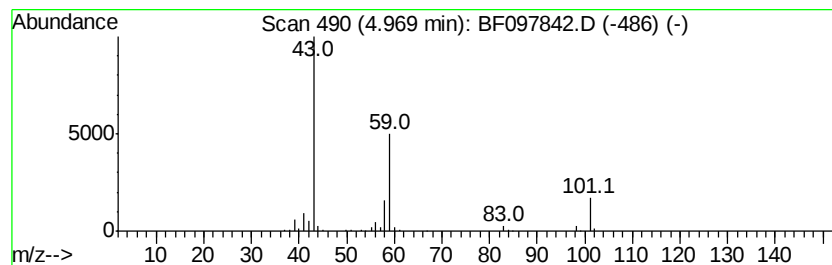
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	20.06 ng	782924	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081817\
Data File : BF097842.D
Acq On : 18 Aug 2017 19:37
Operator : SJ/JU
Sample : PB101580BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB101580BL

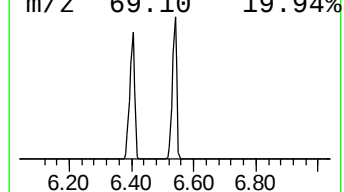
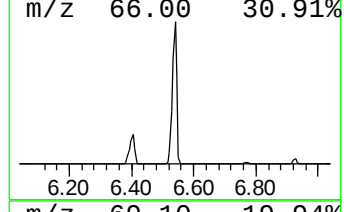
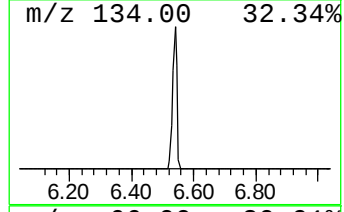
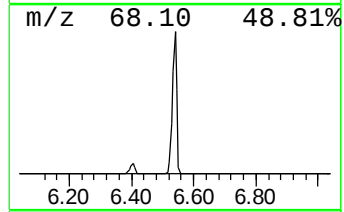
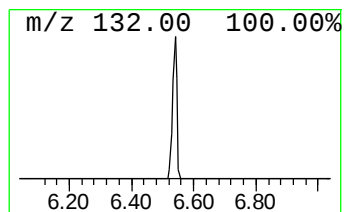
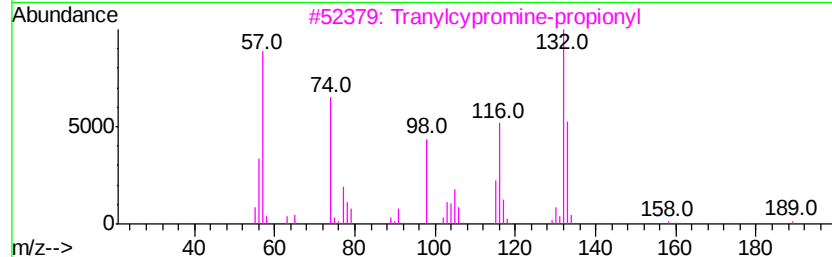
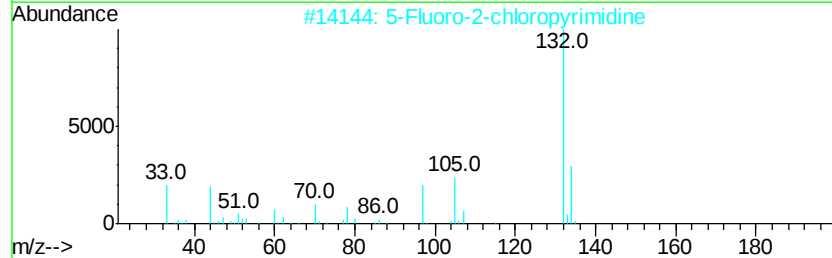
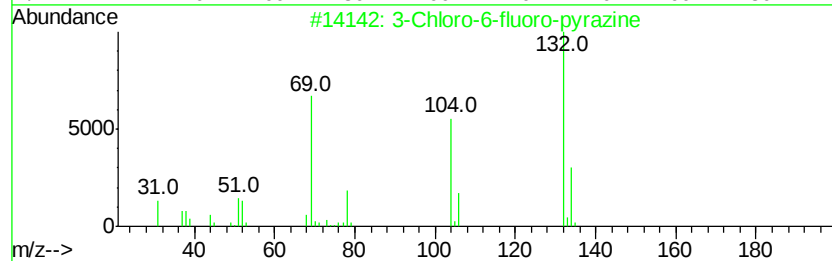
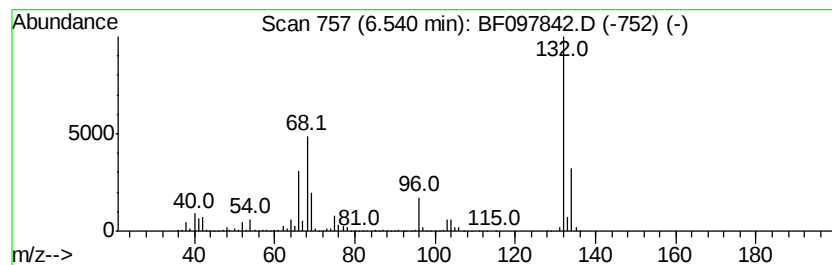
