

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121718\
 Data File : BM018245.D
 Acq On : 17 Dec 2018 12:46
 Operator : JU/SJ
 Sample : J6388-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P001-SS009-0006-01

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	4.687	302	306	315	rBV	53803	74369	3.11%	0.258%
2	5.128	374	381	396	rBV	1454633	2037681	85.10%	7.074%
3	6.693	639	647	660	rBV	1413332	2358814	98.51%	8.189%
4	7.034	698	705	718	rBV	1547441	2394523	100.00%	8.313%
5	7.493	777	783	791	rBV	572546	874277	36.51%	3.035%
6	7.598	796	801	808	rBV3	14034	27573	1.15%	0.096%
7	7.804	829	836	847	rVB	1105543	1774940	74.12%	6.162%
8	8.651	973	980	995	rBV	771704	1385960	57.88%	4.812%
9	10.263	1246	1254	1268	rBV	620851	1134180	47.37%	3.938%
10	12.757	1672	1678	1690	rBV	1535076	2270105	94.80%	7.881%
11	13.633	1820	1827	1837	rBV	55296	97267	4.06%	0.338%
12	14.151	1909	1915	1928	rBV2	881165	1331817	55.62%	4.624%
13	15.657	2165	2171	2183	rBV	1095508	1719235	71.80%	5.969%
14	16.915	2379	2385	2391	rBV	948855	1346513	56.23%	4.675%
15	17.321	2449	2454	2461	rVB6	16778	32448	1.36%	0.113%
16	17.710	2511	2520	2527	rBV7	12015	33558	1.40%	0.117%
