

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
 Data File : BM018303.D
 Acq On : 19 Dec 2018 19:11
 Operator : JU/SJ
 Sample : J6477-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-A1

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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	4.681	301	305	312	rBV	92039	122480	2.87%	0.351%
2	5.122	373	380	394	rBV	2113255	3016508	70.64%	8.650%
3	6.687	639	646	661	rBV	1984623	3320984	77.77%	9.523%
4	7.028	697	704	714	rBV	2146916	3323342	77.83%	9.530%
5	7.487	776	782	791	rVB	369609	583805	13.67%	1.674%
6	7.799	828	835	845	rBV	1562935	2464381	57.71%	7.067%
7	8.646	970	979	997	rBV	1091493	1922882	45.03%	5.514%
8	10.251	1245	1252	1265	rBV	387186	712959	16.70%	2.044%
9	12.751	1670	1677	1689	rBV	2522137	3770206	88.29%	10.811%
10	13.622	1819	1825	1836	rBV	119524	201784	4.73%	0.579%
11	14.145	1908	1914	1924	rBV2	554466	857287	20.08%	2.458%
12	15.651	2164	2170	2181	rBV	1905002	2784516	65.21%	7.985%
13	16.910	2377	2384	2390	rBV	577720	907338	21.25%	2.602%
14	17.821	2533	2539	2549	rBV	492657	755733	17.70%	2.167%
15	18.986	2730	2737	2743	rBV4	54655	119322	2.79%	0.342%
16	19.115	2754	2759	2770	rBV	199380	332051	7.78%	0.952%