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	84.08 ng	3281680	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropamine-propionyl	189	C12H15NO	1000123-86-3	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081817\
Data File : BF097842.D
Acq On : 18 Aug 2017 19:37
Operator : SJ/JU
Sample : PB101580BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB101580BL

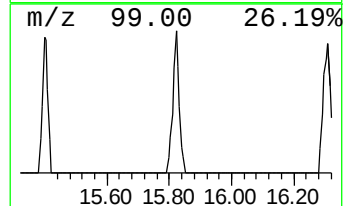
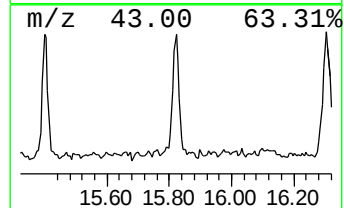
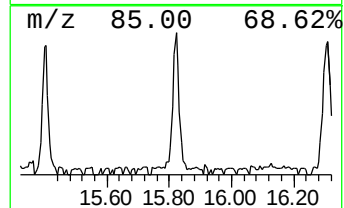
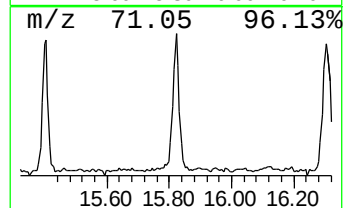
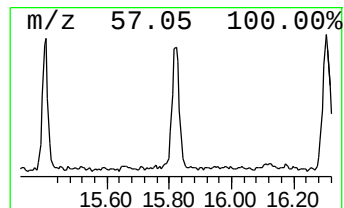
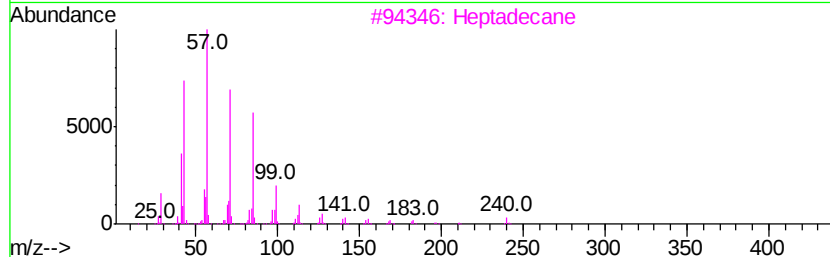
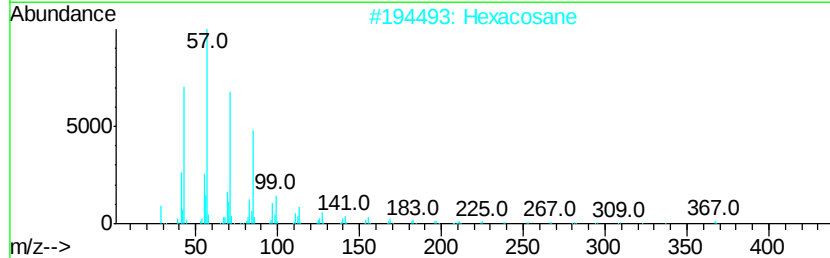
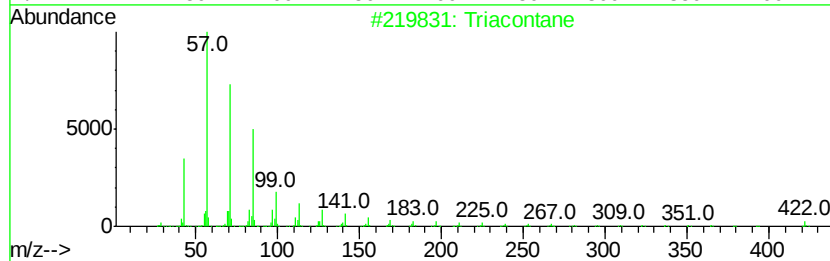
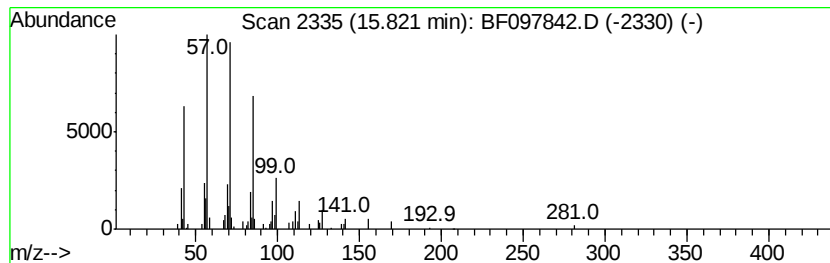
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	2.22 ng	110658	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	90