17	17.827	2536	2540	2551	rVB	154372	239674	10.01%	0.832%
18	18.704	2683	2689	2696	rBV6	52574	105944	4.42%	0.368%
19	18.998	2732	2739	2742	rBV5	38297	77060	3.22%	0.268%
20	19.127	2756	2761	2768	rBV5	81239	148802	6.21%	0.517%
21	19.357	2796	2800	2803	rBV	34162	46031	1.92%	0.160%
22	19.392	2803	2806	2813	rVB2	49095	71359	2.98%	0.248%
23	19.492	2819	2823	2828	rBV4	14551	25153	1.05%	0.087%
24	19.568	2831	2836	2843	rVV	1760777	2131859	89.03%	7.401%
25	19.709	2857	2860	2865	rVB4	48954	51111	2.13%	0.177%
26	19.756	2865	2868	2870	rBV4	23002	25508	1.07%	0.089%
27	19.851	2880	2884	2889	rBV3	153691	210178	8.78%	0.730%
28	20.056	2916	2919	2923	rBV5	21180	24674	1.03%	0.086%
29	20.133	2928	2932	2937	rBV	182425	227583	9.50%	0.790%
30	20.186	2938	2941	2944	rVV4	27545	32241	1.35%	0.112%
31	20.292	2955	2959	2964	rBV7	64726	89682	3.75%	0.311%
32	20.386	2973	2975	2979	rVB4	27552	33340	1.39%	0.116%
33	20.451	2979	2986	2991	rBV5	112885	216236	9.03%	0.751%
34	20.598	3008	3011	3018	rBV5	106750	134036	5.60%	0.465%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.662	3019	3022	3025	rBV4	31844	41425	1.73%	0.144%
36	20.862	3052	3056	3062	rBV2	260714	373106	15.58%	1.295%