17	19.345	2793	2798	2802	rBV2	57203	91895	2.15%	0.264%
18	19.563	2829	2835	2843	rVB	3688373	4270062	100.00%	12.244%
19	19.880	2886	2889	2895	rVB	92614	107057	2.51%	0.307%
20	20.386	2971	2975	2978	rVB	140525	148588	3.48%	0.426%
21	20.851	3050	3054	3063	rBV	461622	598691	14.02%	1.717%
22	21.133	3096	3102	3108	rBV	769308	1094376	25.63%	3.138%
23	21.292	3126	3129	3135	rBV	221945	227917	5.34%	0.654%
24	21.715	3197	3201	3205	rBV	232644	299054	7.00%	0.858%
25	22.162	3273	3277	3284	rVB	201885	254467	5.96%	0.730%
26	22.280	3293	3297	3303	rVB	797373	1032831	24.19%	2.962%
27	22.645	3355	3359	3364	rVB2	190818	250608	5.87%	0.719%
28	23.174	3446	3449	3457	rVB	179403	265257	6.21%	0.761%
29	23.292	3463	3469	3477	rVB2	578298	1037021	24.29%	2.974%

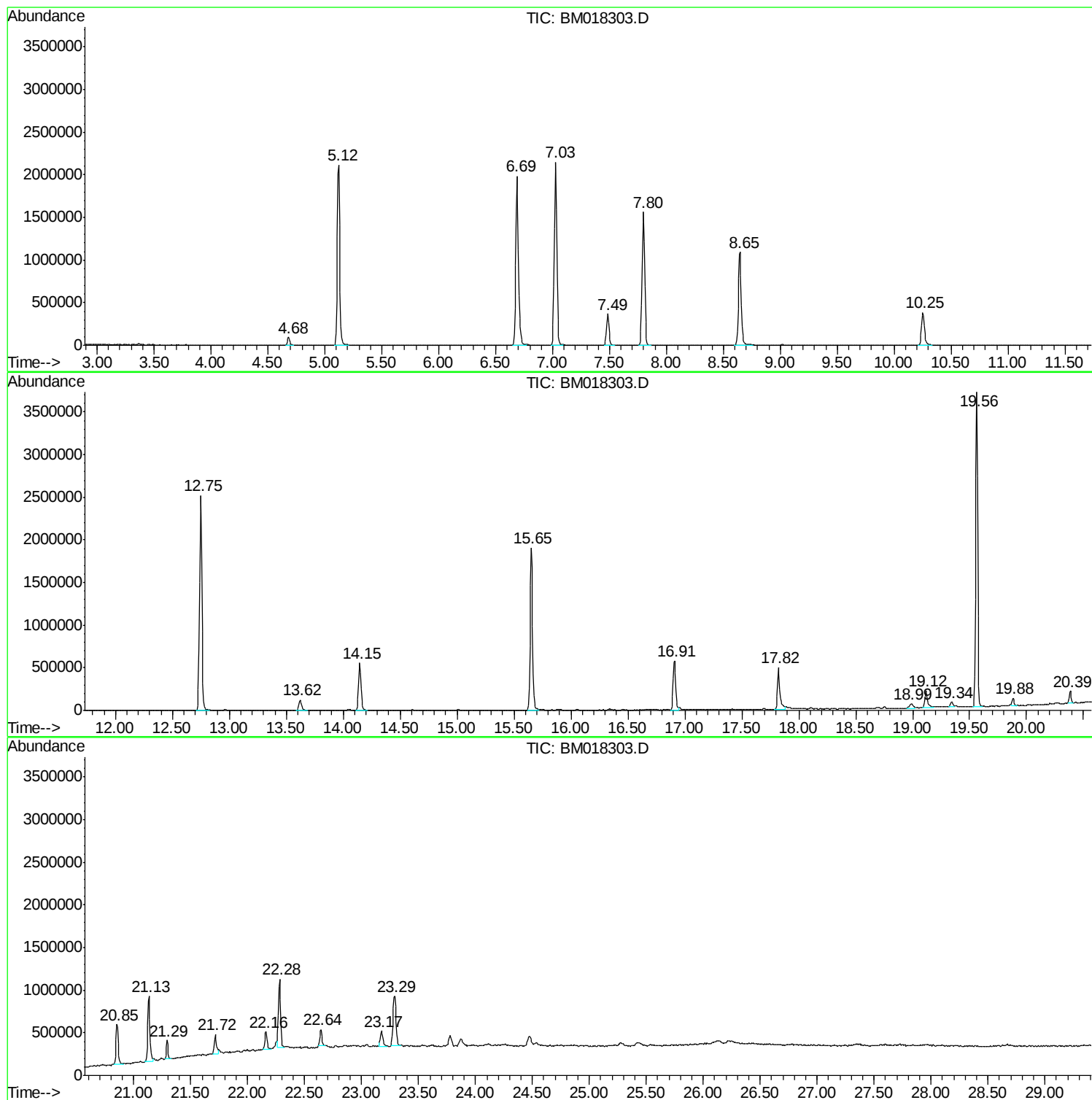
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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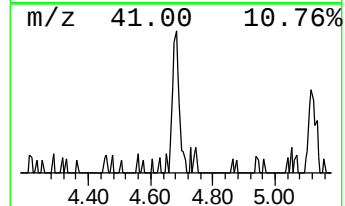
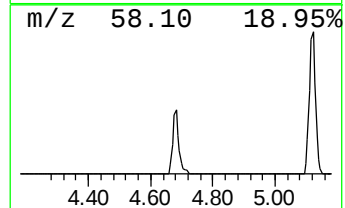
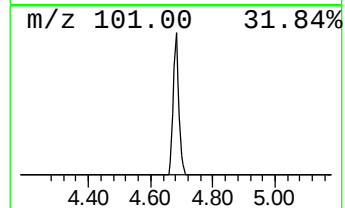
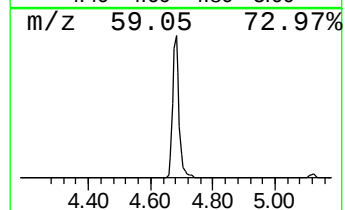
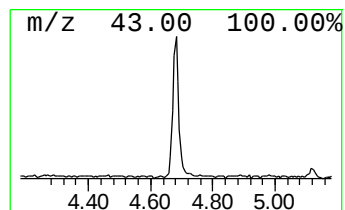
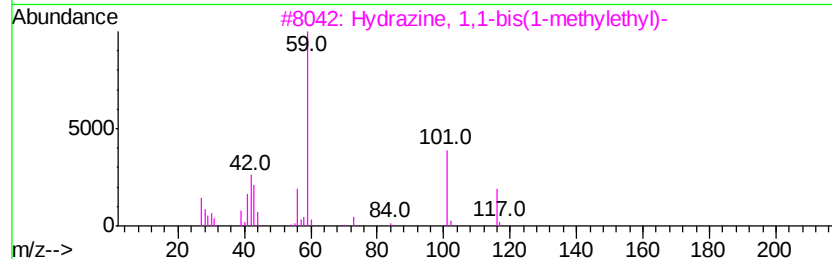
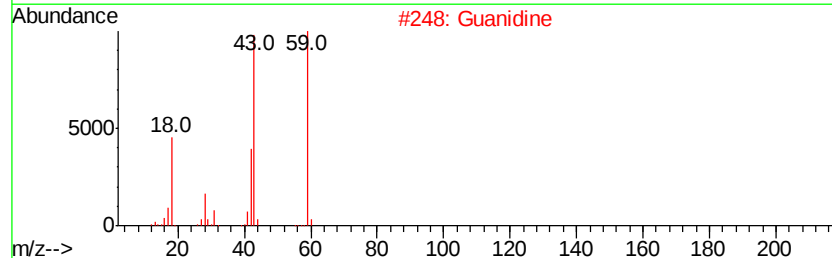
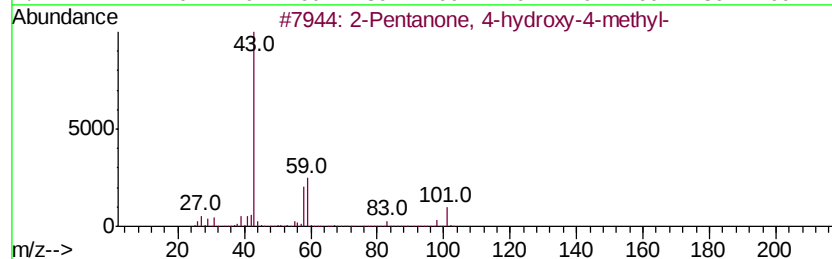
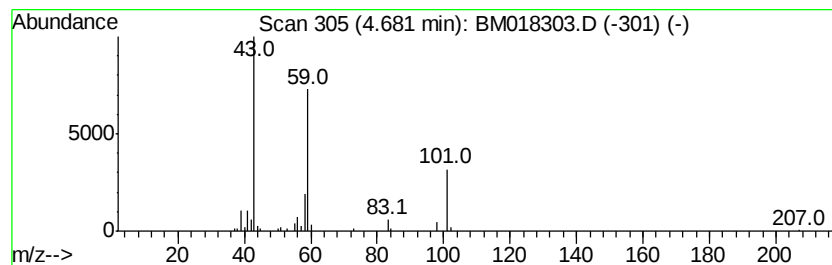