2		Hexacosane	366	C26H54	000630-01-3	87
3		Heptadecane	240	C17H36	000629-78-7	86
4		2-methyloctacosane	408	C29H60	1000376-72-8	86
5		Pentacosane	352	C25H52	000629-99-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081817\
Data File : BF097842.D
Acq On : 18 Aug 2017 19:37
Operator : SJ/JU
Sample : PB101580BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB101580BL

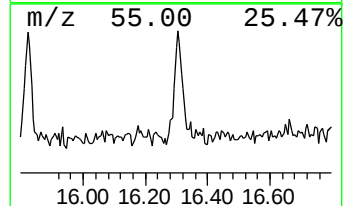
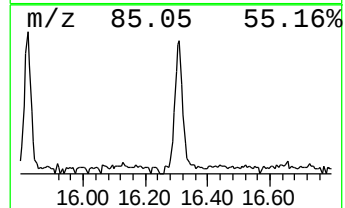
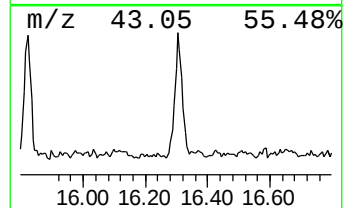
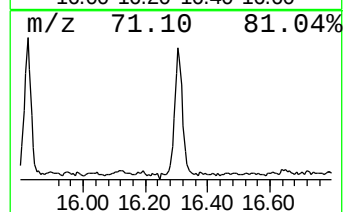
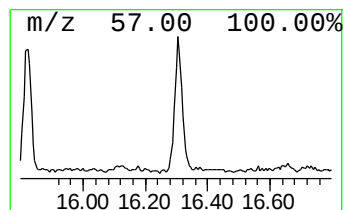
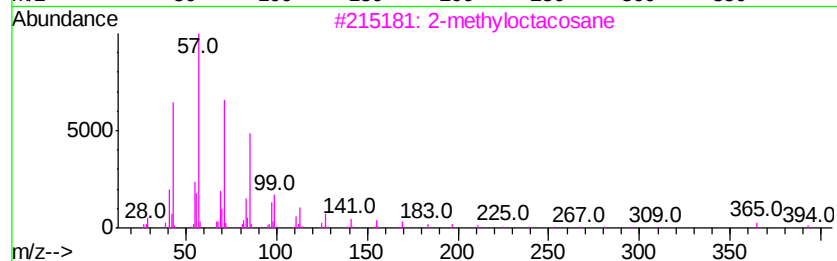
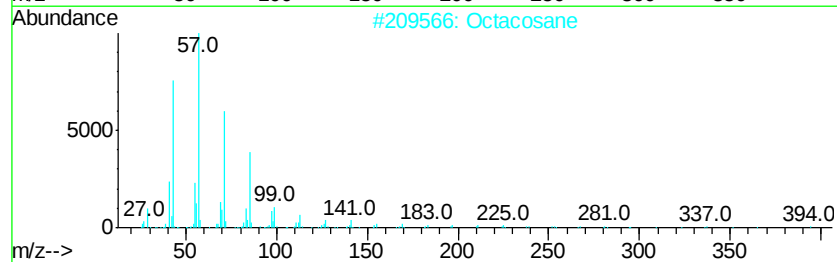
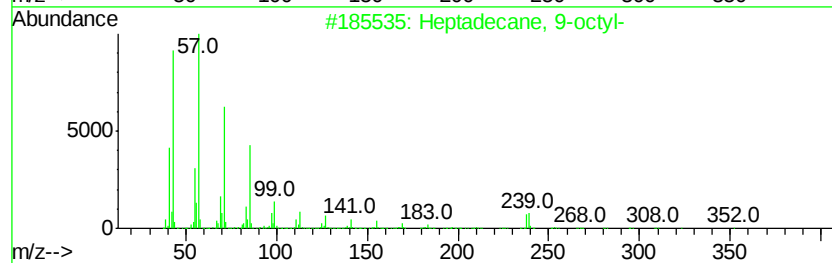
