

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
 Data File : BF088605.D
 Acq On : 2 Jul 2016 6:28
 Operator : UM/SJ
 Sample : H3831-10
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-20-COMP

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-BF063016.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	1.667	3	7	9	rVB	4223265	5529232	100.00%	13.432%
2	1.735	12	13	23	rVB	594050	912331	16.50%	2.216%
3	1.861	23	24	39	rVB	2402936	5301017	95.87%	12.878%
4	2.055	39	41	80	rVB	158176	825210	14.92%	2.005%
5	3.061	127	129	143	rVB	45841	99647	1.80%	0.242%
6	4.993	295	298	303	rVB	223621	369291	6.68%	0.897%
7	5.404	331	334	337	rBV	2476557	3247387	58.73%	7.889%
8	6.444	421	425	427	rBV	2858110	3331749	60.26%	8.094%
9	6.582	434	437	439	rBV	2568547	3532671	63.89%	8.582%
10	6.810	454	457	459	rBV	835687	791855	14.32%	1.924%
11	6.970	468	471	473	rVB	2240187	2791141	50.48%	6.781%
12	7.370	503	506	508	rBV	1923267	1993235	36.05%	4.842%
13	8.090	567	569	571	rVB	1191268	1001332	18.11%	2.433%
14	9.176	661	664	666	rVB	2944458	3686518	66.67%	8.956%
15	9.565	695	698	700	rBV	235873	243594	4.41%	0.592%
16	9.839	720	722	725	rVB	988218	942645	17.05%	2.290%
17	10.628	788	791	793	rBV	1750594	1708793	30.90%	4.151%
18	11.199	839	841	843	rBV	80296	75296	1.36%	0.183%
19	11.313	849	851	853	rVB2	685208	772561	13.97%	1.877%
20	12.902	987	990	993	rBV	2438920	2347511	42.46%	5.703%
21	13.828	1068	1071	1078	rBV	58013	122358	2.21%	0.297%
22	13.942	1078	1081	1083	rBV	819829	721543	13.05%	1.753%
23	15.348	1201	1204	1206	rBV	383629	567886	10.27%	1.380%
24	16.868	1334	1337	1341	rVB	97272	187853	3.40%	0.456%
25	17.028	1348	1351	1355	rVB	32313	61298	1.11%	0.149%

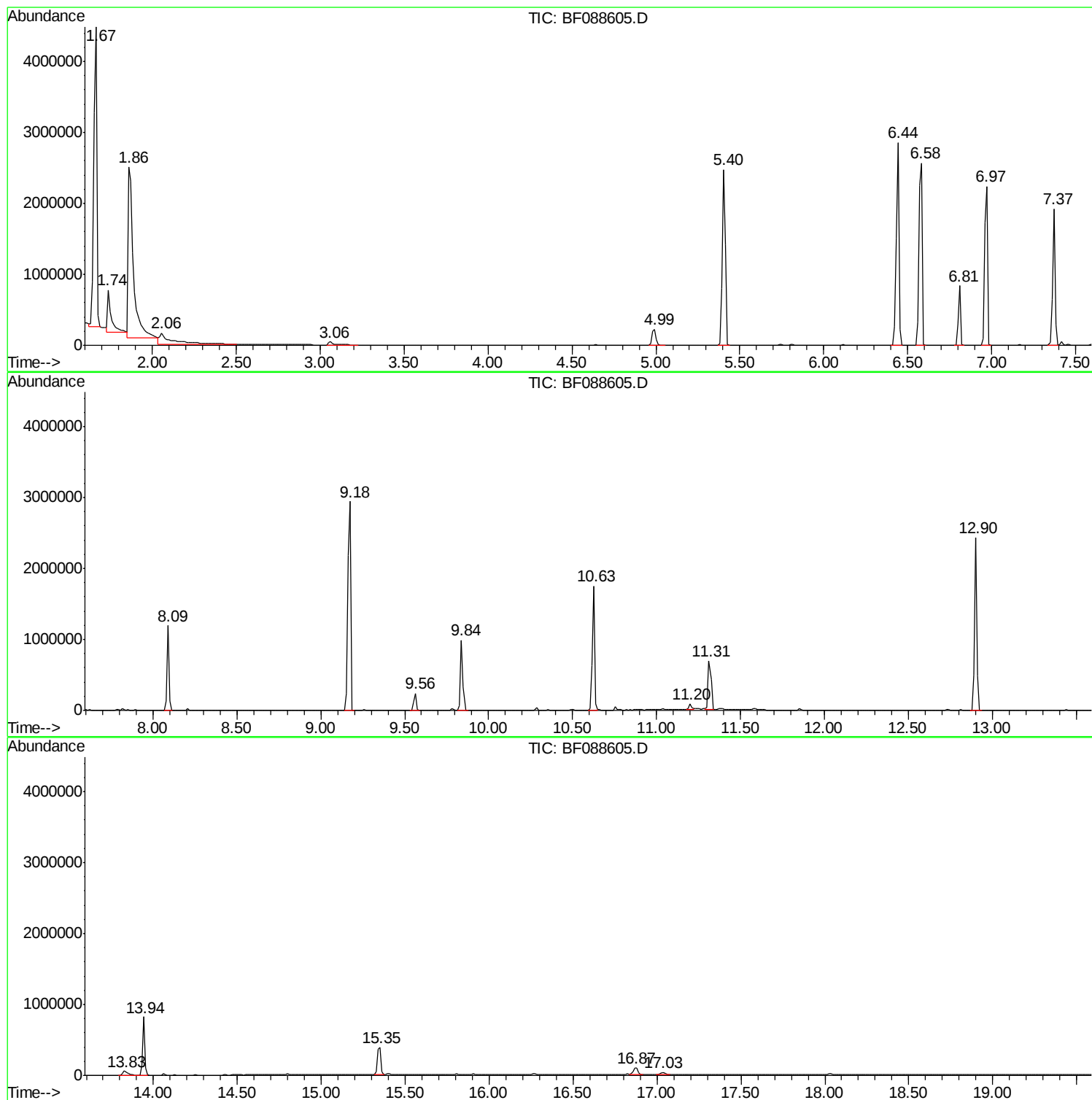
Sum of corrected areas: 41163954

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

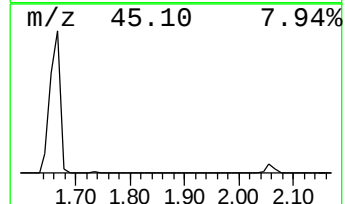
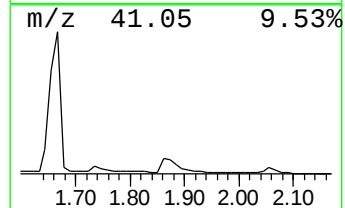
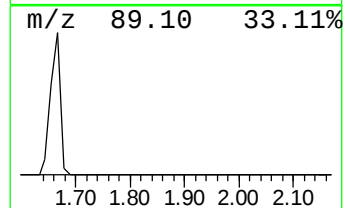
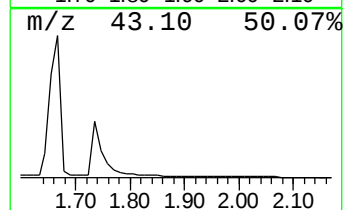
