

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
 Data File : BF095549.D
 Acq On : 30 May 2017 22:33
 Operator : SJ/MA
 Sample : I3302-07
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NM12-COMP-0-6

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-BF050217.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	5.089	533	536	554	rBV	59458	158419	7.34%	0.958%
2	5.707	637	641	668	rBV	610932	1702773	78.86%	10.302%
3	7.295	907	911	926	rBV	557146	1487268	68.88%	8.998%
4	7.407	926	930	958	rVB	1131299	2159243	100.00%	13.064%
5	7.736	982	986	999	rBV	390279	482182	22.33%	2.917%
6	7.972	1021	1026	1051	rVB	1128220	1451998	67.25%	8.785%
7	8.648	1136	1141	1173	rBV	385048	985316	45.63%	5.961%
8	9.766	1327	1331	1351	rBV	258992	600702	27.82%	3.634%
9	11.536	1627	1632	1655	rBV	840543	1605786	74.37%	9.715%
10	12.242	1747	1752	1767	rBV	81818	177254	8.21%	1.072%
11	12.601	1808	1813	1827	rBV2	334638	616809	28.57%	3.732%
12	13.424	1947	1953	1959	rBV2	24108	33221	1.54%	0.201%
13	13.901	2030	2034	2059	rBV	359391	771869	35.75%	4.670%
14	14.195	2080	2084	2094	rBV	23120	34676	1.61%	0.210%
15	15.006	2217	2222	2243	rVV	262817	516203	23.91%	3.123%
16	15.895	2369	2373	2379	rBV3	27103	43699	2.02%	0.264%
17	15.953	2379	2383	2396	rVB4	67741	131307	6.08%	0.794%
18	16.789	2521	2525	2534	rBV	92061	131155	6.07%	0.793%
19	17.042	2563	2568	2572	rBV5	19010	32546	1.51%	0.197%
20	17.089	2572	2576	2586	rVB	108677	155103	7.18%	0.938%
21	17.312	2610	2614	2626	rBV	972385	1190526	55.14%	7.203%
22	17.553	2651	2655	2661	rVB6	18775	32709	1.51%	0.198%
23	17.689	2674	2678	2686	rVB6	18414	32161	1.49%	0.195%
24	17.983	2725	2728	2731	rBV	55135	59873	2.77%	0.362%
25	18.553	2822	2825	2834	rVB4	35291	67741	3.14%	0.410%
26	18.677	2840	2846	2850	rBV	405344	613640	28.42%	3.713%