37	20.927	3064	3067	3072	rVB6	56559	71699	2.99%	0.249%
38	21.139	3098	3103	3113	rBV	1044774	1625706	67.89%	5.644%
39	21.298	3127	3130	3136	rVB2	67104	75106	3.14%	0.261%
40	21.468	3156	3159	3165	rVB6	78181	108764	4.54%	0.378%
41	21.721	3199	3202	3206	rBV	312494	372740	15.57%	1.294%
42	22.168	3275	3278	3282	rVB	162560	187635	7.84%	0.651%
43	22.386	3312	3315	3320	rVB4	130300	164006	6.85%	0.569%
44	22.650	3356	3360	3364	rBV	296994	378172	15.79%	1.313%
45	23.186	3448	3451	3456	rVB4	122270	175860	7.34%	0.611%
46	23.297	3464	3470	3485	rVB	789909	1501085	62.69%	5.211%
47	23.486	3497	3502	3511	rVB2	417210	693978	28.98%	2.409%
48	23.792	3551	3554	3559	rVB2	163201	250828	10.48%	0.871%

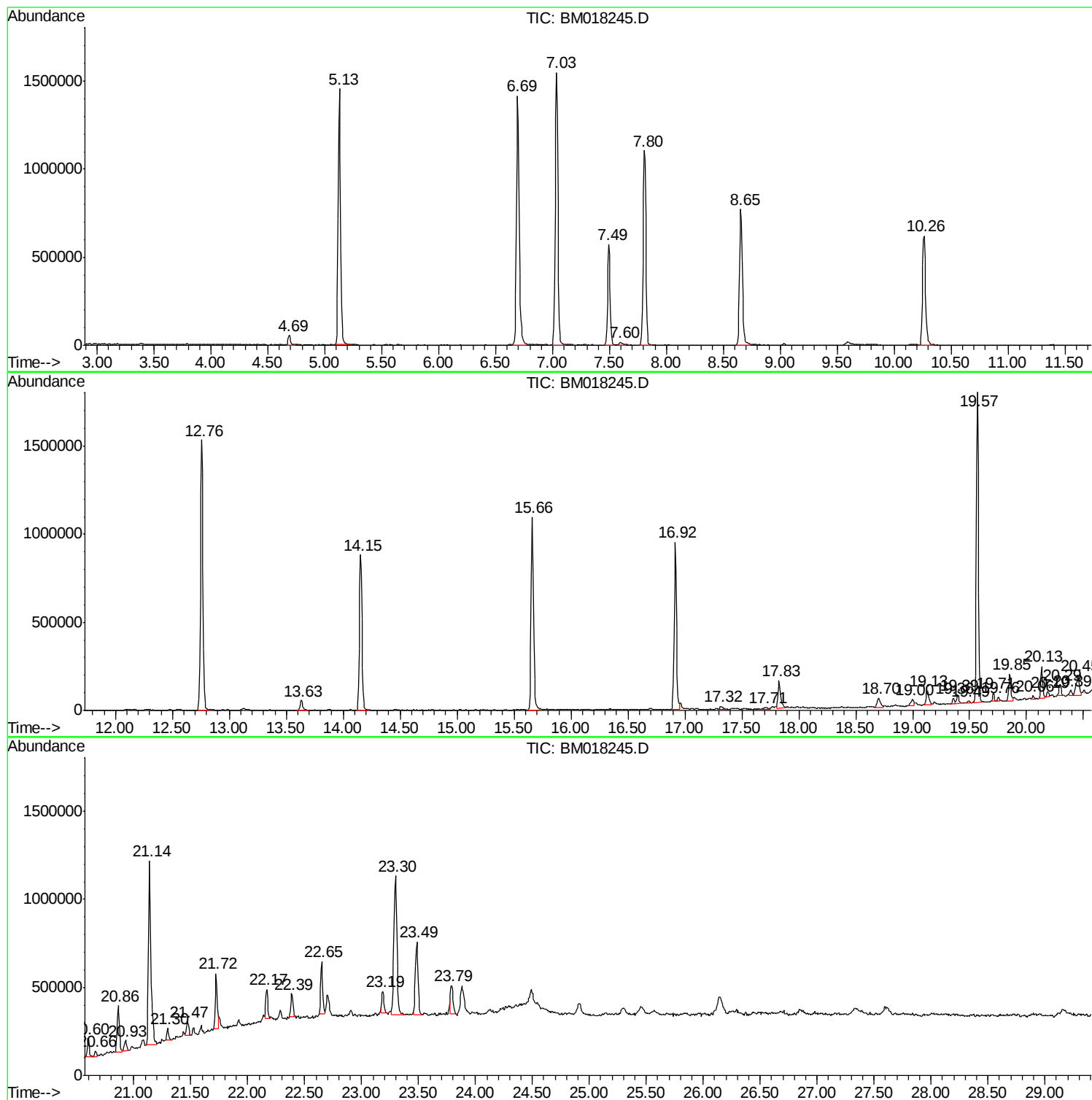
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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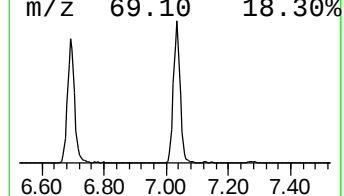
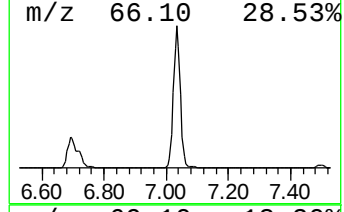
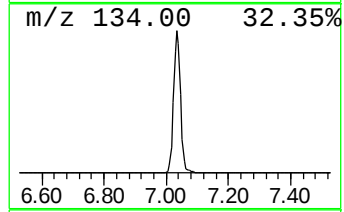
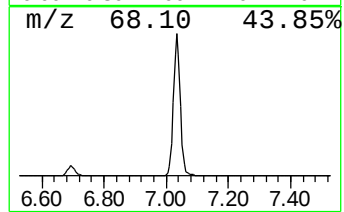
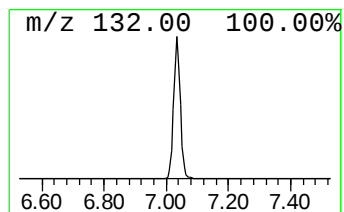
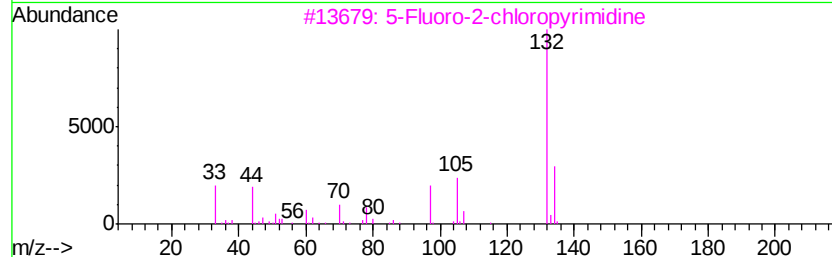
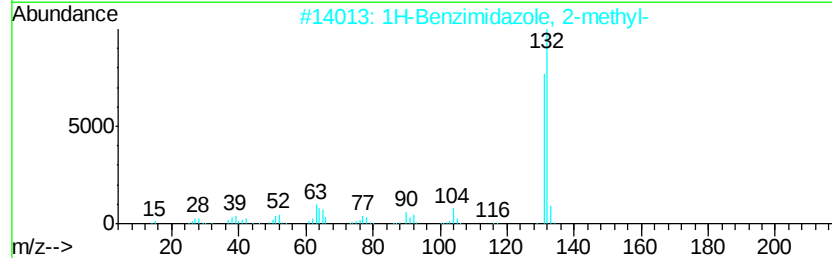
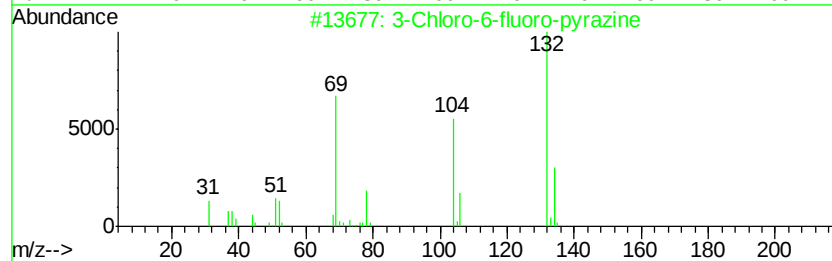