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	4.20 ng	122480	1,4-Dichlorobenzene-d4	7.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Guanidine	59	CH5N3	000113-00-8	43
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7N02	016504-58-8	37
5			Dimethadione	129	C5H7N03	000695-53-4	33



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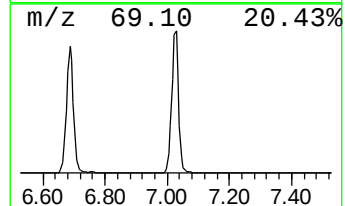
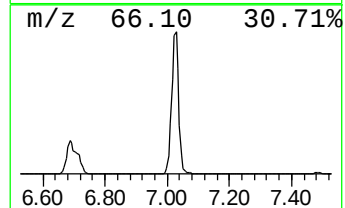
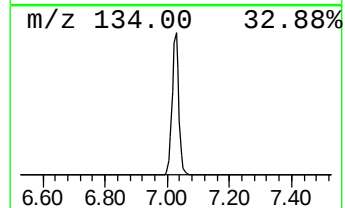
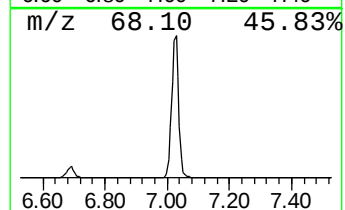
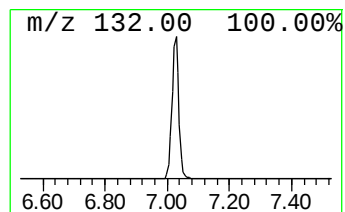
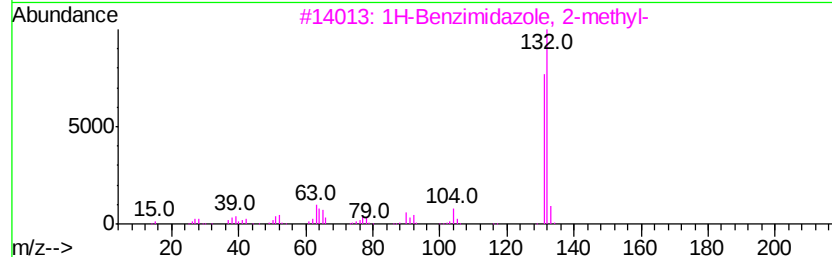
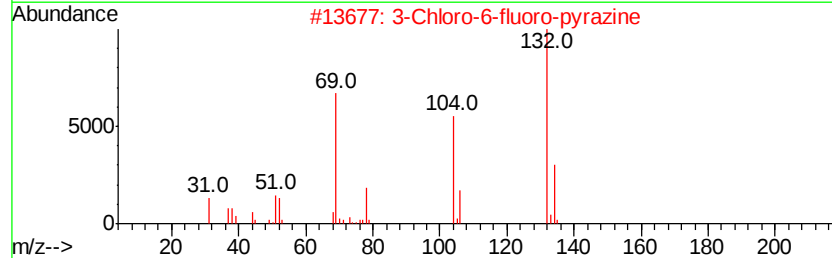
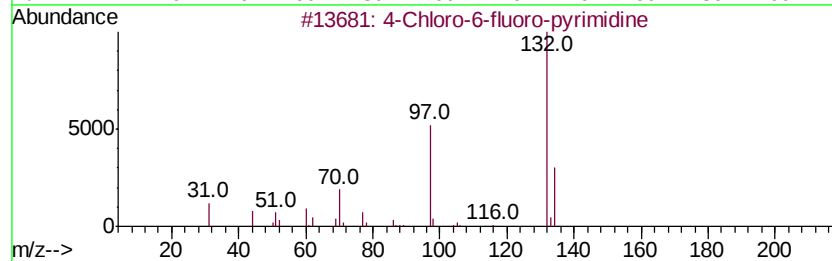
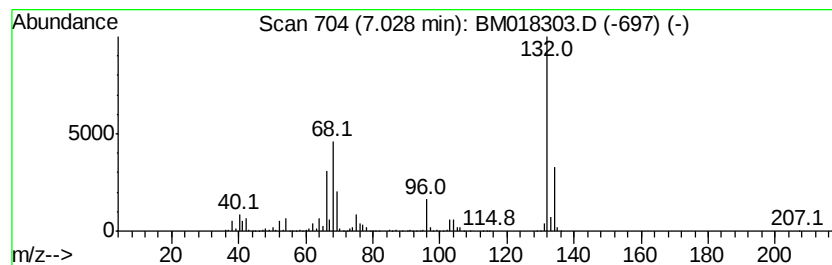
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Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	113.85 ng	3323340	1,4-Dichlorobenzene-d4	7.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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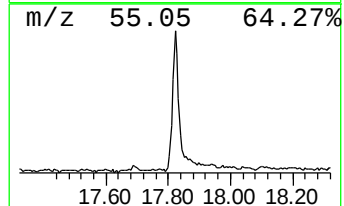
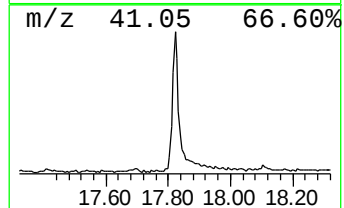
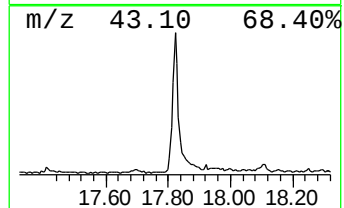
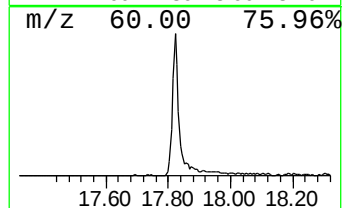
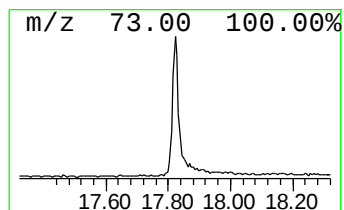