27	19.341	2955	2959	2962	rBV3	46356	52744	2.44%	0.319%
28	19.712	3018	3022	3025	rVB5	20359	25688	1.19%	0.155%
29	19.783	3030	3034	3040	rVV	45552	71524	3.31%	0.433%
30	19.865	3044	3048	3052	rBV6	26792	35634	1.65%	0.216%
31	19.953	3059	3063	3066	rBV	62183	93734	4.34%	0.567%
32	20.065	3079	3082	3085	rBV	92024	89066	4.12%	0.539%
33	20.241	3110	3112	3117	rVB	37753	40491	1.88%	0.245%
34	20.306	3119	3123	3127	rBV	36156	47141	2.18%	0.285%

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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-BF050217.M
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35	20.353	3127	3131	3139	rBV	250821	352423	16.32%	2.132%
36	20.583	3167	3170	3175	rVB4	47219	63189	2.93%	0.382%
37	20.788	3201	3205	3211	rBV	88389	120200	5.57%	0.727%
38	21.465	3316	3320	3326	rVB8	32649	53464	2.48%	0.323%
39	21.724	3358	3364	3372	rVB3	113198	209213	9.69%	1.266%

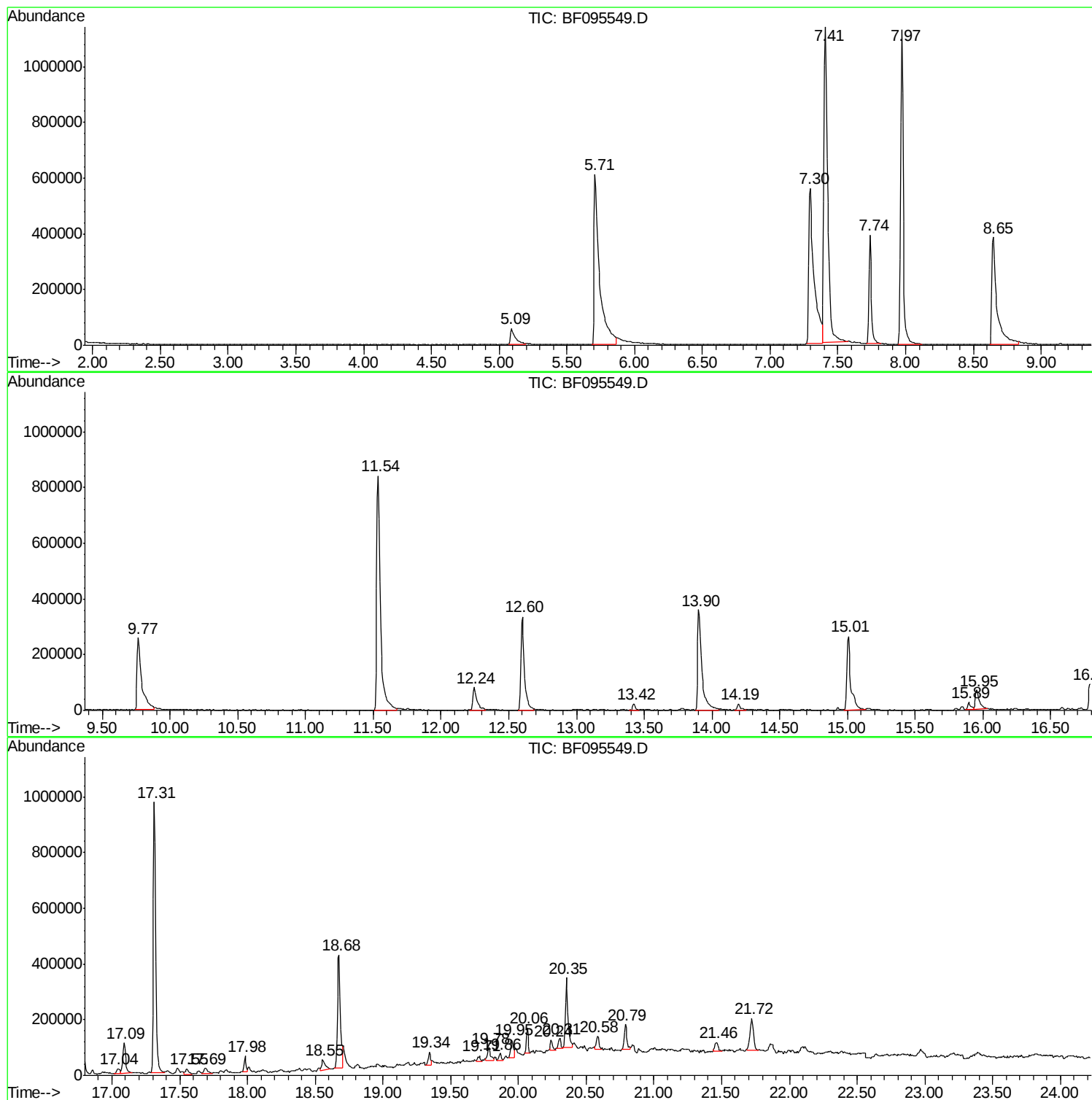
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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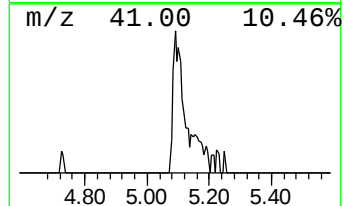
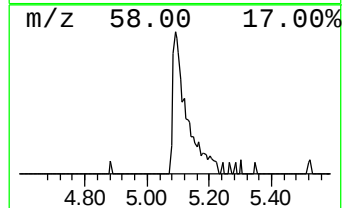
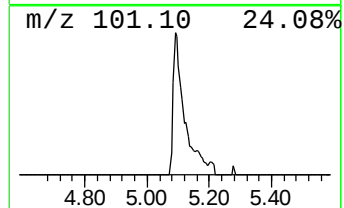
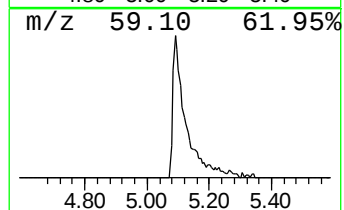
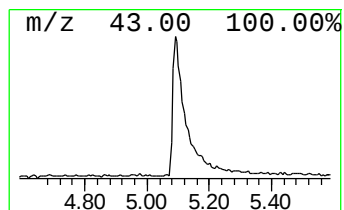
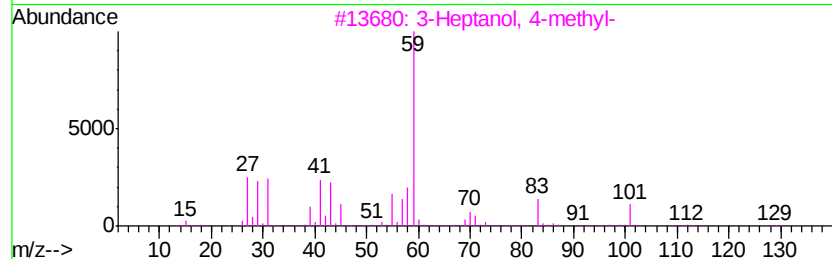
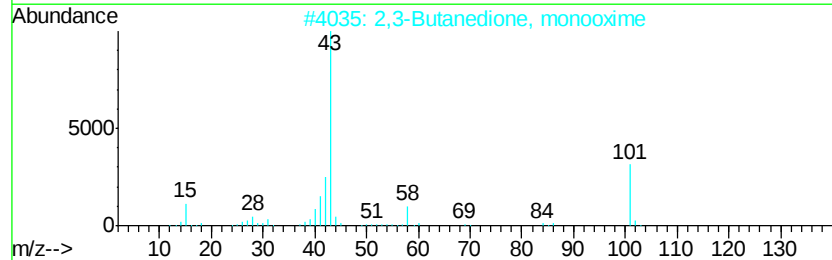
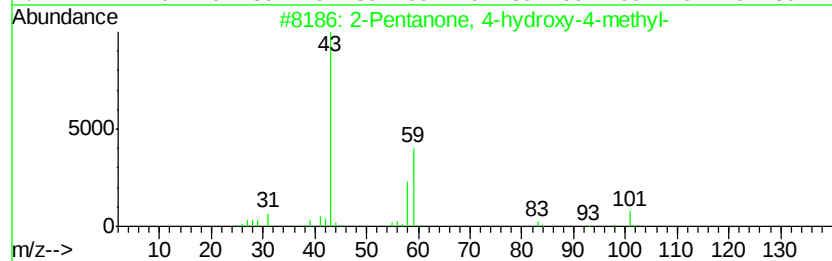
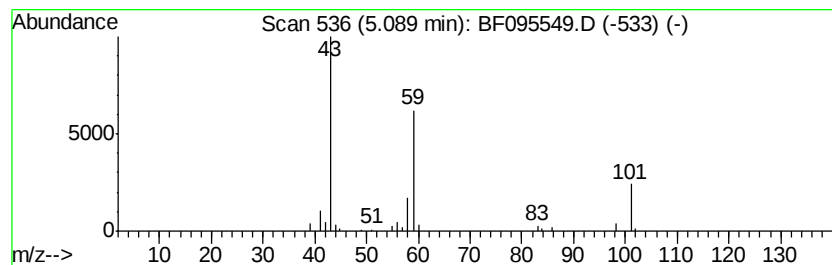
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.57 ng	158419	1,4-Dichlorobenzene-d4	7.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3			3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25
4			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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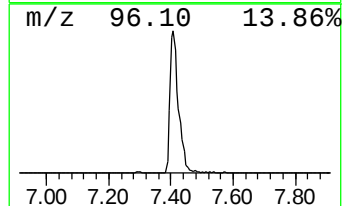
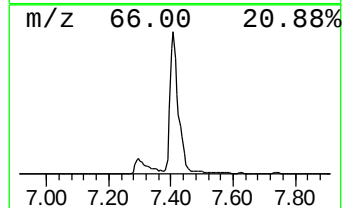