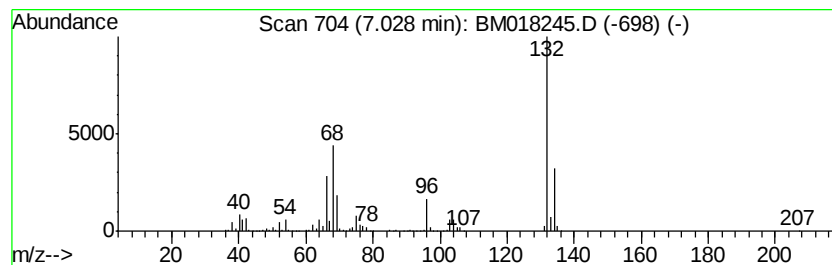
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	54.78 ng	2394520	1,4-Dichlorobenzene-d4	7.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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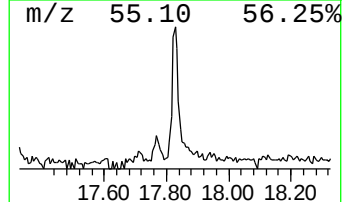
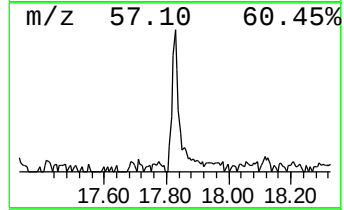
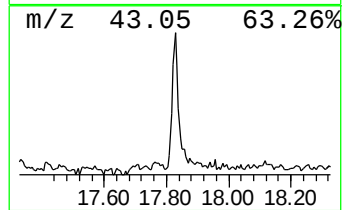
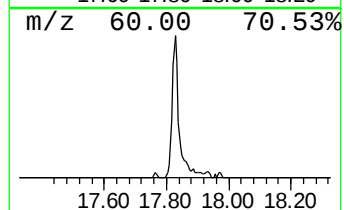
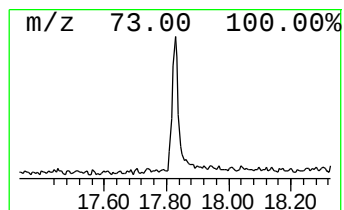
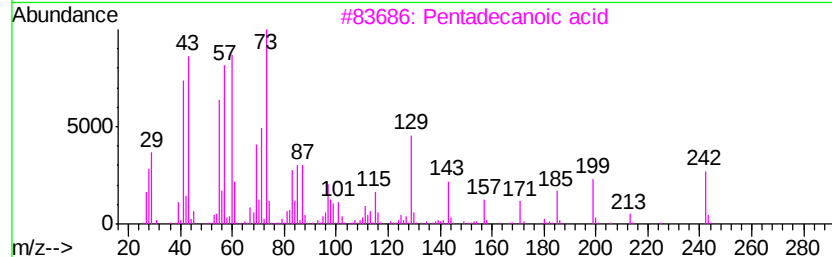
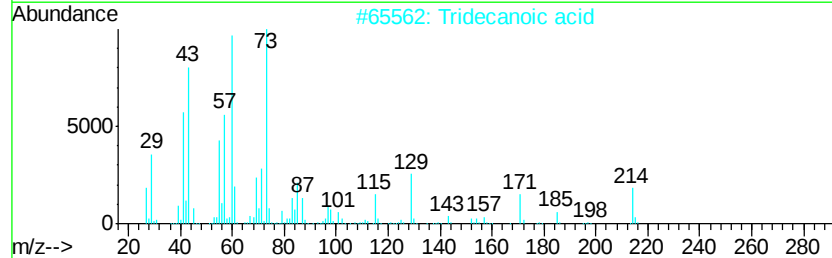
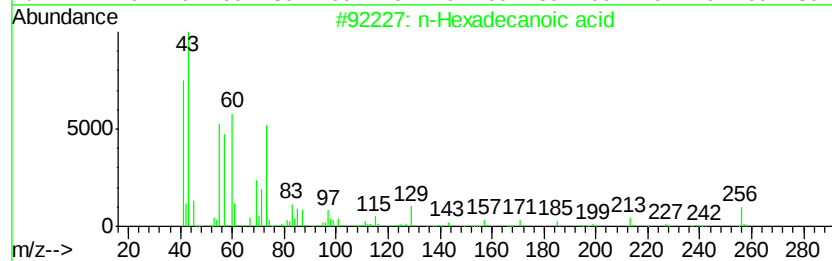
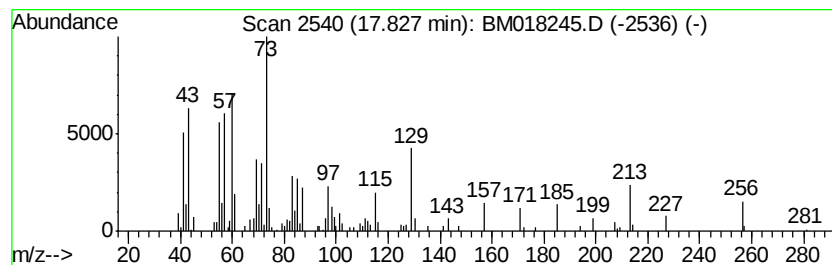
Instrument :
BNA_M
ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.83	3.56 ng	239674	Phenanthrene-d10		16.92
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	53



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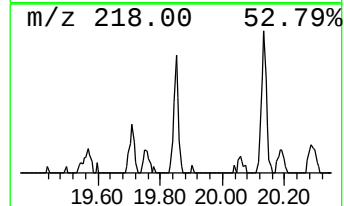
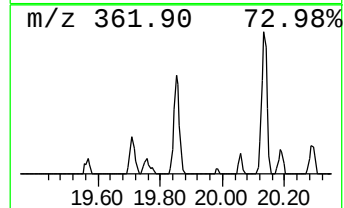
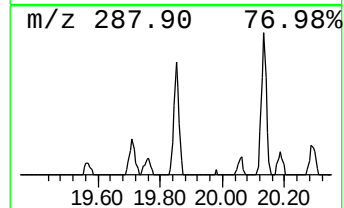
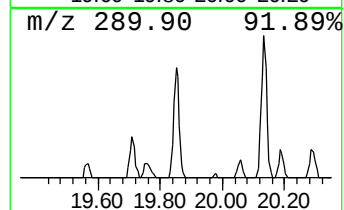
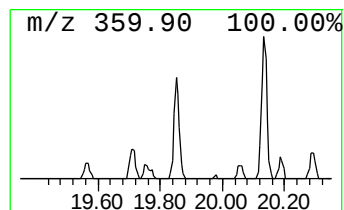
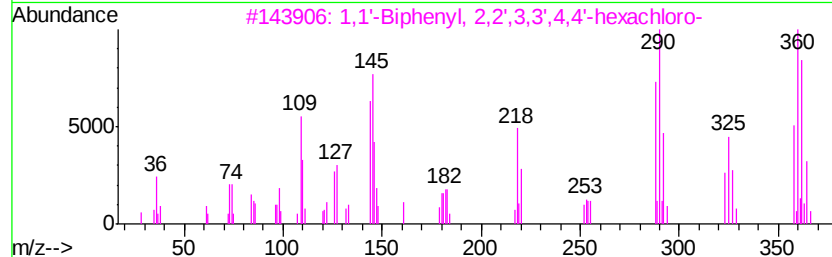
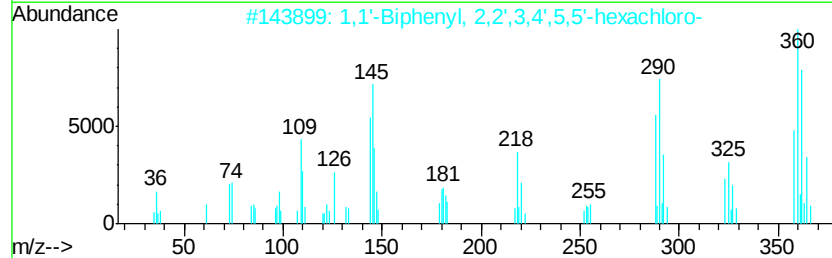
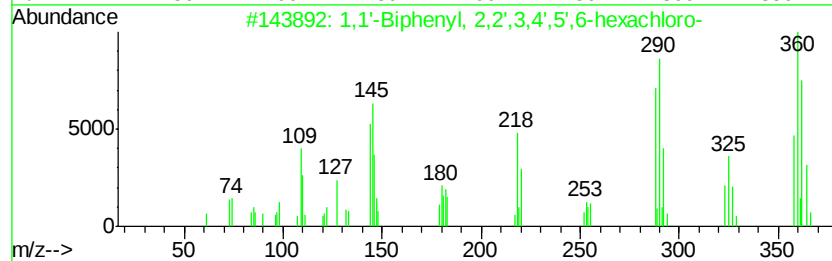