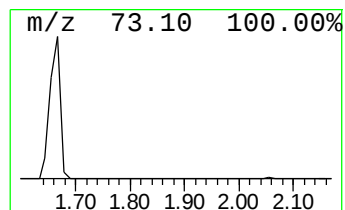
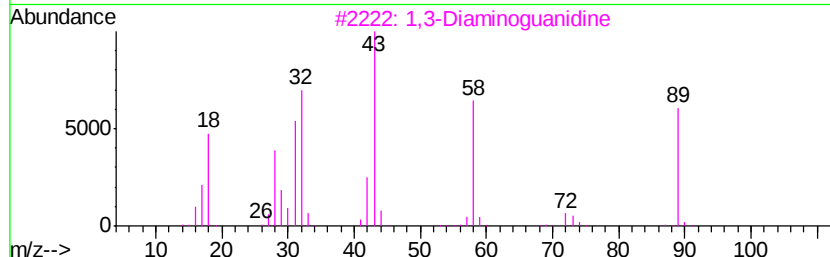
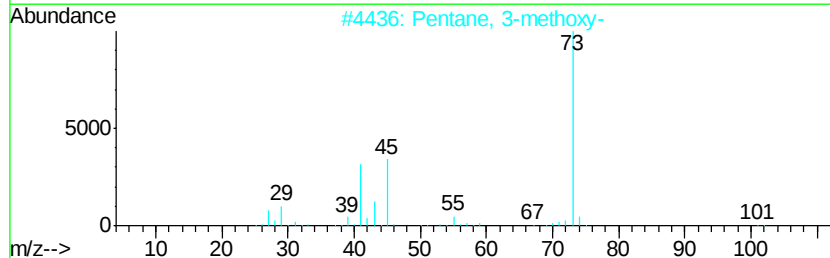
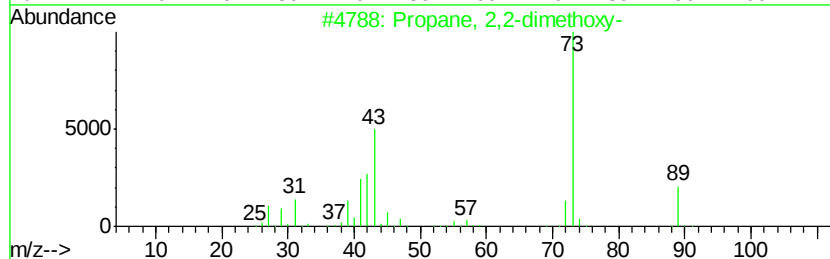
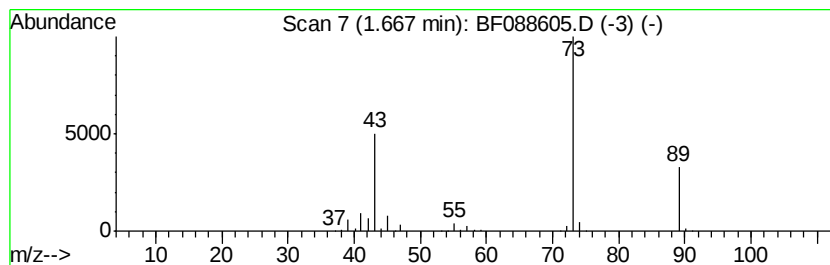
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	139.65 ng	5529230	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

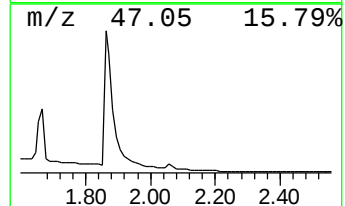
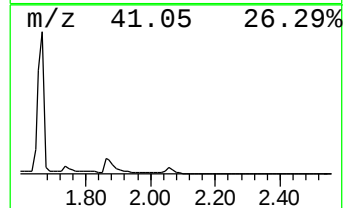
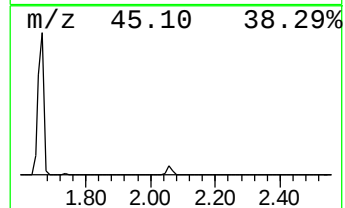
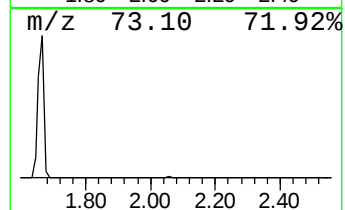
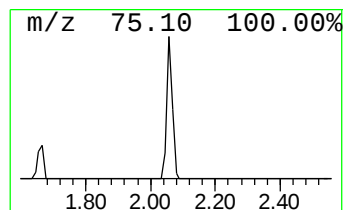
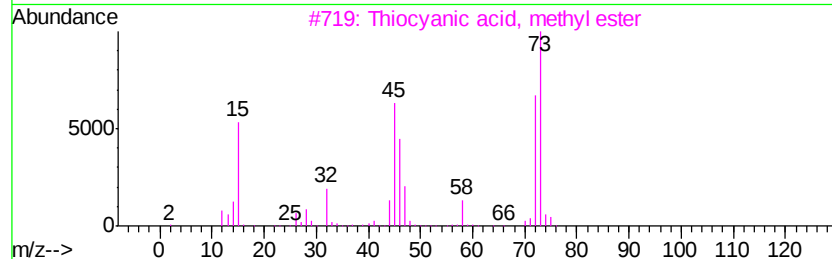
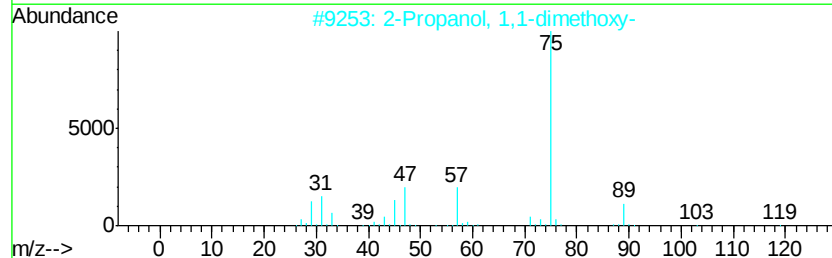
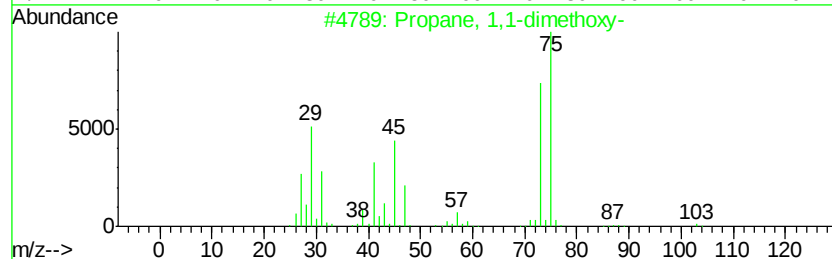
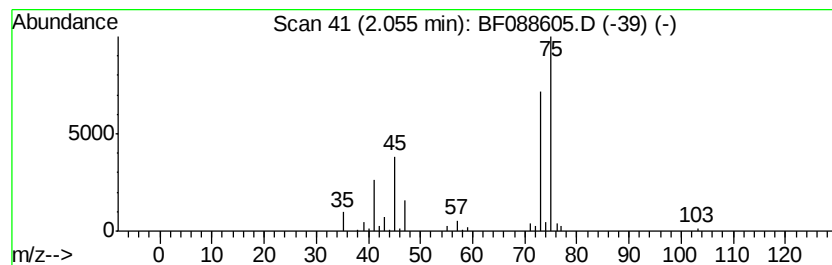
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	20.84 ng	825210	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	33
3		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	27
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

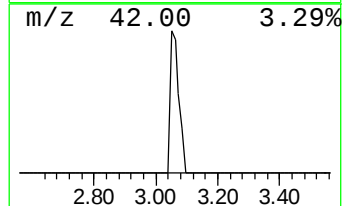