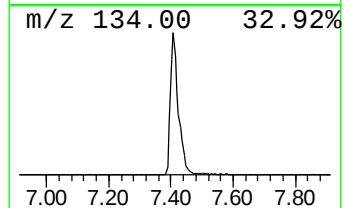
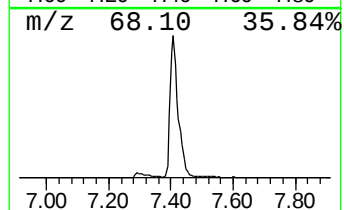
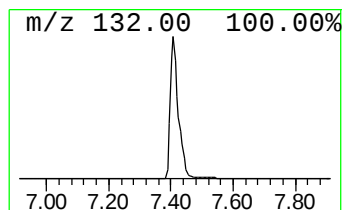
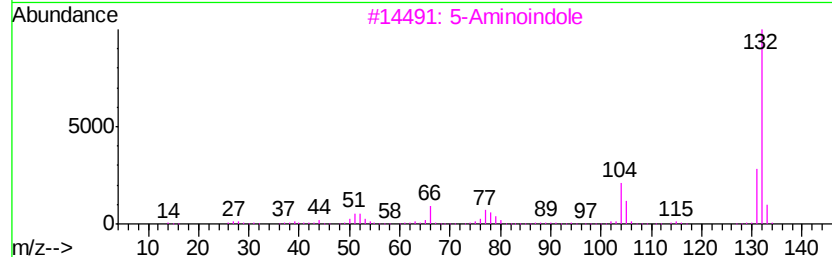
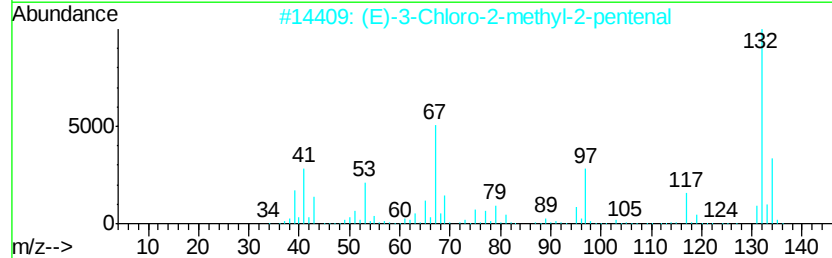
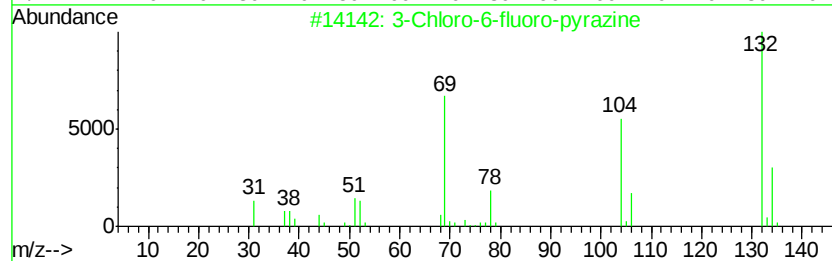
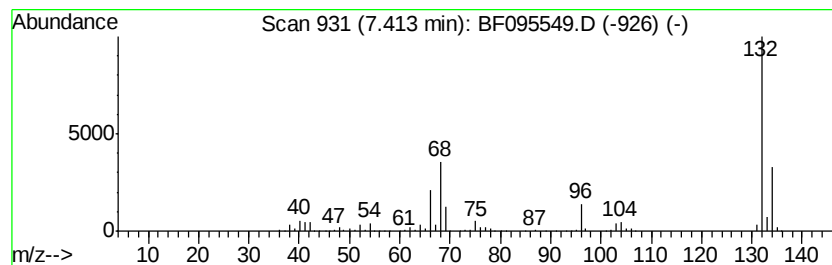
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	89.56 ng	2159240	1,4-Dichlorobenzene-d4	7.74

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	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Xenon	132	Xe	007440-63-3	9



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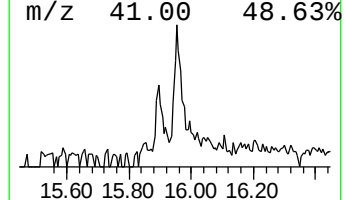
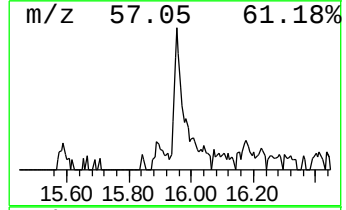
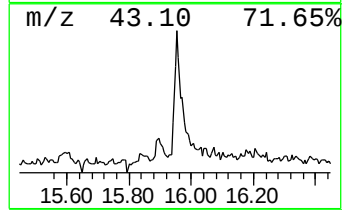
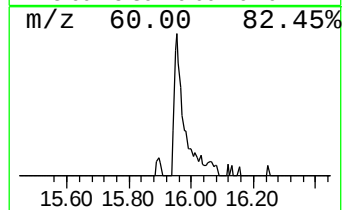
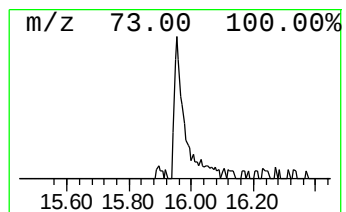
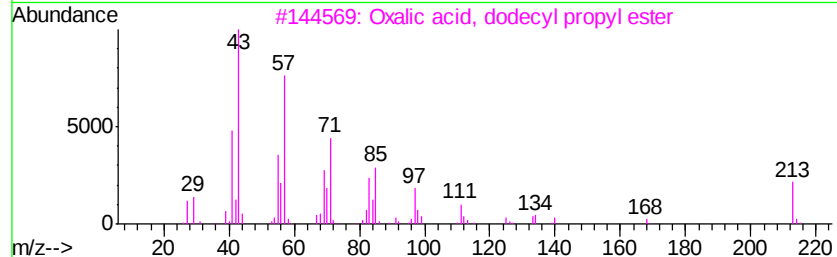
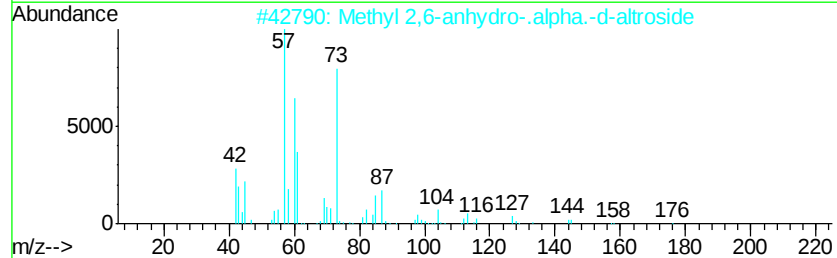
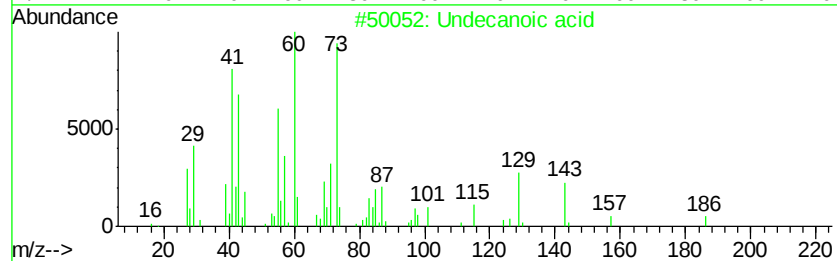
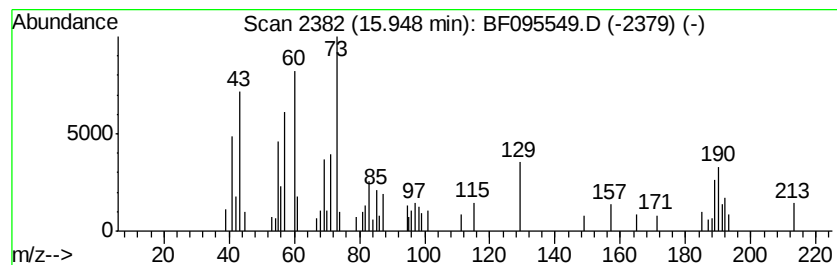
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.95 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	5.09 ng	131307	Phenanthrene-d10	15.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Undecanoic acid	186	C11H22O2	000112-37-8	47
2		Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	27
3		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	11
4		Undecane, 2-methyl-	170	C12H26	007045-71-8	10
5		Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	10



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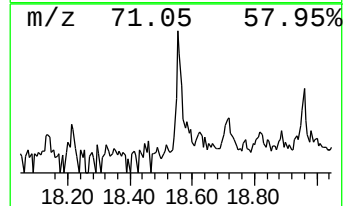
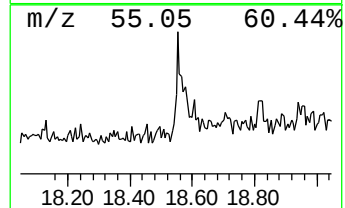
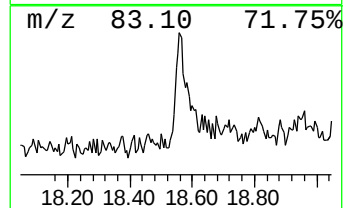
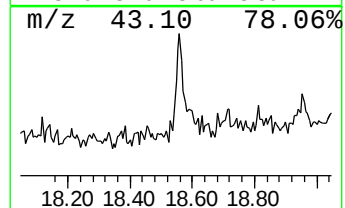
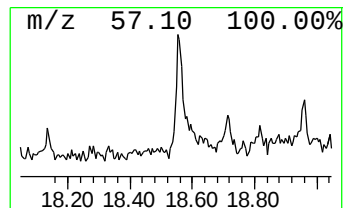
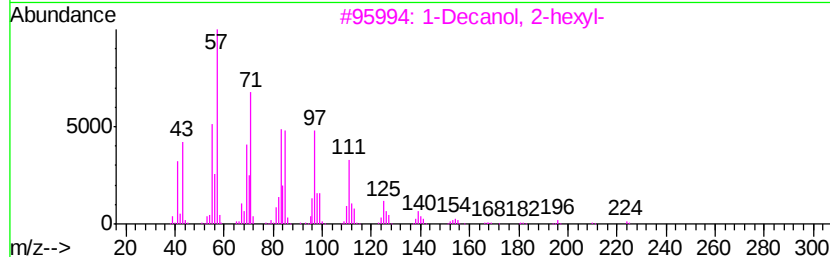
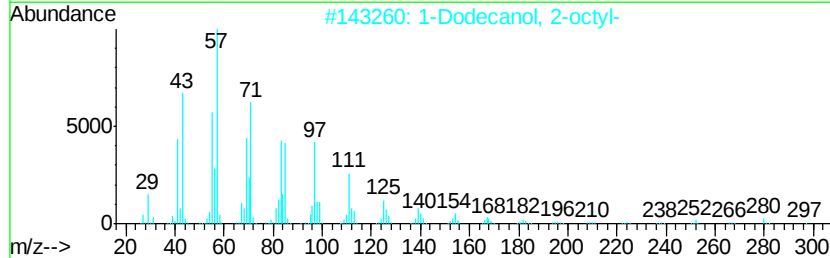