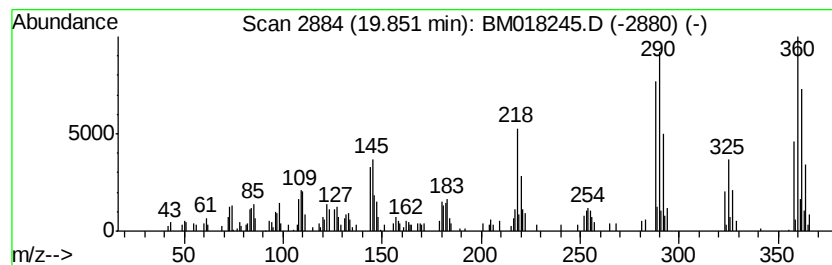
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,1'-Biphenyl, 2,2',3,4',5'... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.85	2.59 ng	210178	Chrysene-d12	21.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2,2',3,4',5',6-he...	358	C12H4Cl6	038380-04-0	99
2		1,1'-Biphenyl, 2,2',3,4',5,5'-he...	358	C12H4Cl6	051908-16-8	99
3		1,1'-Biphenyl, 2,2',3,3',4,4'-he...	358	C12H4Cl6	038380-07-3	99
4		1,1'-Biphenyl, 2,2',3,3',6,6'-he...	358	C12H4Cl6	038411-22-2	99
5		1,1'-Biphenyl, 3,3',4,4',5,5'-he...	358	C12H4Cl6	032774-16-6	98



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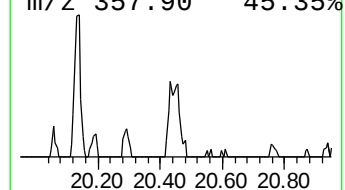
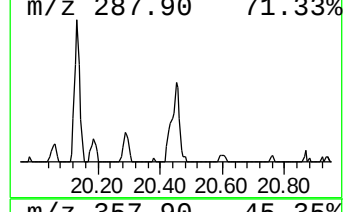
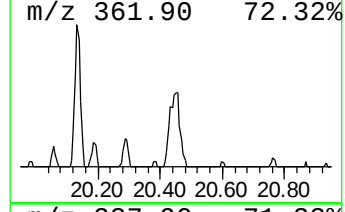
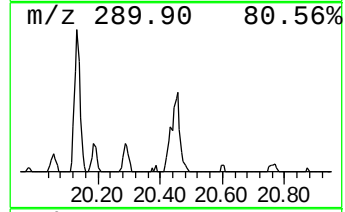
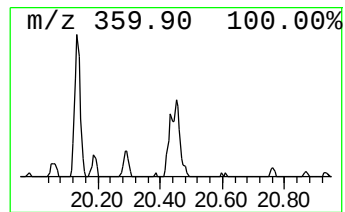
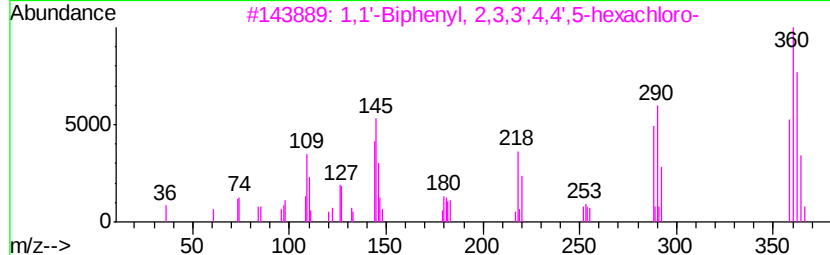
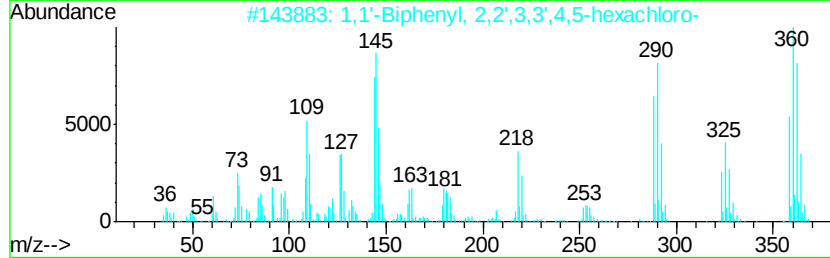
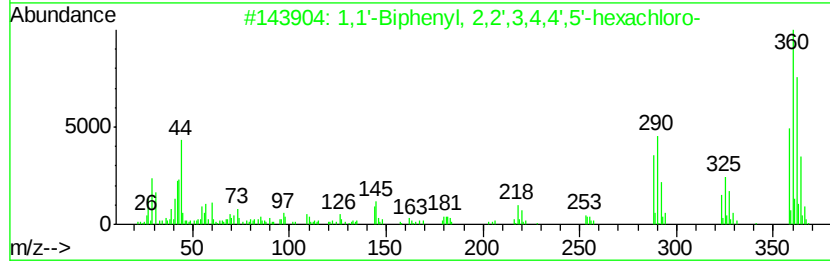
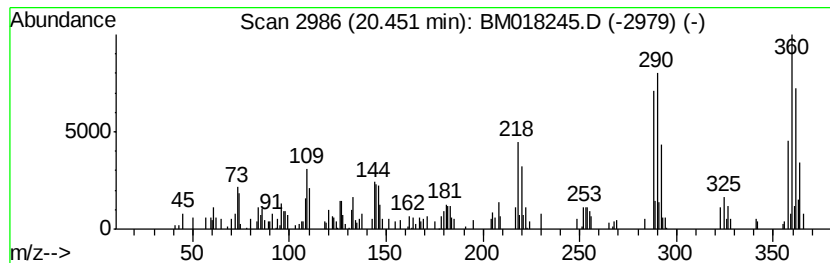
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,1'-Biphenyl, 2,2',3,4,4',... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.45	2.66 ng	216236	Chrysene-d12	21.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2,2',3,4,4',5'-he...	358	C12H4Cl6	035065-28-2	96