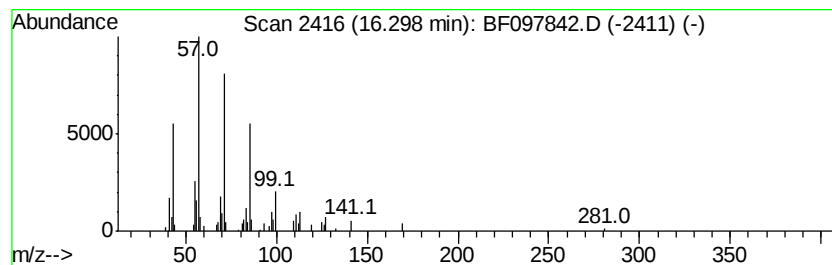
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	2.53 ng	126324	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Octacosane	394	C28H58	000630-02-4	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081817\
Data File : BF097842.D
Acq On : 18 Aug 2017 19:37
Operator : SJ/JU
Sample : PB101580BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB101580BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
3-Penten-2-one, 4...	4.34	2.4	ng	92430	1	6.77	780632	20.0
2-Pentanone, 4-hy...	4.97	20.1	ng	782924	1	6.77	780632	20.0
unknown6.54	6.54	84.1	ng	3281680	1	6.77	780632	20.0
Triacontane	15.82	2.2	ng	110658	6	15.36	997462	20.0
Heptadecane, 9-oc...	16.30	2.5	ng	126324	6	15.36	997462	20.0