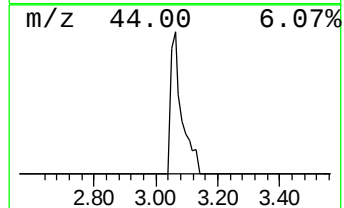
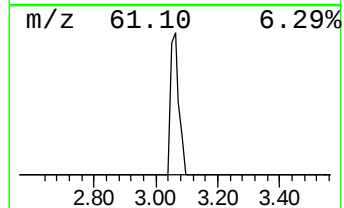
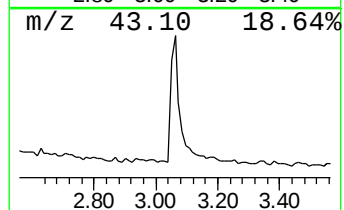
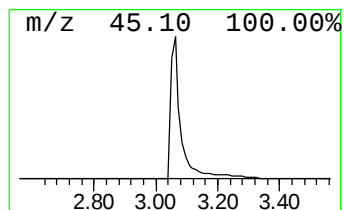
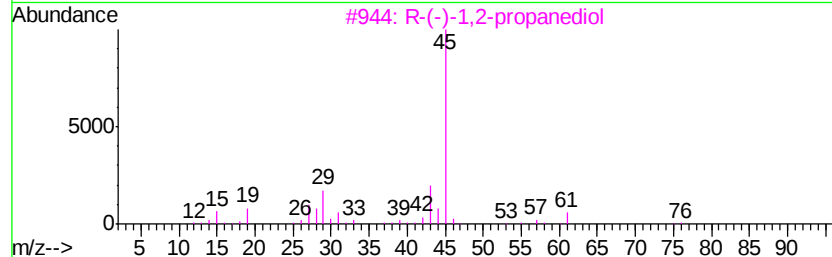
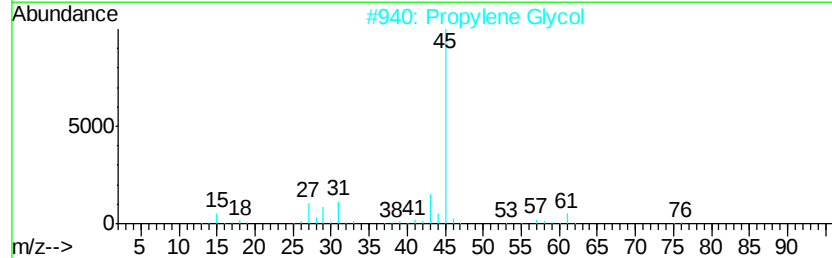
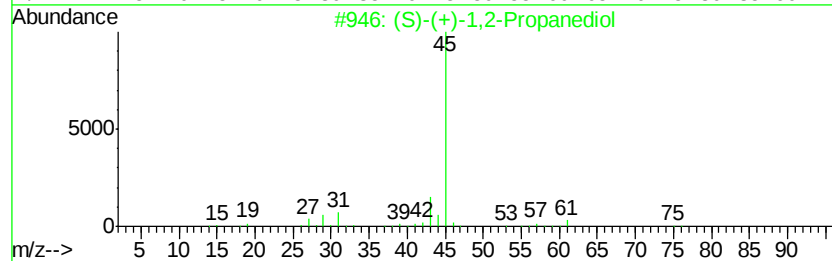
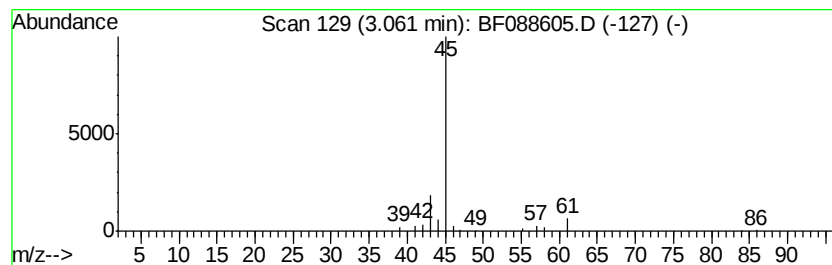
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 (S)-(+)-1,2-Propanediol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	2.52 ng	99647	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
2		Propylene Glycol	76	C3H8O2	000057-55-6	43
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
4		2-Heptanol	116	C7H16O	000543-49-7	9
5		2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

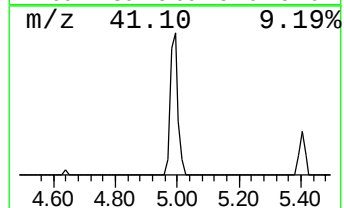
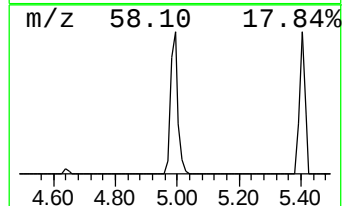
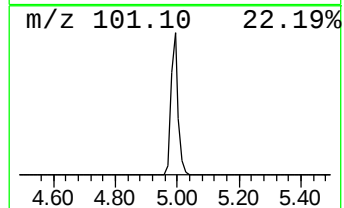
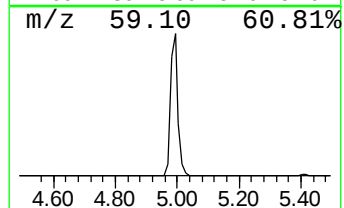
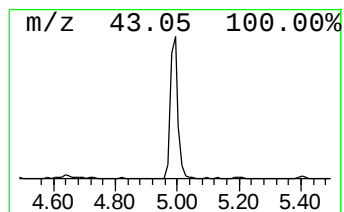
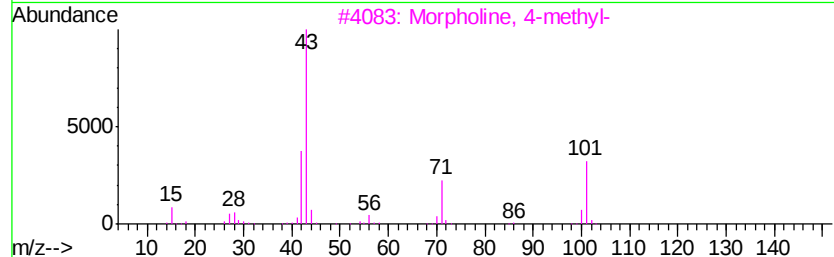