2		1,1'-Biphenyl, 2,2',3,3',4,5-hex...	358	C12H4Cl6	055215-18-4	94
3		1,1'-Biphenyl, 2,3,3',4,4',5-hex...	358	C12H4Cl6	038380-08-4	94
4		1,1'-Biphenyl, 2,2',3,4,4',5',6-he...	358	C12H4Cl6	038380-04-0	94
5		1,1'-Biphenyl, 2,2',3,3',4,6'-he...	358	C12H4Cl6	038380-05-1	94



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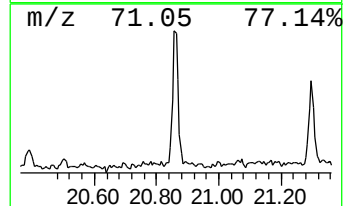
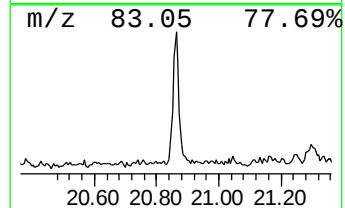
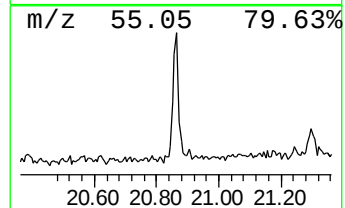
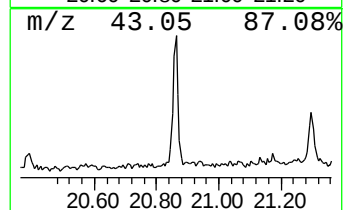
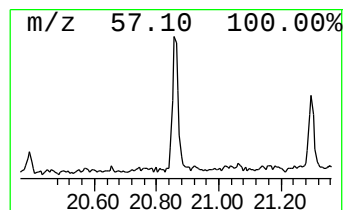
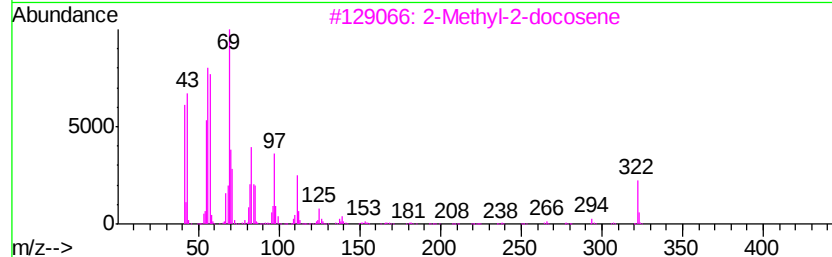
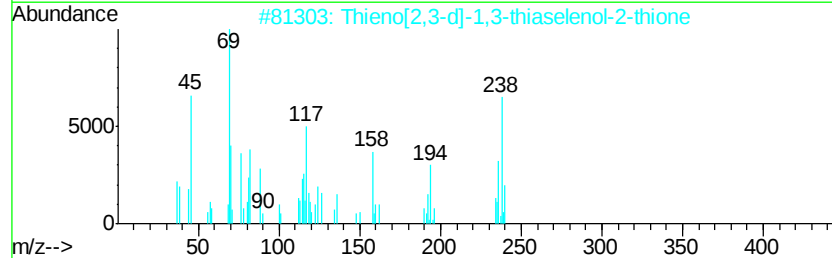
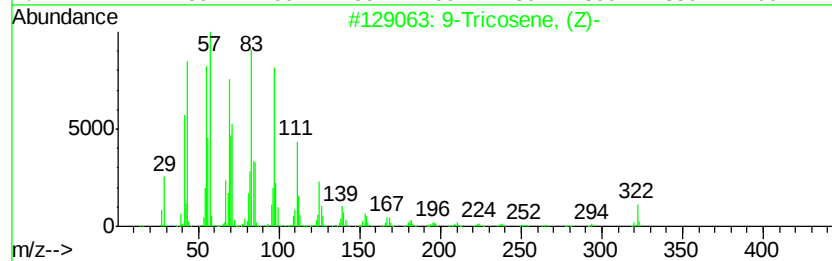
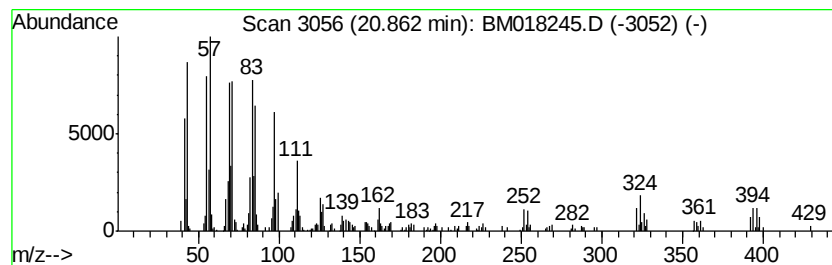
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Tricosene, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	4.59 ng	373106	Chrysene-d12	21.14

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-			322	C23H46	027519-02-4	96
2	Thieno[2,3-d]-1,3-thiaselenol-2-...			238	C5H2S3Se	081803-09-0	56
3	2-Methyl-2-docosene			322	C23H46	1000131-16-9	45