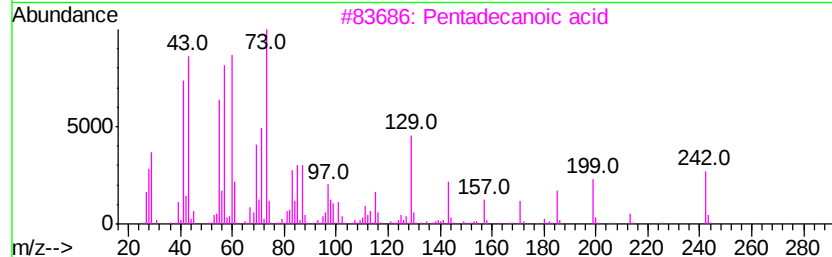
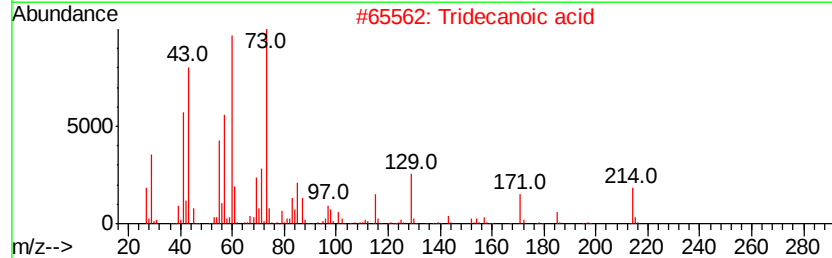
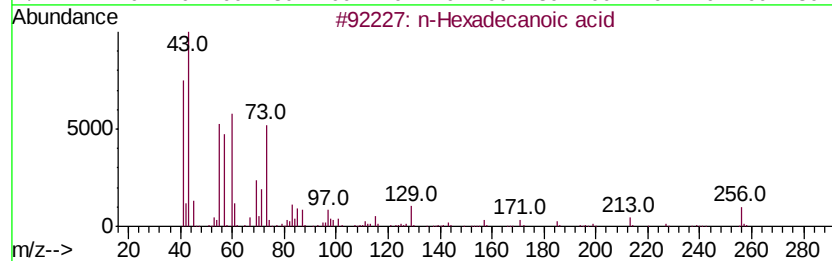
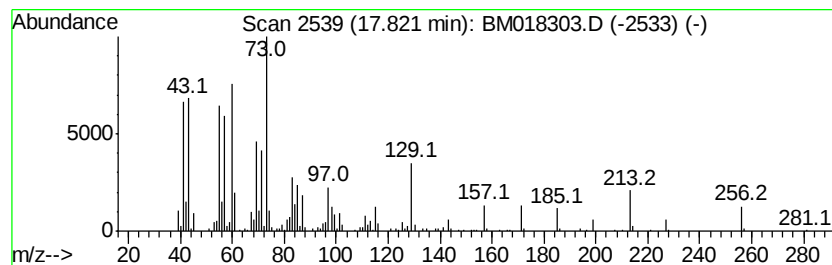
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	16.66 ng	755733	Phenanthrene-d10	16.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	68
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25
5		Hexadecane	226	C16H34	000544-76-3	11



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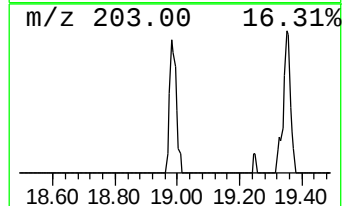
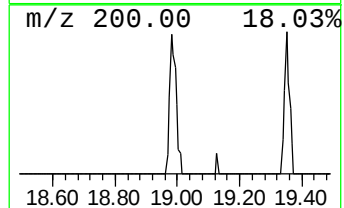
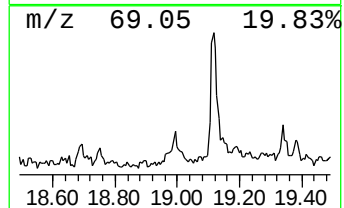
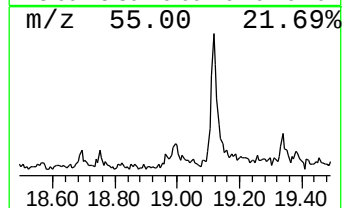
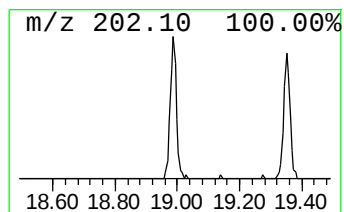
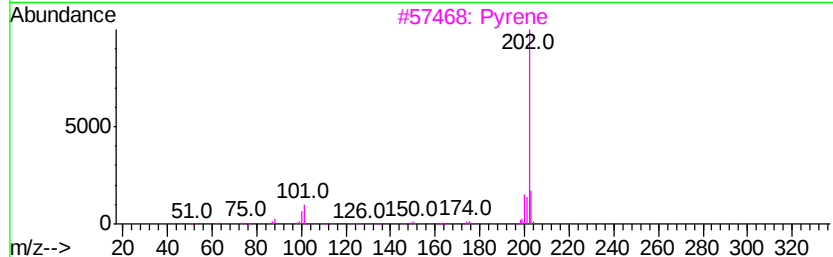
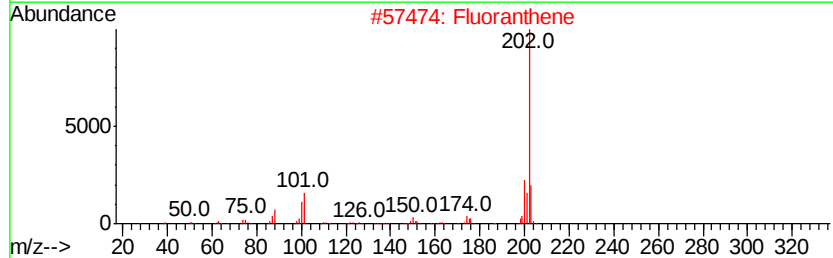
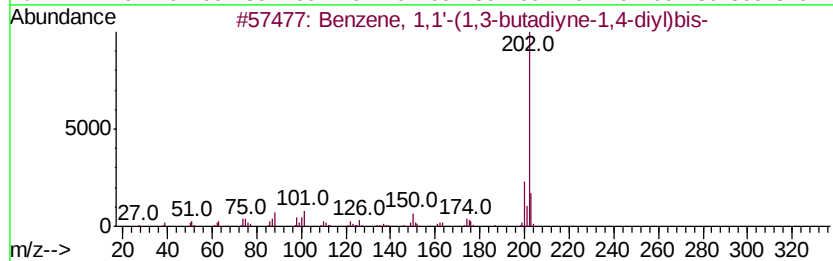
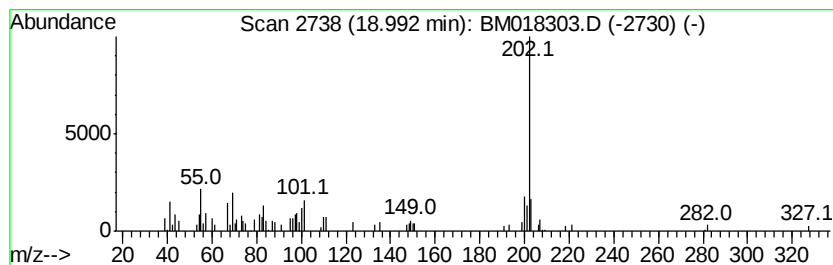
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Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.99	2.63 ng	119322	Phenanthrene-d10	16.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
2		Fluoranthene	202	C16H10	000206-44-0	68
3		Pyrene	202	C16H10	000129-00-0	64
4		3H-Benzo[4,5]furo[3,2-d]pyrimidi...	202	C10H6N2OS	062208-70-2	47
5		1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	45