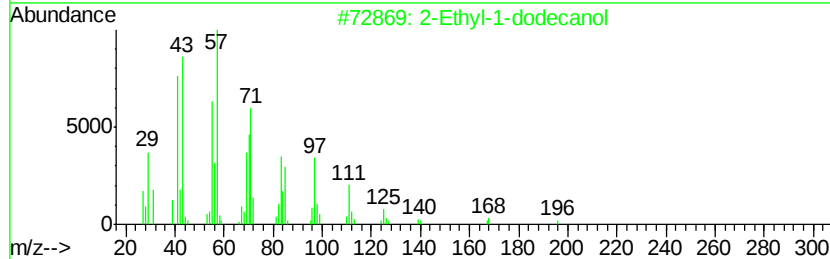
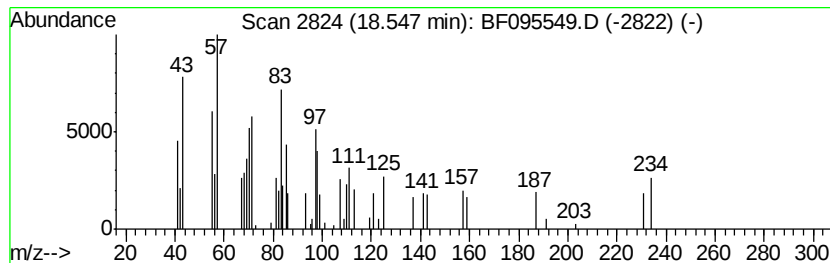
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Ethyl-1-dodecanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	2.21 ng	67741	Chrysene-d12	18.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Ethyl-1-dodecanol	214 C14H30O	019780-33-7	86
2	1-Dodecanol, 2-octyl-	298 C20H42O	005333-42-6	72
3	1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6	68
4	Tetratriacontyl trifluoroacetate	591 C36H69F3O2	1000351-75-3	58
5	Dotriacontyl heptafluorobutyrate	662 C36H65F7O2	1000351-84-2	58



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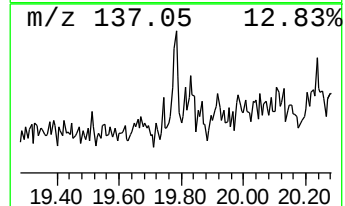
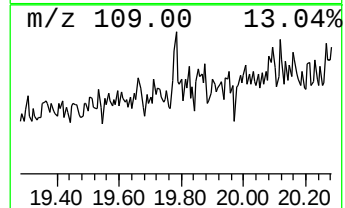
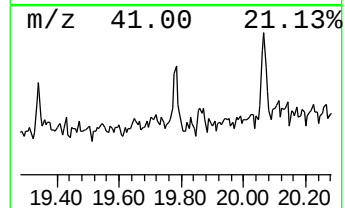
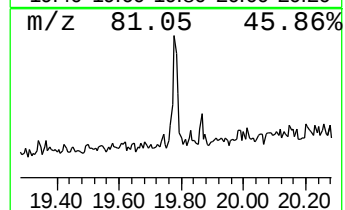
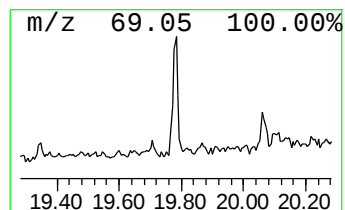
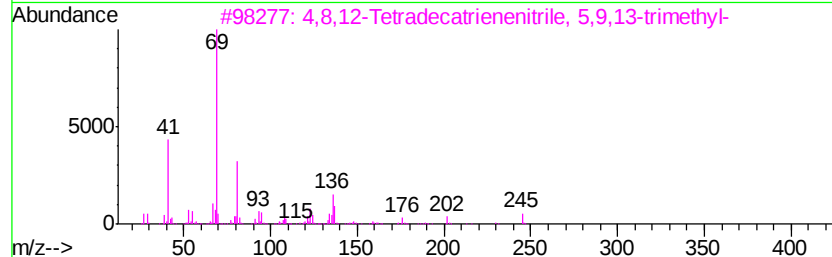
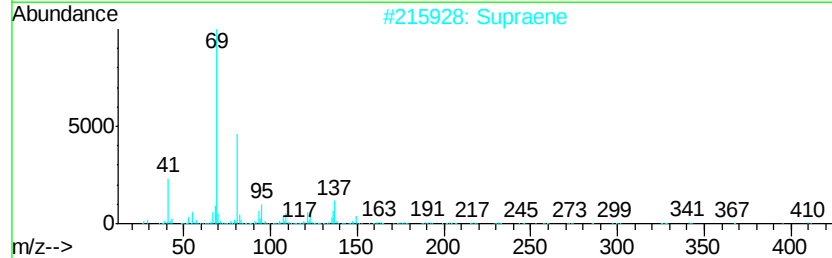
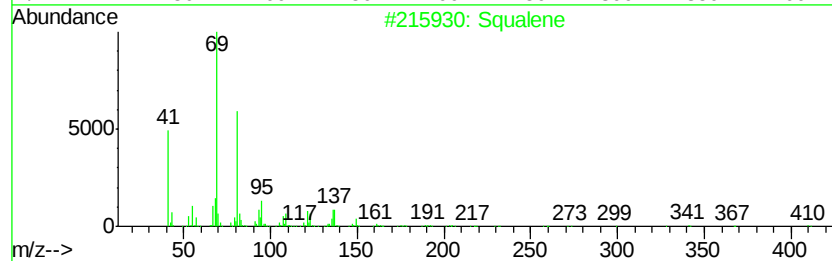
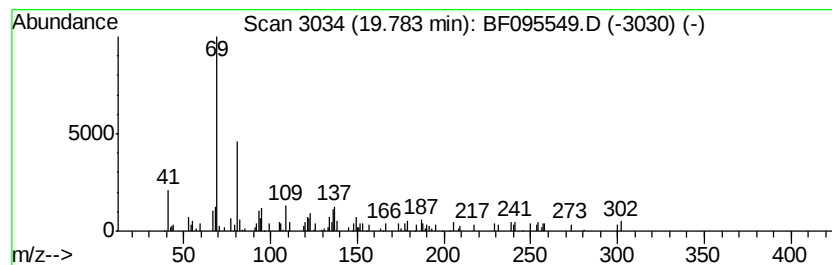
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.78	4.06 ng	71524	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	64
2		Supraene	410	C30H50	007683-64-9	64
3		4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	59
4		2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	59
5		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095549.D
Acq On : 30 May 2017 22:33
Operator : SJ/MA
Sample : I3302-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM12-COMP-0-6

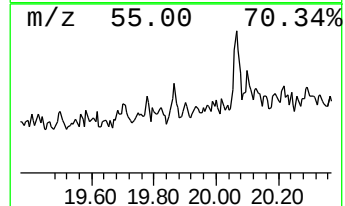
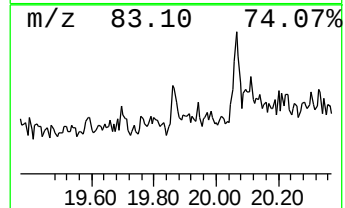
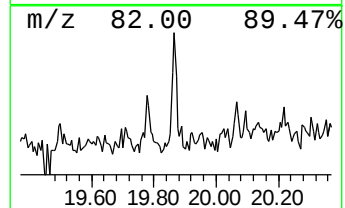
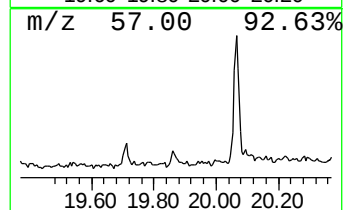
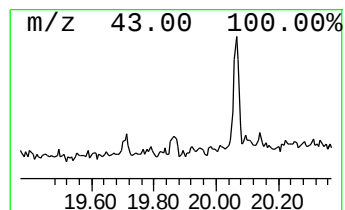
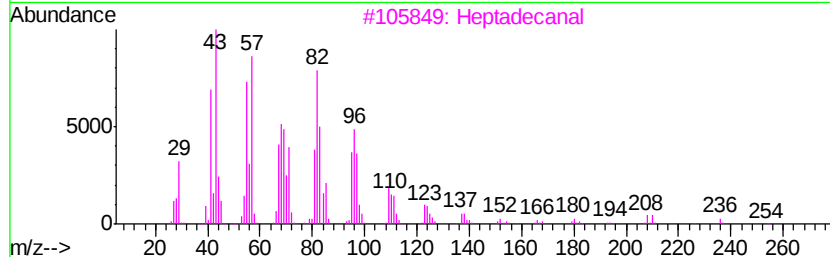
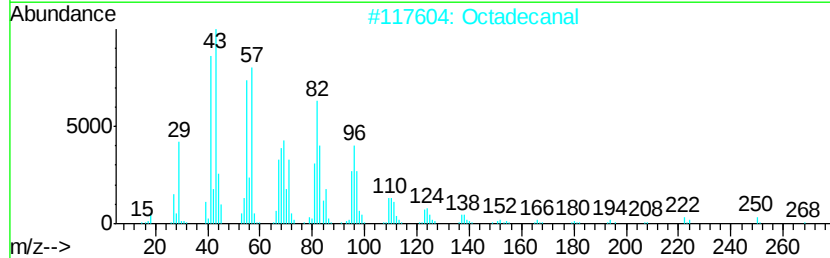