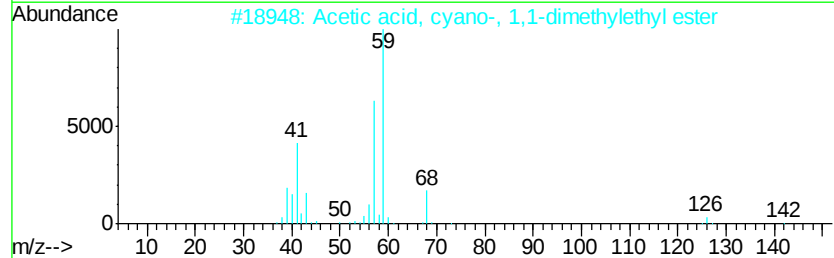
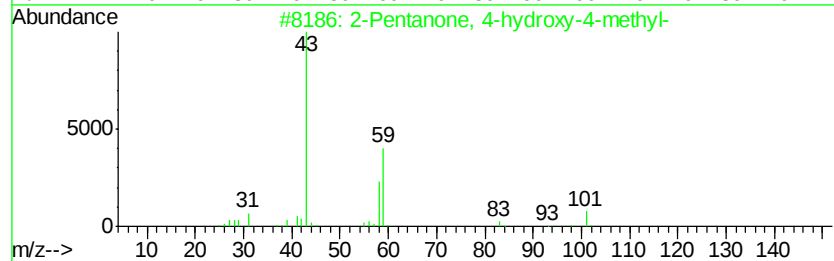
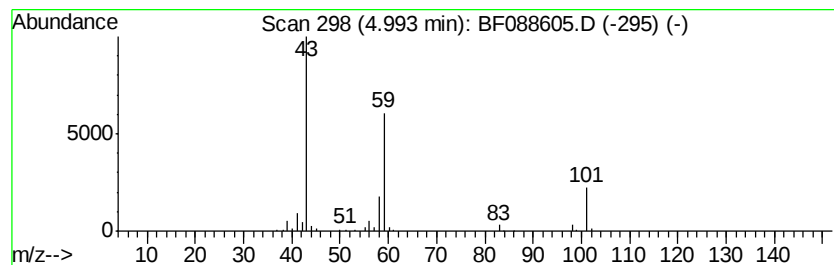
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	9.33 ng	369291	1,4-Dichlorobenzene-d4	6.81

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-dimethy...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Butane	58	C4H10	000106-97-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

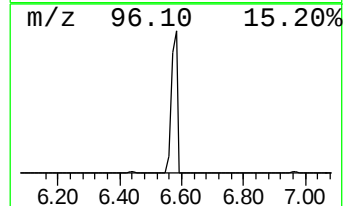
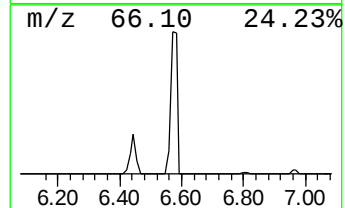
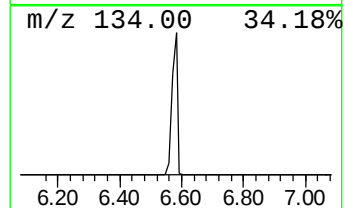
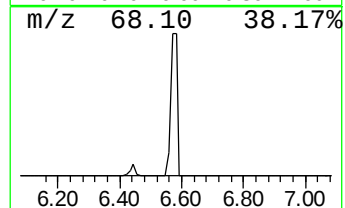
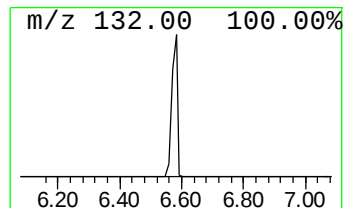
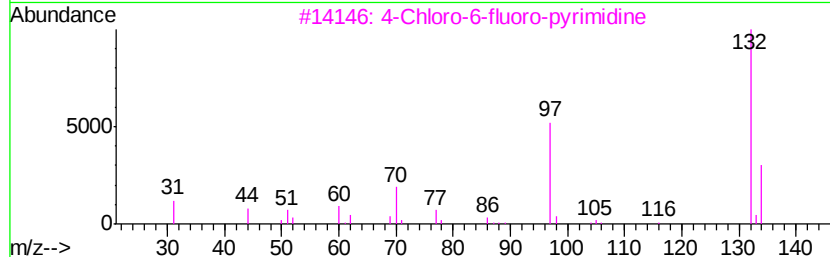
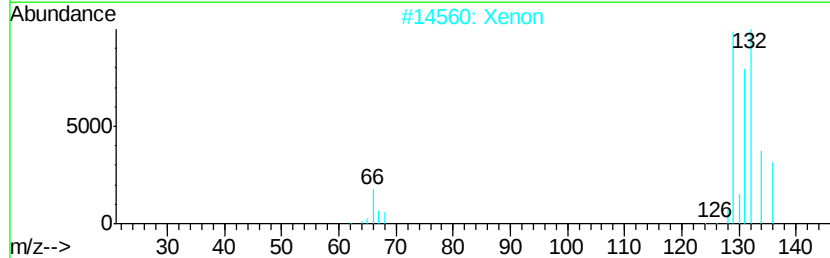
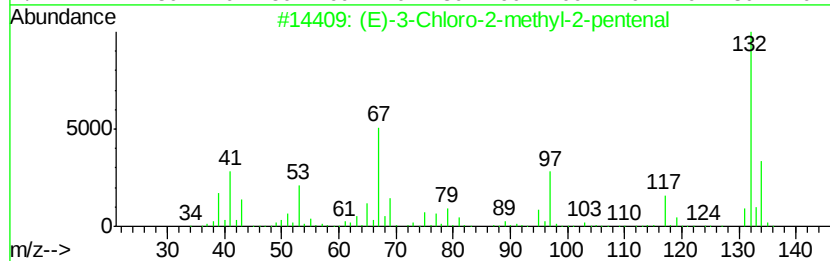
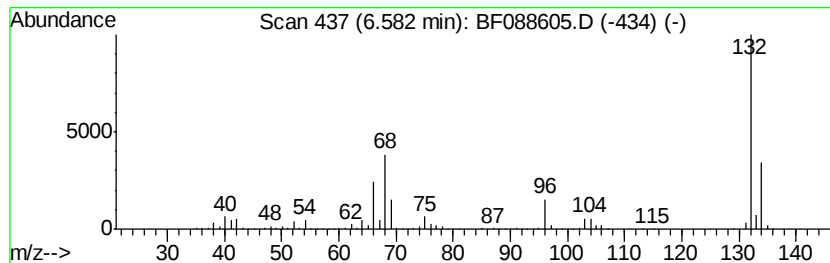
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	89.23 ng	3532670	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Xenon	132	Xe	007440-63-3	9
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