4	5-Methyl-Z-5-docosene			322	C23H46	1000131-17-1	45
5	Hexadecanoic acid, 2-hydroxy-, m...			286	C17H34O3	016742-51-1	40



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121718\
Data File : BM018245.D
Acq On : 17 Dec 2018 12:46
Operator : JU/SJ
Sample : J6388-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

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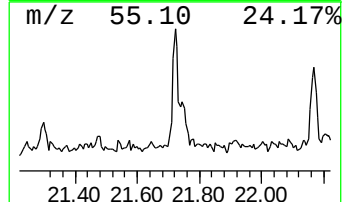
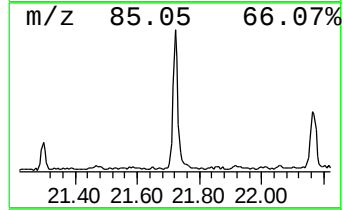
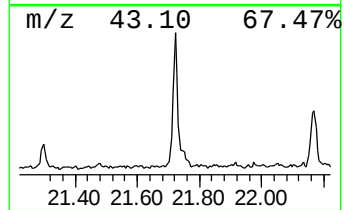
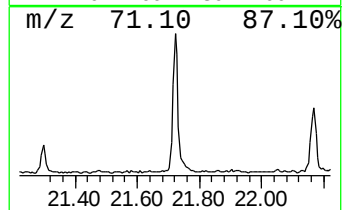
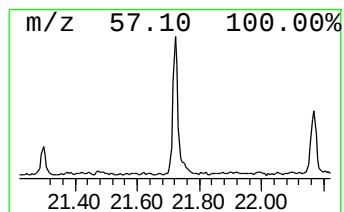
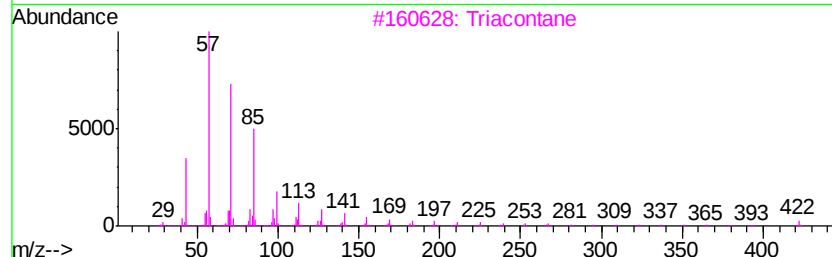
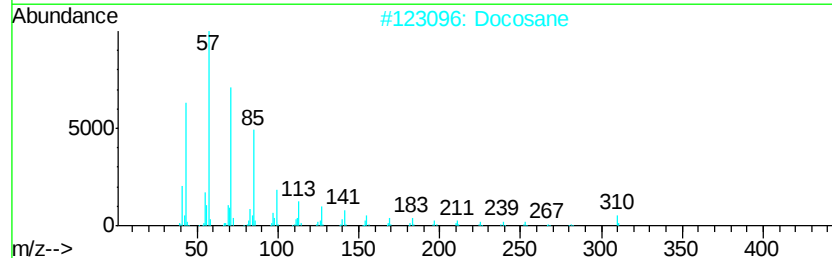
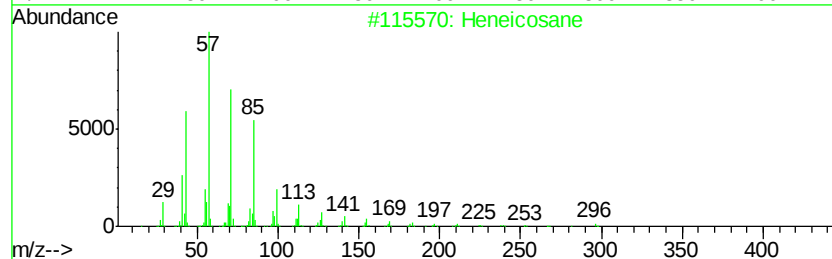
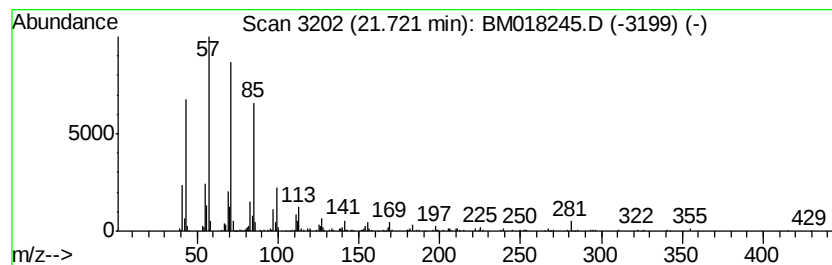
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	4.59 ng	372740	Chrysene-d12	21.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Docosane		310	C22H46	000629-97-0	90
3	Triacontane		422	C30H62	000638-68-6	86
4	Nonacosane		408	C29H60	000630-03-5	83
5	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121718\
Data File : BM018245.D
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ClientSampleId :