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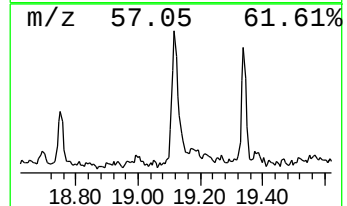
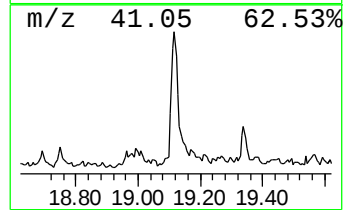
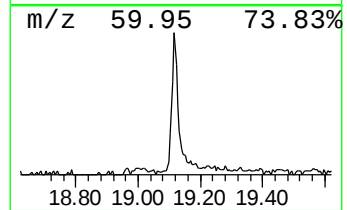
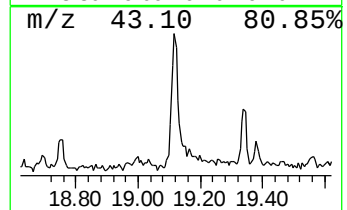
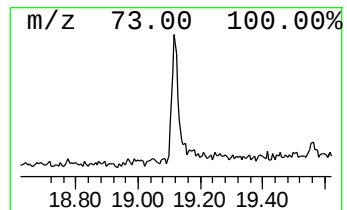
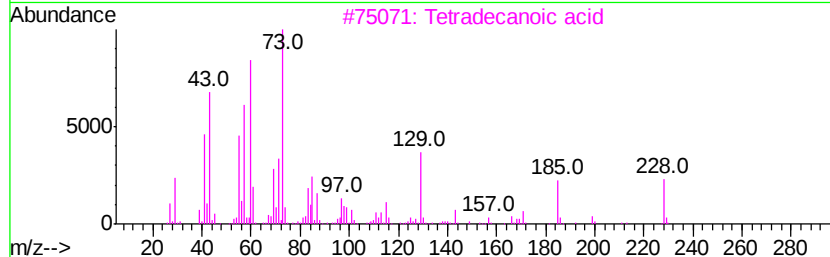
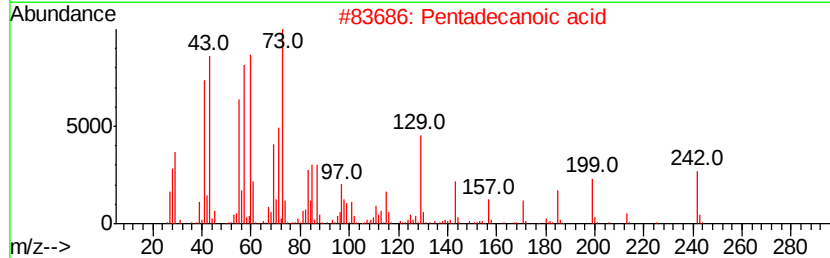
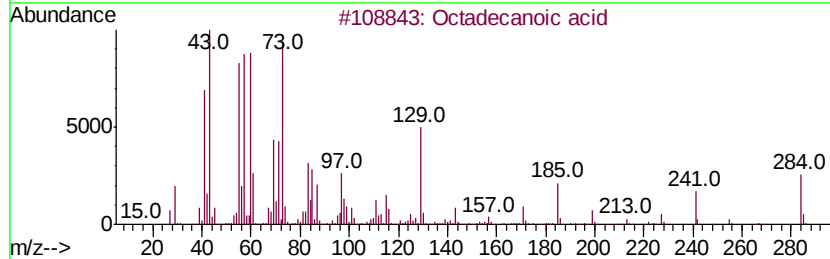
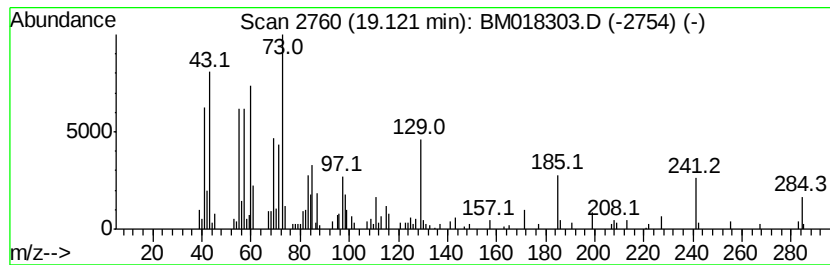
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Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.12	6.07 ng	332051	Chrysene-d12		21.13
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64



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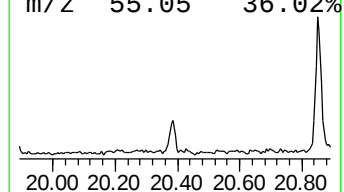
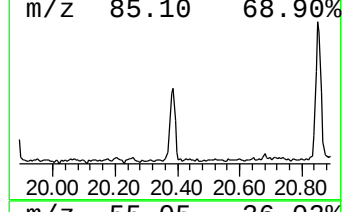
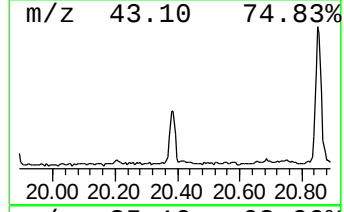
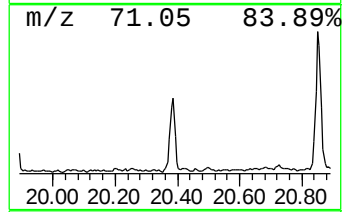
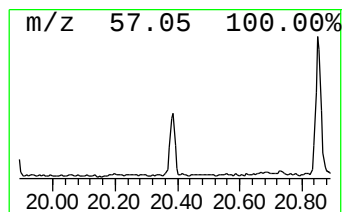
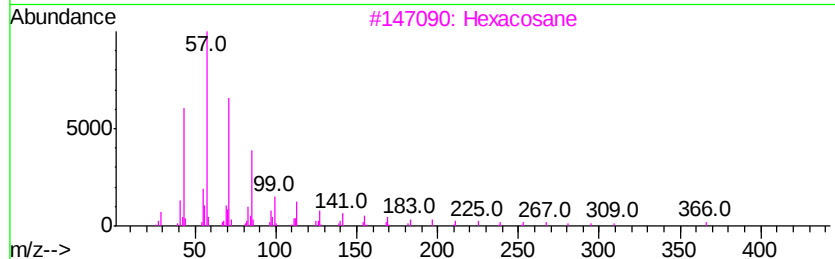
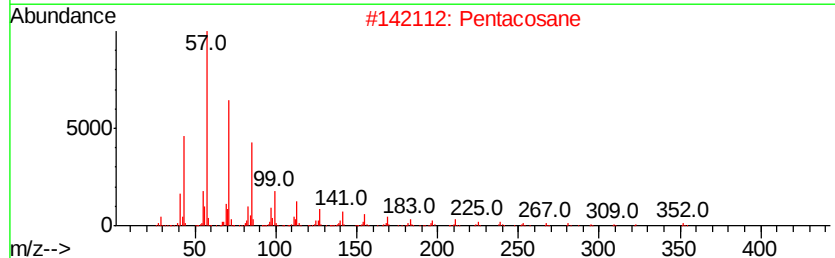
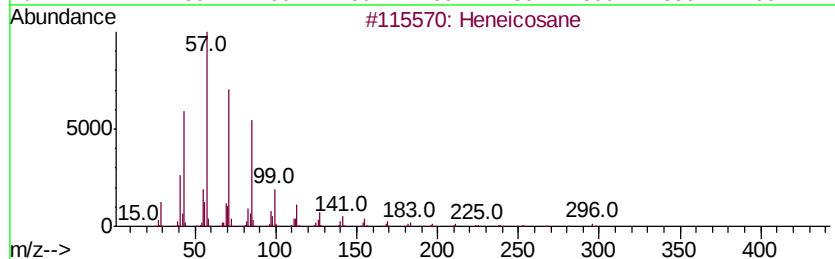
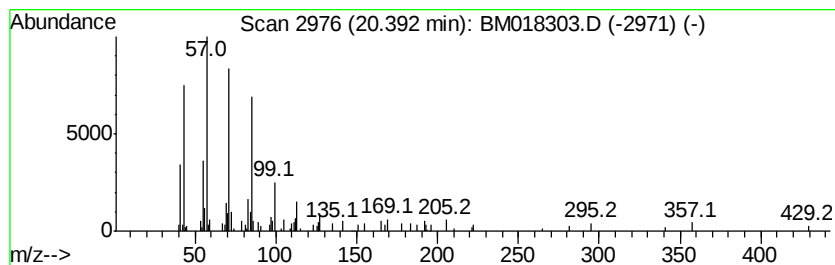
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.39	2.72 ng	148588	Chrysene-d12	21.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Pentacosane		352	C25H52	000629-99-2	90