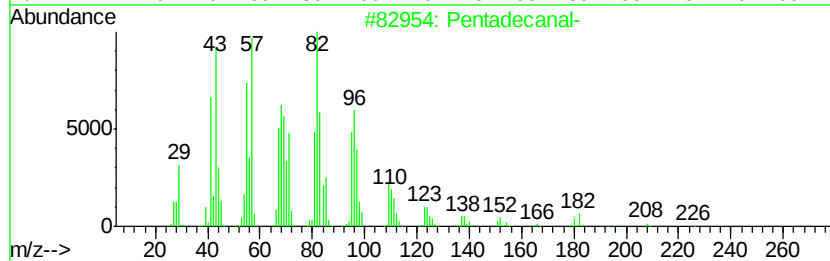
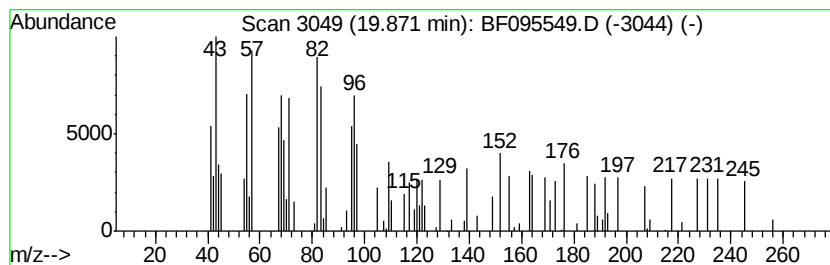
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecanal- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.87	2.02 ng	35634	Perylene-d12	20.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanal-		226	C15H30O	002765-11-9	53
2	Octadecanal		268	C18H36O	000638-66-4	53
3	Heptadecanal		254	C17H34O	1000376-70-0	53
4	1,19-Eicosadiene		278	C20H38	014811-95-1	49
5	2,5a-Methano-5aH-pyrido[1,2-b][1...		167	C10H17NO	054980-46-0	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
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Acq On : 30 May 2017 22:33
Operator : SJ/MA
Sample : I3302-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

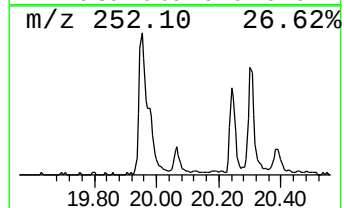
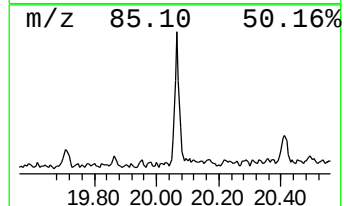
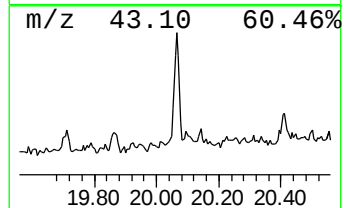
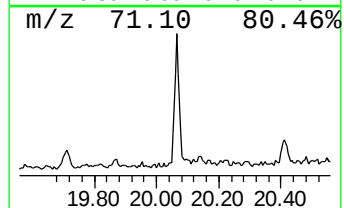
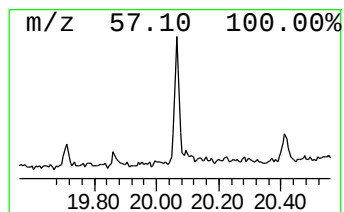
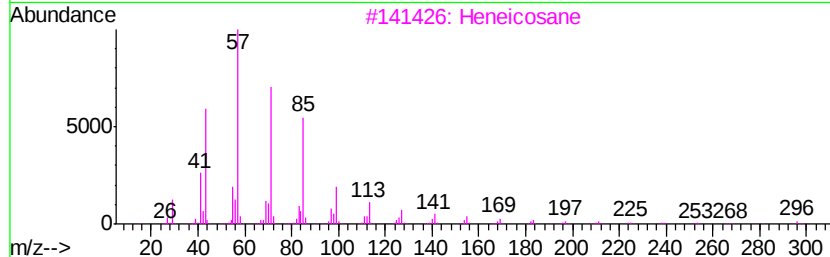
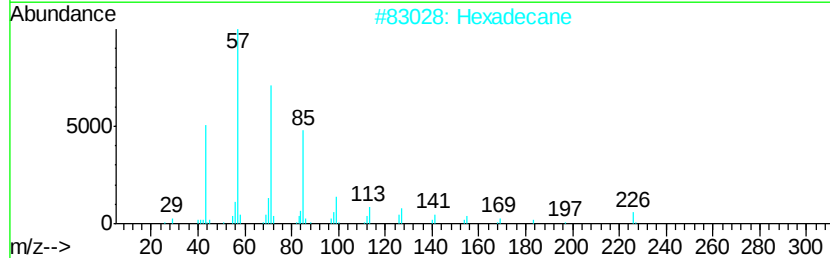
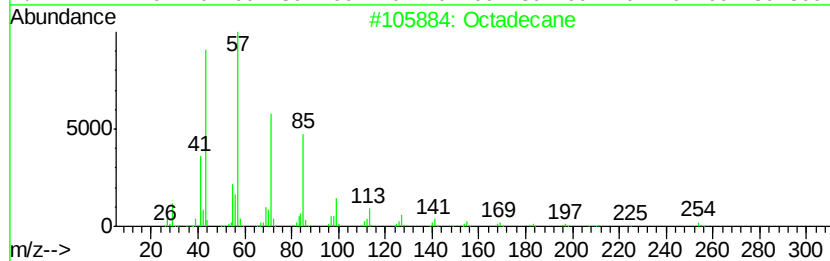
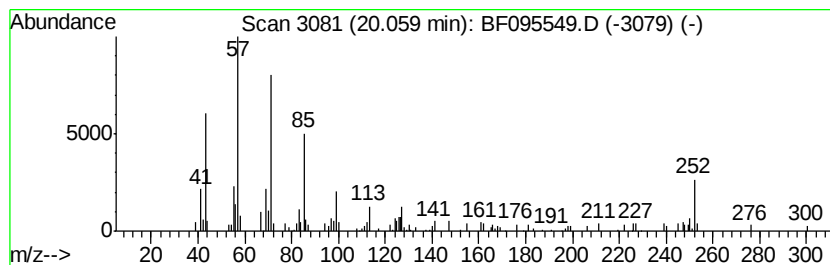
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
20.06	5.05 ng	89066	Perylene-d12		20.35
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Pentacosane	352	C25H52	000629-99-2	83
5	Triacontane	422	C30H62	000638-68-6	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095549.D
Acq On : 30 May 2017 22:33
Operator : SJ/MA
Sample : I3302-07
Misc :
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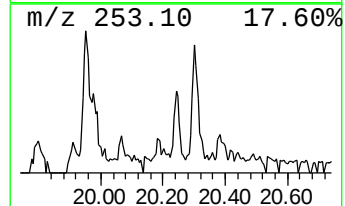
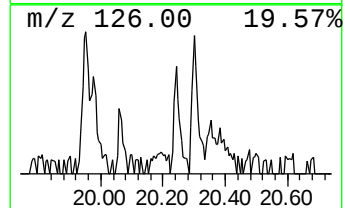
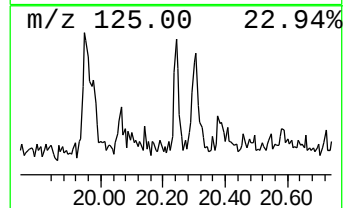
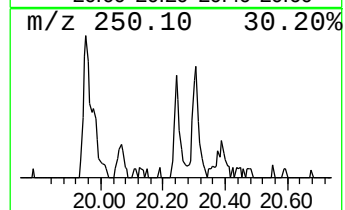
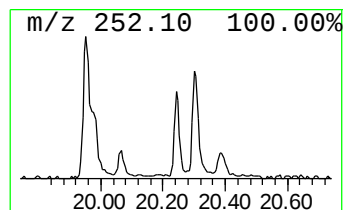
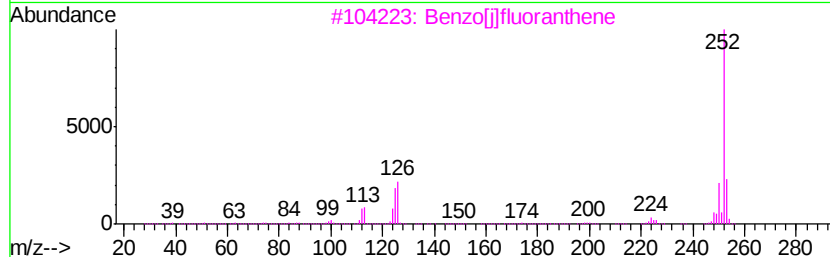
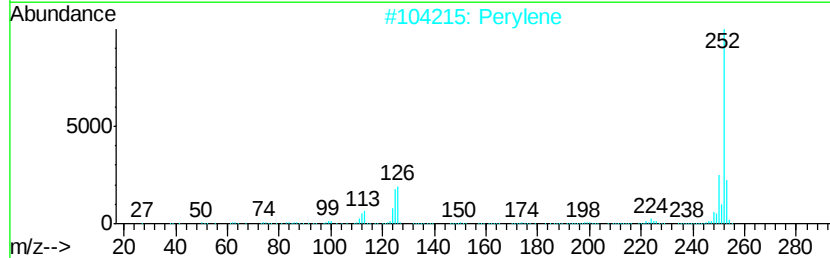