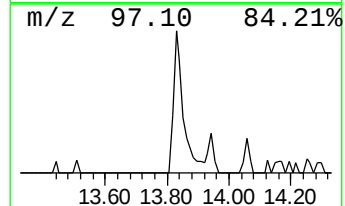
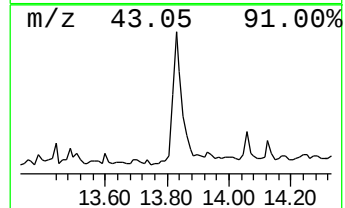
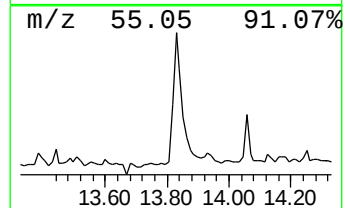
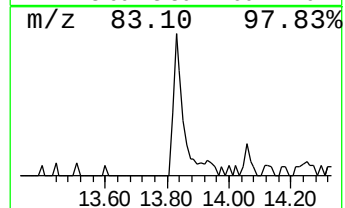
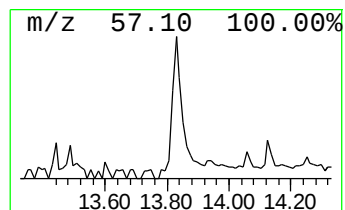
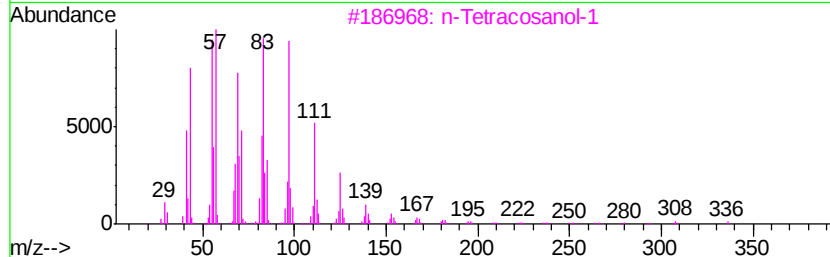
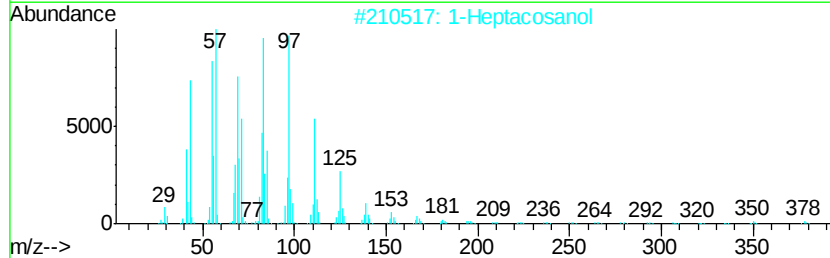
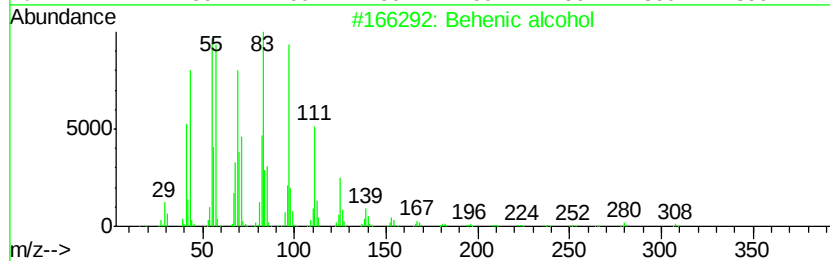
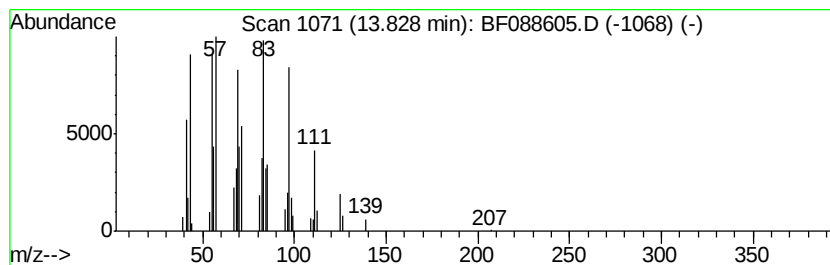
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Behenic alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.39 ng	122358	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	94
2		1-Heptacosanol	396	C27H56O	002004-39-9	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

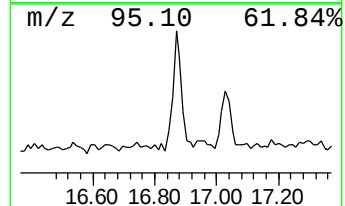
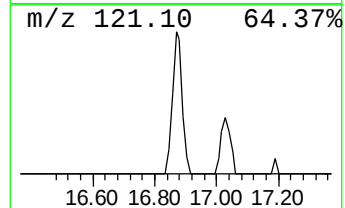
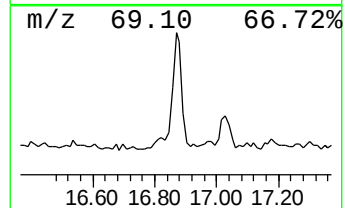
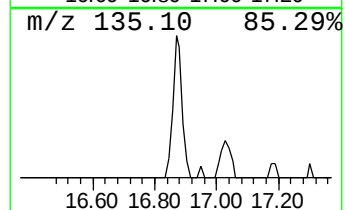
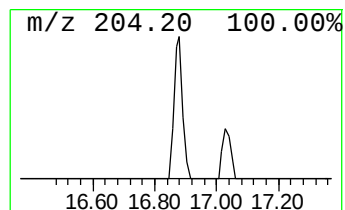
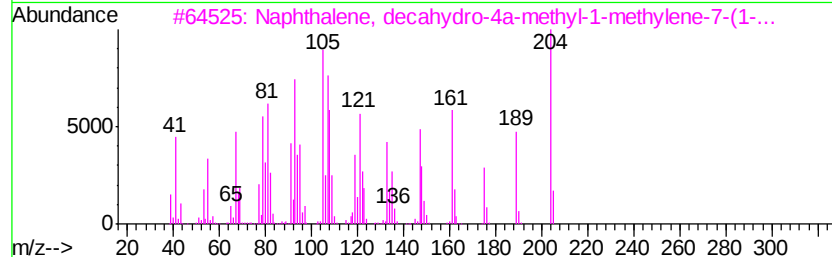
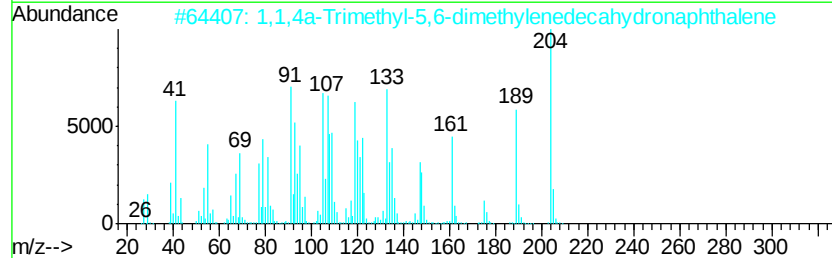
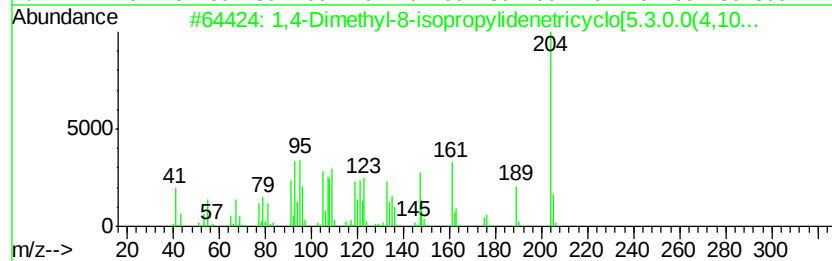