3	Hexacosane		366	C26H54	000630-01-3	87
4	Tetracosane		338	C24H50	000646-31-1	87
5	Octacosane		394	C28H58	000630-02-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018303.D
Acq On : 19 Dec 2018 19:11
Operator : JU/SJ
Sample : J6477-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-A1

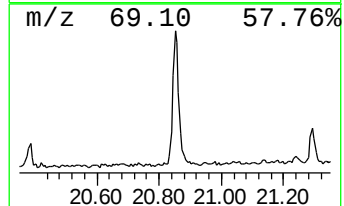
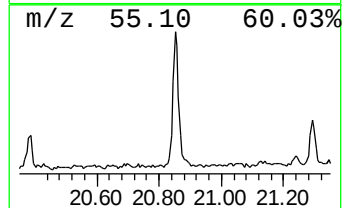
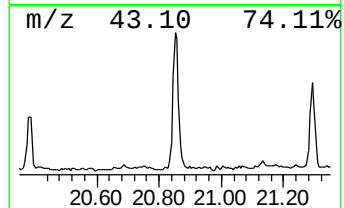
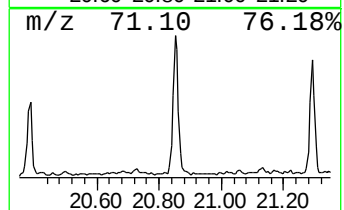
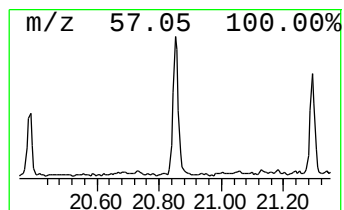
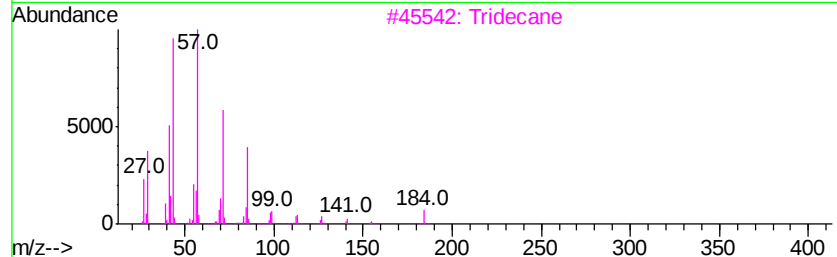
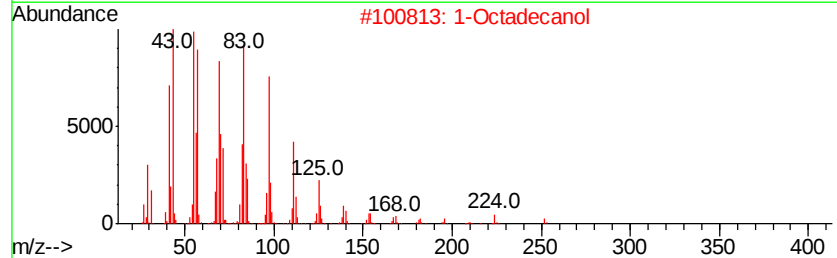
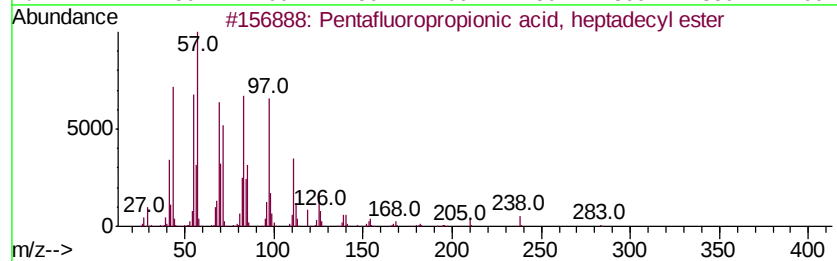
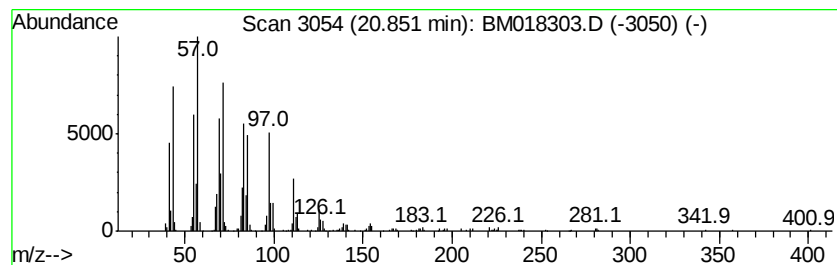
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	10.94 ng	598691	Chrysene-d12	21.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	62
2		1-Octadecanol	270	C18H38O	000112-92-5	60
3		Tridecane	184	C13H28	000629-50-5	60
4		1-Tricosene	322	C23H46	018835-32-0	60
5		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	60



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018303.D
Acq On : 19 Dec 2018 19:11
Operator : JU/SJ
Sample : J6477-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