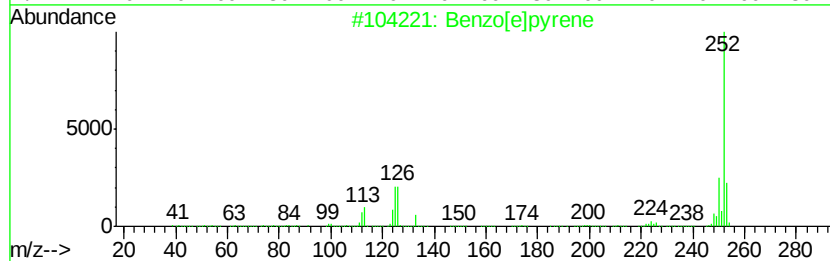
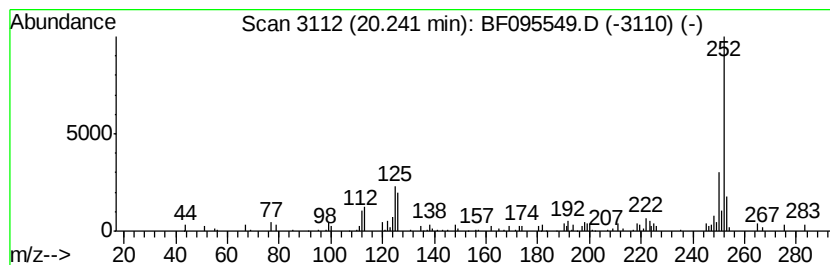
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.24	2.30 ng	40491	Perylene-d12	20.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Benzo[e]pyrene	252 C20H12	000192-97-2	96
2	Perylene	252 C20H12	000198-55-0	94
3	Benzo[j]fluoranthene	252 C20H12	000205-82-3	93
4	Benz[e]acephenanthrylene	252 C20H12	000205-99-2	93
5	Benzo[a]pyrene	252 C20H12	000050-32-8	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
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Acq On : 30 May 2017 22:33
Operator : SJ/MA
Sample : I3302-07
Misc :
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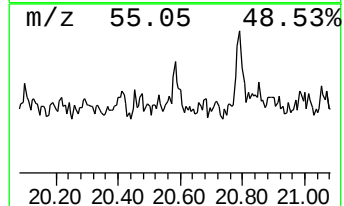
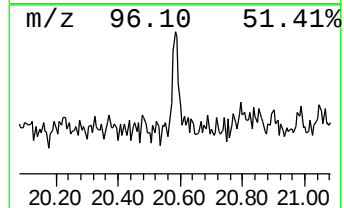
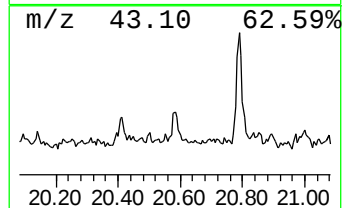
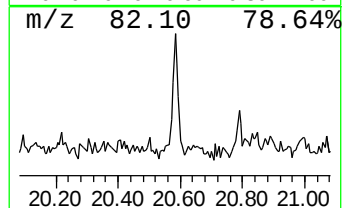
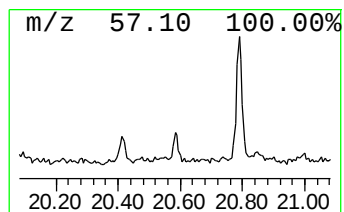
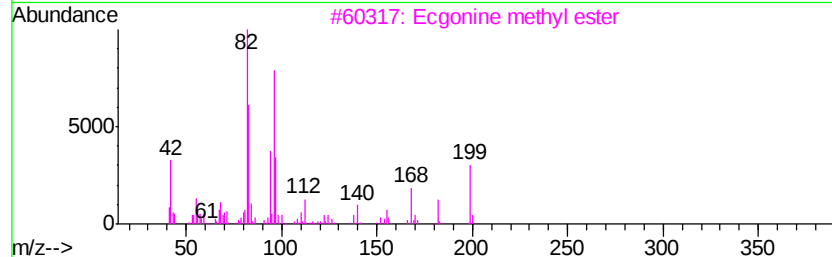
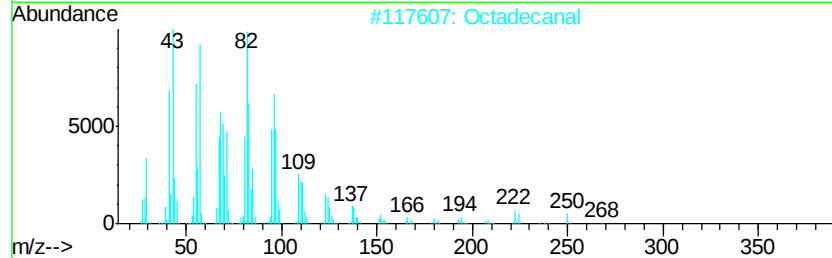
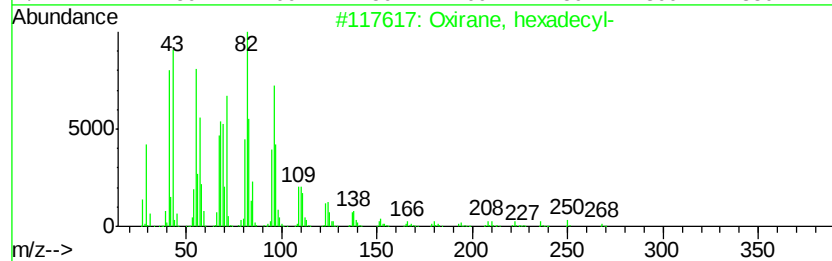
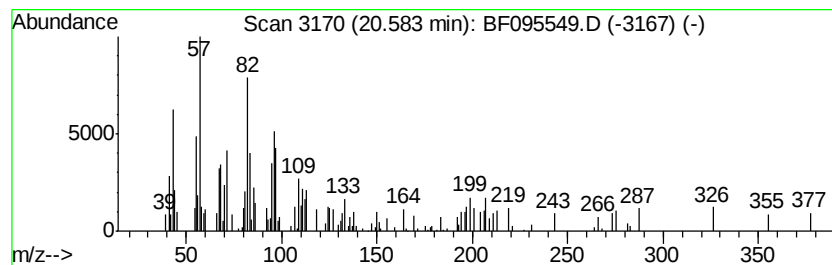
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.58	3.59 ng	63189	Perylene-d12	20.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Oxirane, hexadecyl-	268 C18H36O	007390-81-0 78
2		Octadecanal	268 C18H36O	000638-66-4 62
3		Ecgonine methyl ester	199 C10H17NO3	106293-60-1 49
4		Pentadecanal-	226 C15H30O	002765-11-9 49
5		E-11(13-Methyl)tetradecen-1-ol a...	268 C17H32O2	1000130-80-4 46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095549.D
Acq On : 30 May 2017 22:33
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Sample : I3302-07
Misc :
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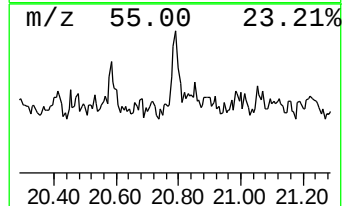
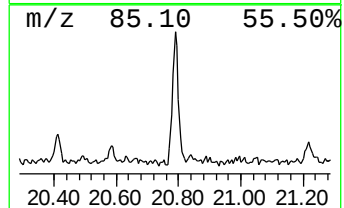
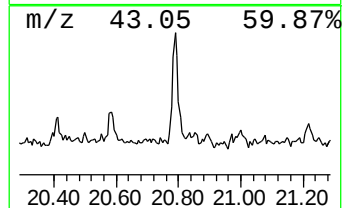