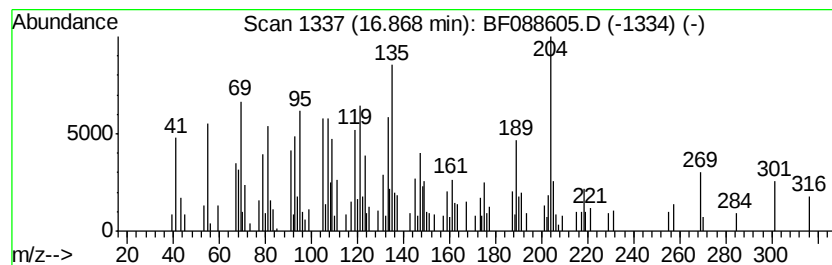
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,4-Dimethyl-8-isopropylide... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.87	6.62 ng	187853	Perylene-d12	15.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	86
2			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	53
3			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	49
4			1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	46
5			1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

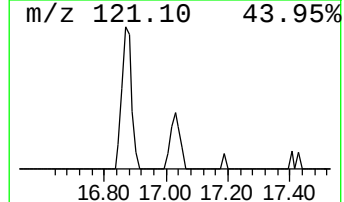
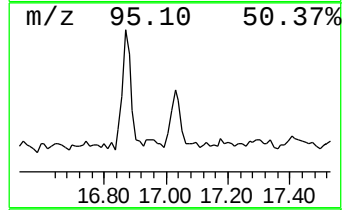
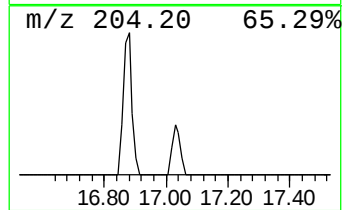
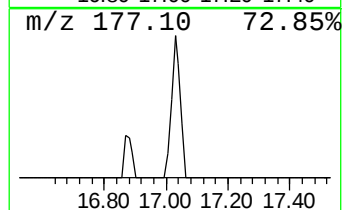
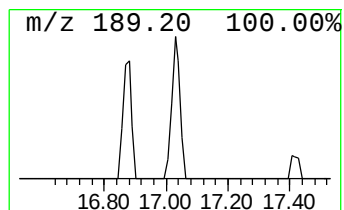
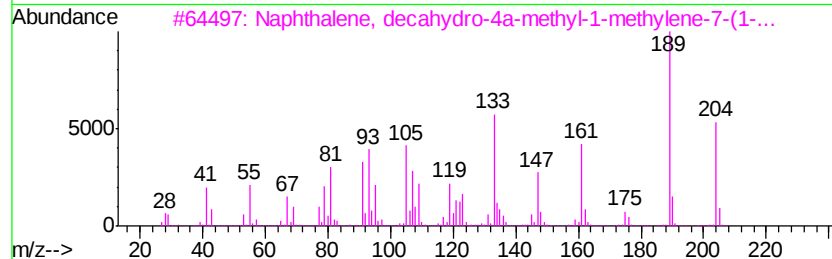
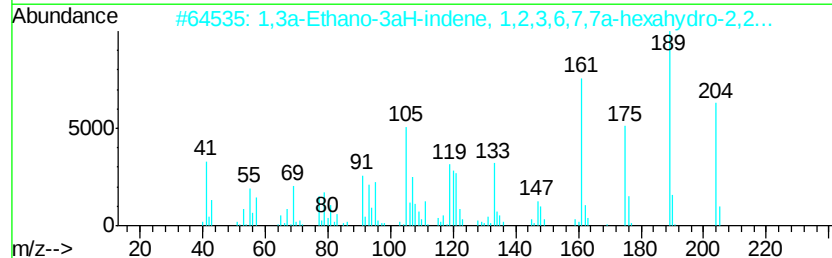
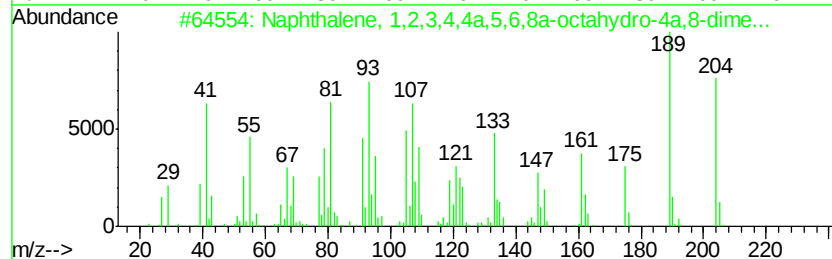
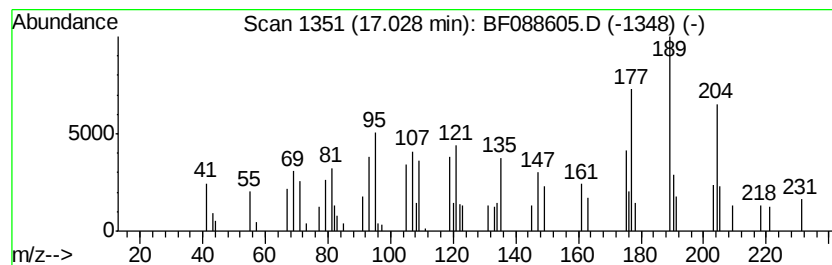
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Naphthalene, 1,2,3,4,4a,5,6... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	2.16 ng	61298	Perylene-d12	15.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	55
2		1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	50
3		Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	49
4		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	45
5		Cedrene-V6	204	C15H24	1000162-76-8	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088605.D
Acq On : 2 Jul 2016 6:28
Operator : UM/SJ
Sample : H3831-10
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
unknown1.67	1.67	139.7	ng	5529230	1	6.81	791855	20.0
Propane, 1,1-dime...	2.06	20.8	ng	825210	1	6.81	791855	20.0
(S)-(+)-1,2-Propa...	3.06	2.5	ng	99647	1	6.81	791855	20.0
2-Pentanone, 4-hy...	4.99	9.3	ng	369291	1	6.81	791855	20.0
unknown6.58	6.58	89.2	ng	3532670	1	6.81	791855	20.0
Behenic alcohol	13.83	3.4	ng	122358	5	13.94	721543	20.0
1,4-Dimethyl-8-is...	16.87	6.6	ng	187853	6	15.35	567886	20.0
Naphthalene, 1,2,...	17.03	2.2	ng	61298	6	15.35	567886	20.0