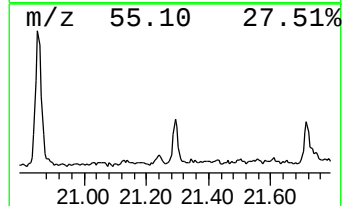
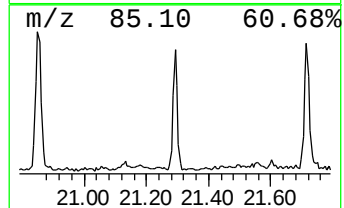
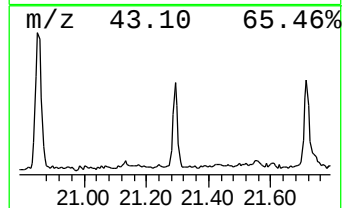
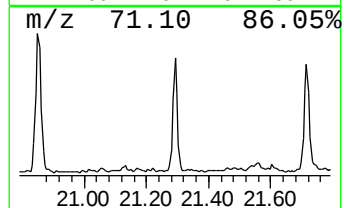
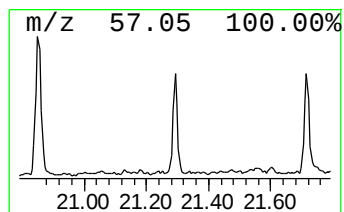
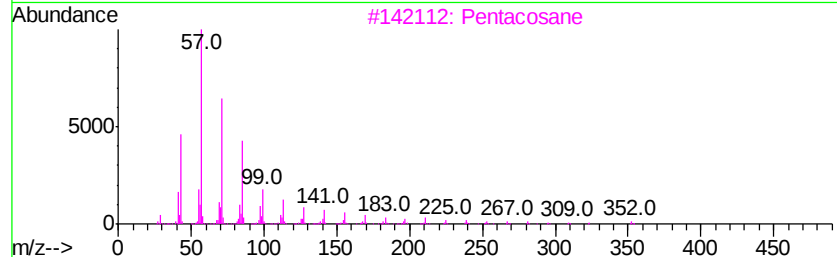
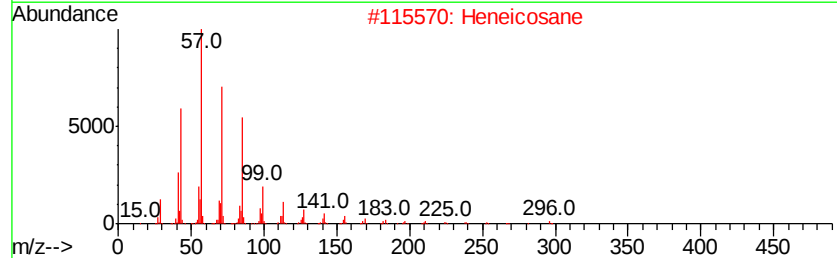
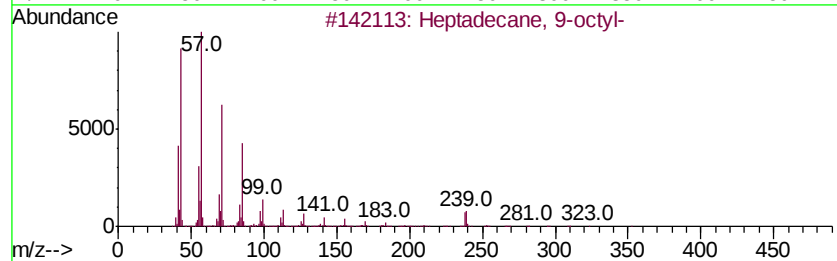
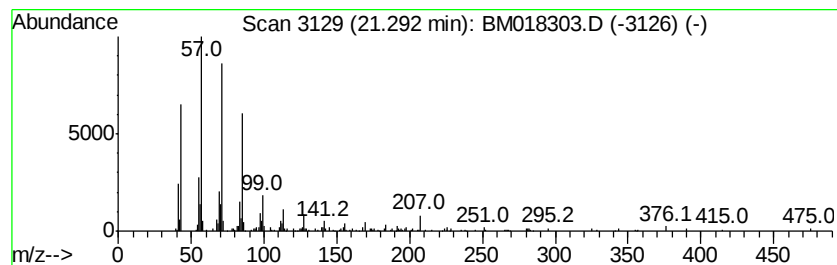
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.17 ng	227917	Chrysene-d12	21.13
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Heptadecane, 9-octyl-	352 C25H52	007225-64-1 91
2		Heneicosane	296 C21H44	000629-94-7 91
3		Pentacosane	352 C25H52	000629-99-2 91
4		Nonacosane	408 C29H60	000630-03-5 91
5		Docosane, 11-butyl-	366 C26H54	013475-76-8 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018303.D
Acq On : 19 Dec 2018 19:11
Operator : JU/SJ
Sample : J6477-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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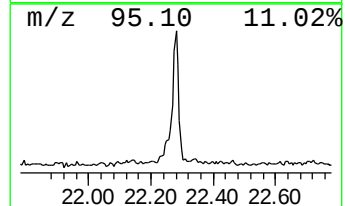
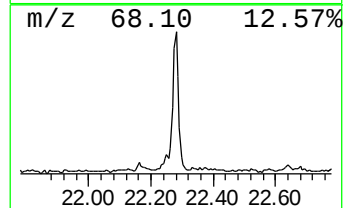
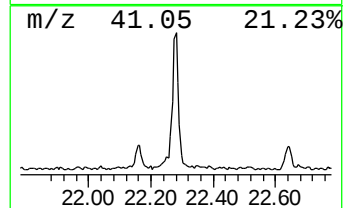
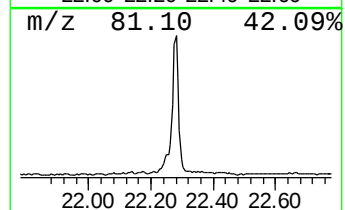
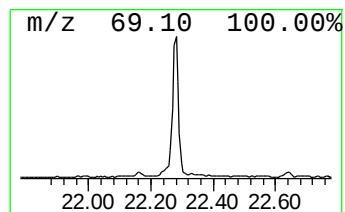
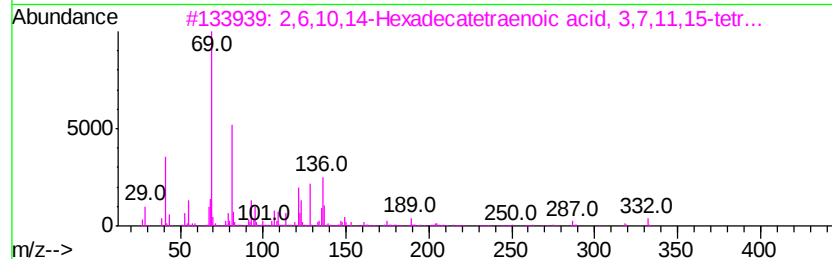
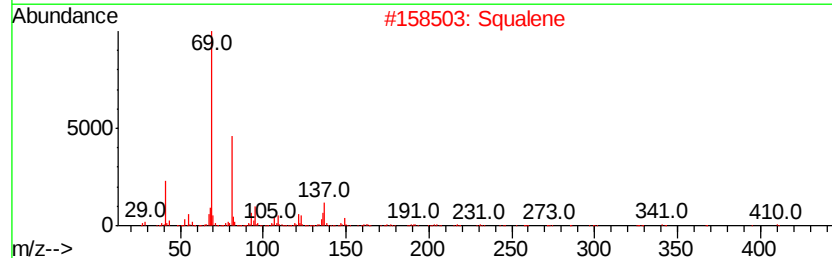