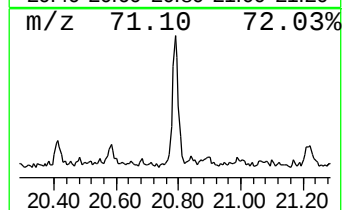
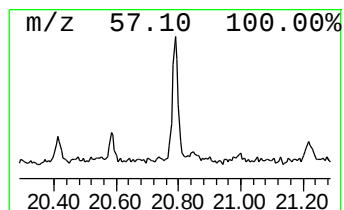
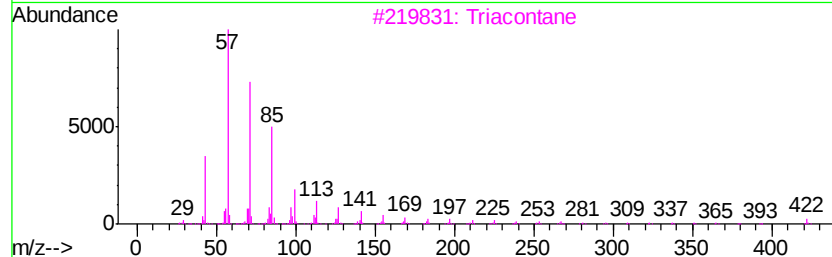
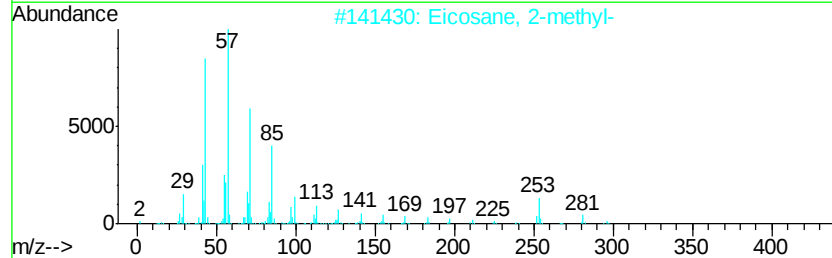
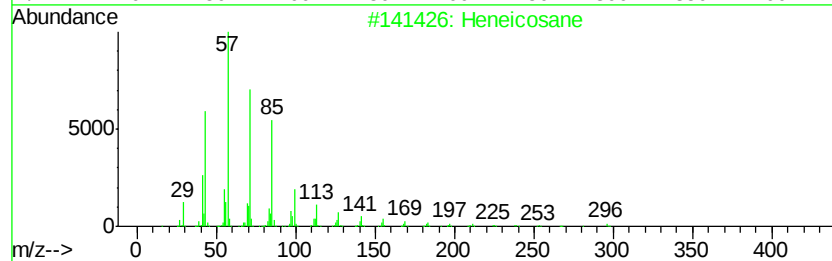
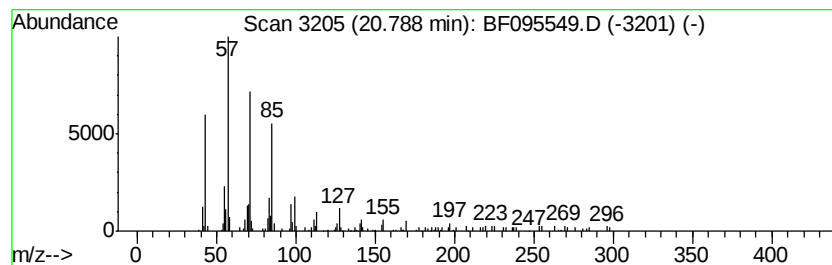
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	6.82 ng	120200	Perylene-d12	20.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Eicosane, 2-methyl-	296	C21H44	001560-84-5	95
3			Triacontane	422	C30H62	000638-68-6	91
4			Hexatriacontane	507	C36H74	000630-06-8	91
5			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095549.D
Acq On : 30 May 2017 22:33
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Misc :
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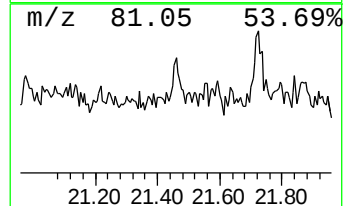
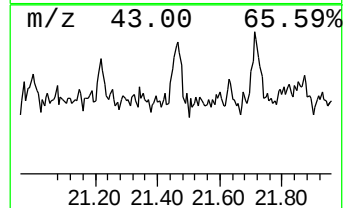
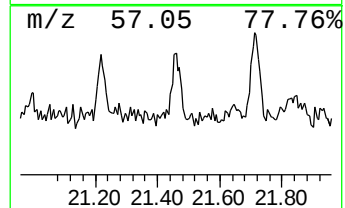
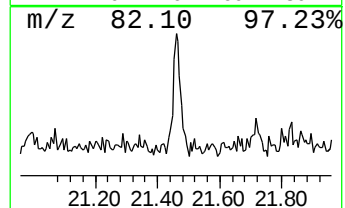
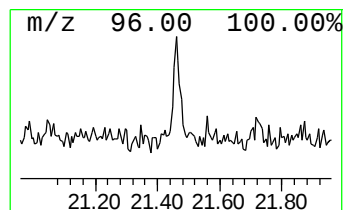
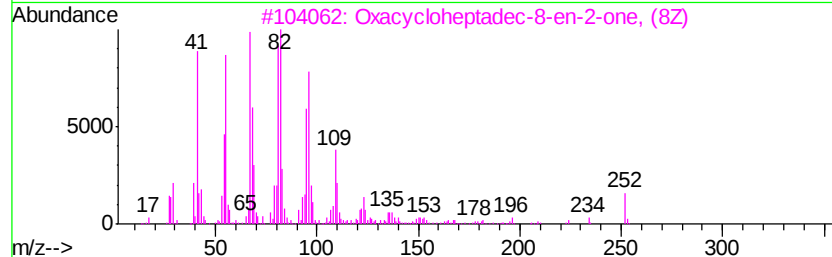
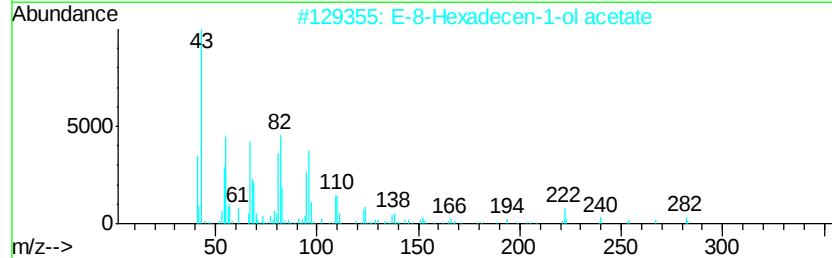
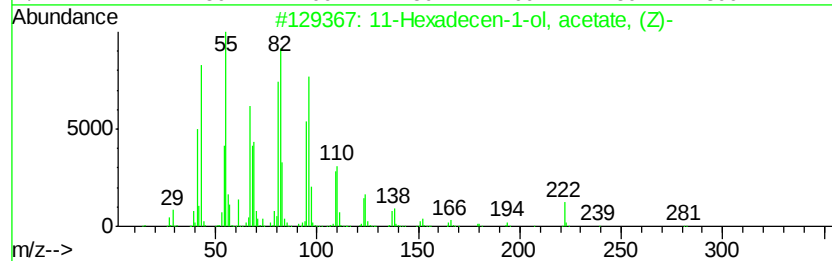
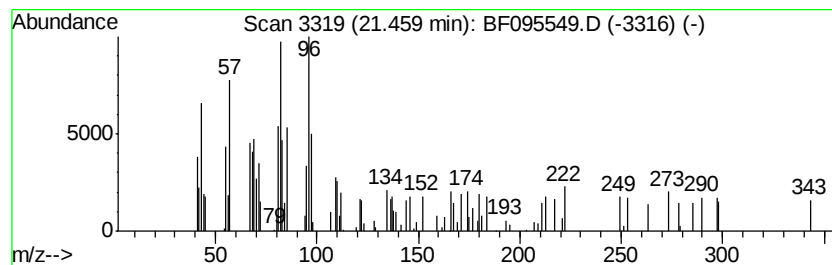
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 11-Hexadecen-1-ol, acetate,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.46	3.03 ng	53464	Perylene-d12	20.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Hexadecen-1-ol, acetate, (Z)-	282	C18H34O2	034010-21-4	53
2			E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	49
3			Oxacycloheptadec-8-en-2-one, (8Z)	252	C16H28O2	000123-69-3	49
4			E-11-Hexadecen-1-ol	240	C16H32O	1000130-89-8	49
5			7-Hexadecen-1-ol, acetate, (Z)-	282	C18H34O2	023192-42-9	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095549.D
Acq On : 30 May 2017 22:33