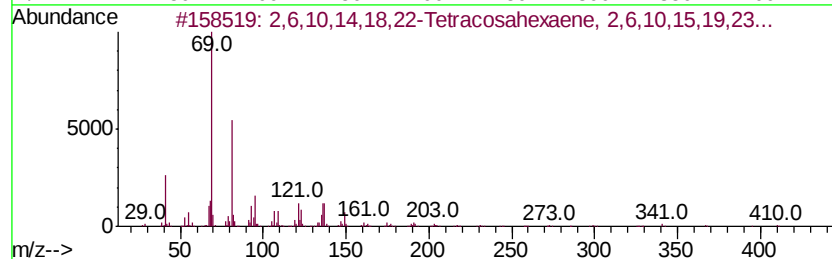
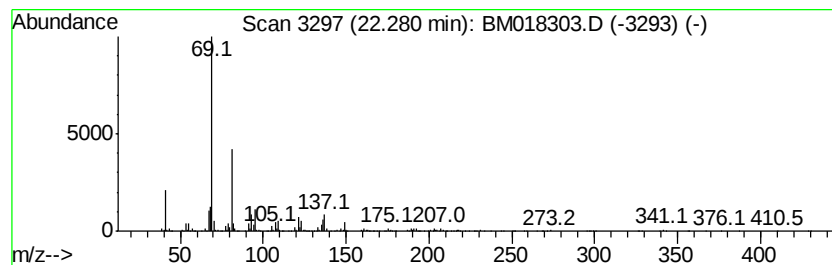
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	19.92 ng	1032830	Perylene-d12	23.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	94		
2	Squalene	410	C30H50	007683-64-9	90		
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78		
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72		
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72		



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121918\
Data File : BM018303.D
Acq On : 19 Dec 2018 19:11
Operator : JU/SJ
Sample : J6477-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-A1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	4.2	ng	122480	1	7.49	583805	20.0
unknown7.03	7.03	113.8	ng	3323340	1	7.49	583805	20.0
n-Hexadecanoic acid	17.82	16.7	ng	755733	4	16.91	907338	20.0
Benzene, 1,1'-(1,...	18.99	2.6	ng	119322	4	16.91	907338	20.0
Octadecanoic acid	19.12	6.1	ng	332051	5	21.13	1094380	20.0
Heneicosane	20.39	2.7	ng	148588	5	21.13	1094380	20.0
Pentafluoropropio...	20.85	10.9	ng	598691	5	21.13	1094380	20.0
Heptadecane, 9-oc...	21.29	4.2	ng	227917	5	21.13	1094380	20.0
2,6,10,14,18,22-T...	22.28	19.9	ng	1032830	6	23.29	1037020	20.0