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Sample : I3302-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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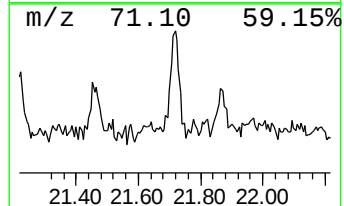
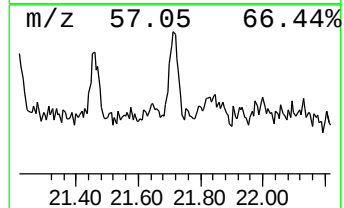
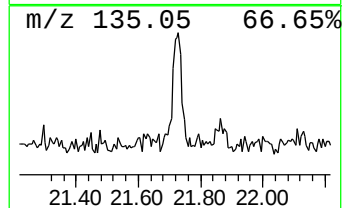
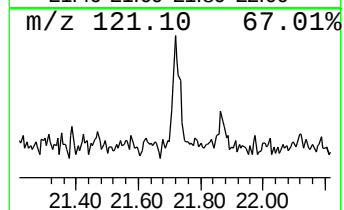
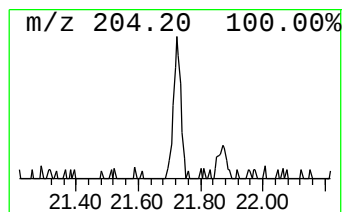
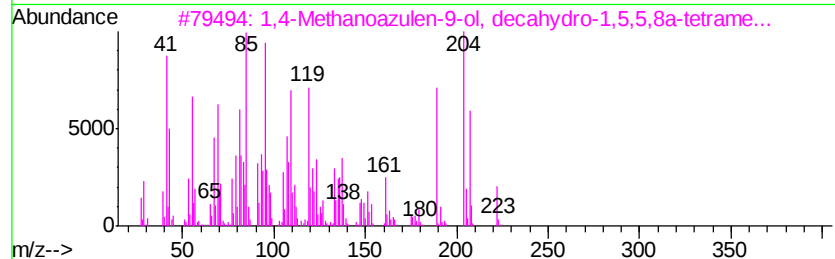
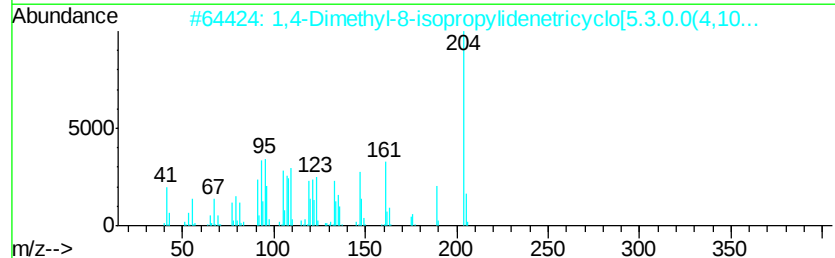
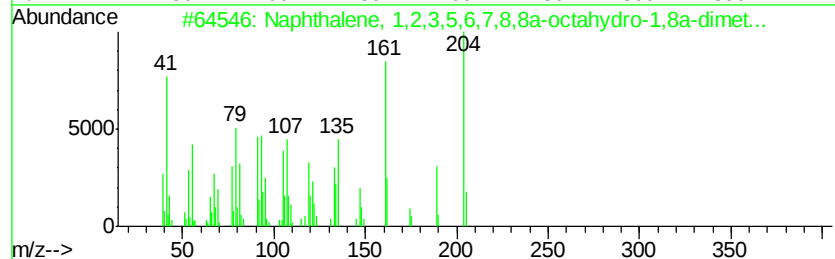
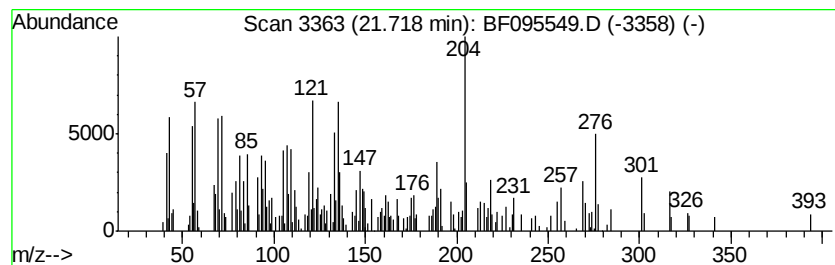
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Naphthalene, 1,2,3,5,6,7,8,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	11.87 ng	209213	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	70
2		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	46
3		1,4-Methanoazulen-9-ol, decahydr...	222	C15H26O	000465-24-7	44
4		1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	38
5		2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053017\
Data File : BF095549.D
Acq On : 30 May 2017 22:33
Operator : SJ/MA
Sample : I3302-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM12-COMP-0-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	5.09	6.6 ng		158419	1	7.74	482182	20.0
unknown7.41	7.41	89.6 ng		2159240	1	7.74	482182	20.0
unknown15.95	15.95	5.1 ng		131307	4	15.01	516203	20.0
2-Ethyl-1-dodecanol	18.55	2.2 ng		67741	5	18.68	613640	20.0
Squalene	19.78	4.1 ng		71524	6	20.35	352423	20.0
Pentadecanal-	19.87	2.0 ng		35634	6	20.35	352423	20.0
Octadecane	20.06	5.0 ng		89066	6	20.35	352423	20.0
Benzo[e]pyrene	20.24	2.3 ng		40491	6	20.35	352423	20.0
Oxirane, hexadecyl-	20.58	3.6 ng		63189	6	20.35	352423	20.0
Heneicosane	20.79	6.8 ng		120200	6	20.35	352423	20.0
11-Hexadecen-1-ol...	21.46	3.0 ng		53464	6	20.35	352423	20.0
Naphthalene, 1,2,...	21.72	11.9 ng		209213	6	20.35	352423	20.0