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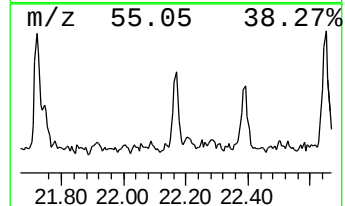
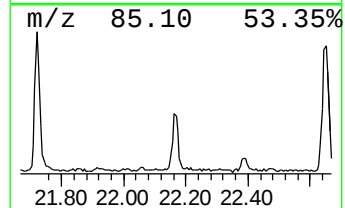
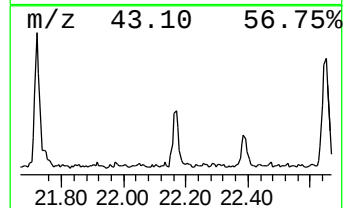
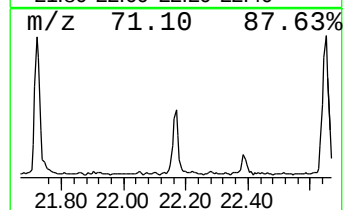
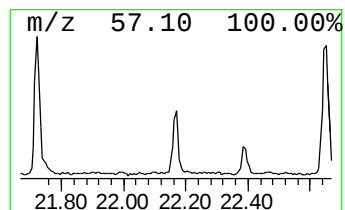
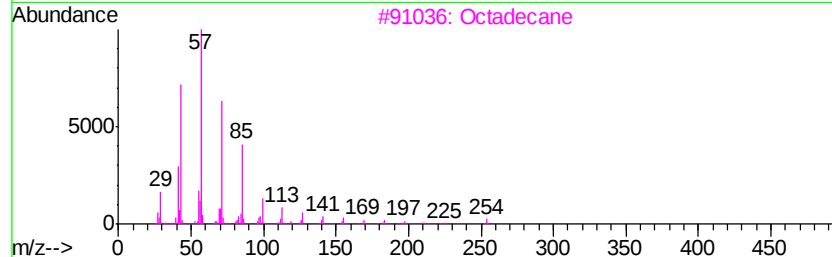
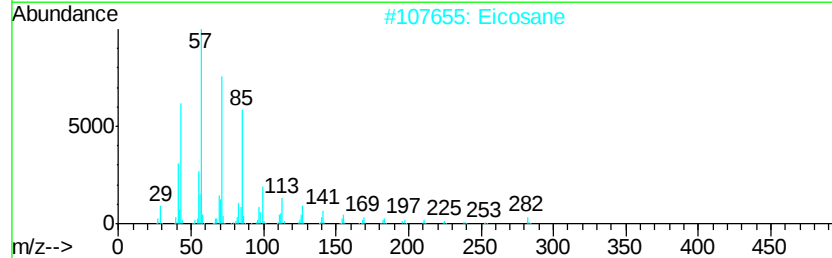
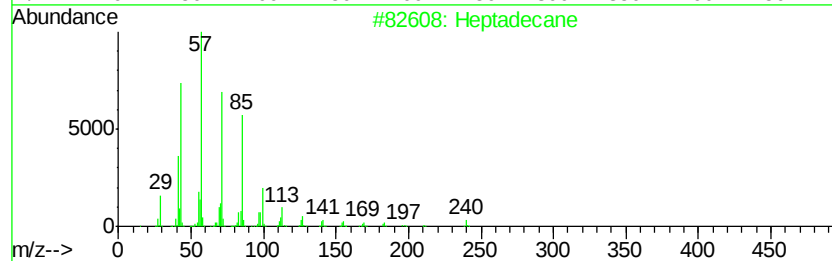
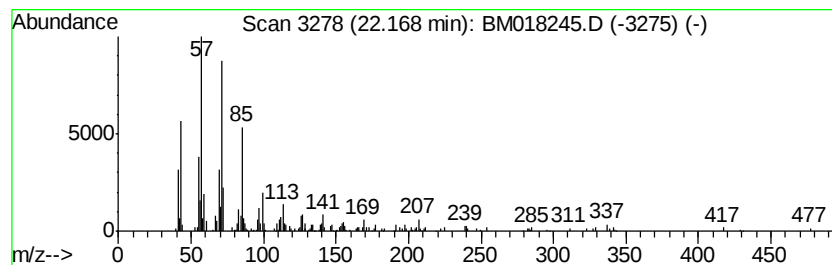
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.17	2.31 ng	187635	Chrysene-d12	21.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	89
2	Eicosane		282	C20H42	000112-95-8	86
3	Octadecane		254	C18H38	000593-45-3	86
4	Tetradecane		198	C14H30	000629-59-4	70
5	Docosane		310	C22H46	000629-97-0	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121718\
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Misc :
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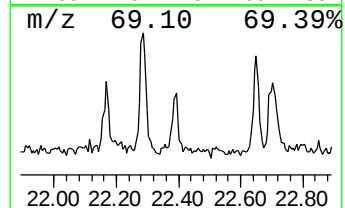
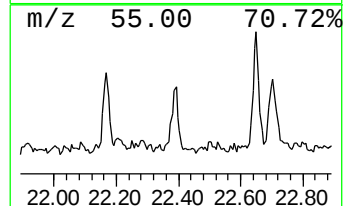
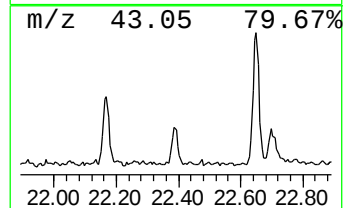
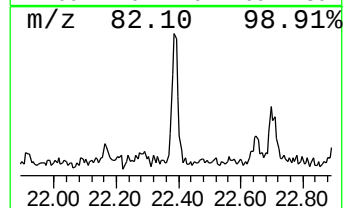
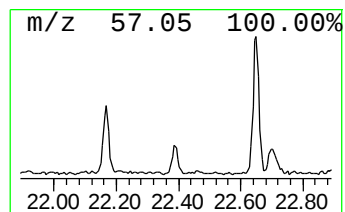
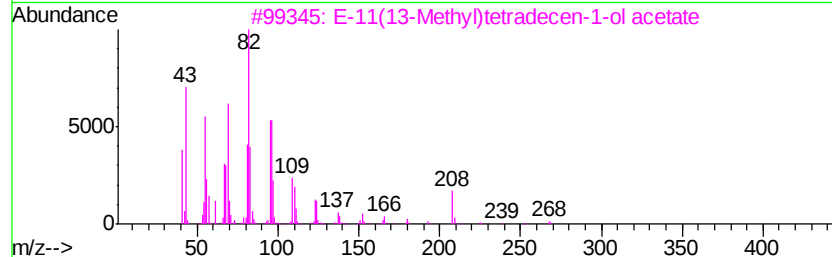
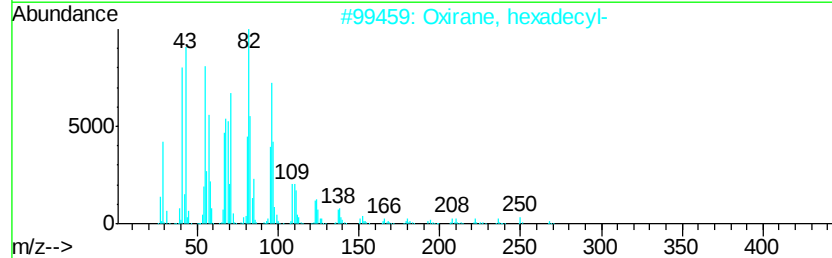
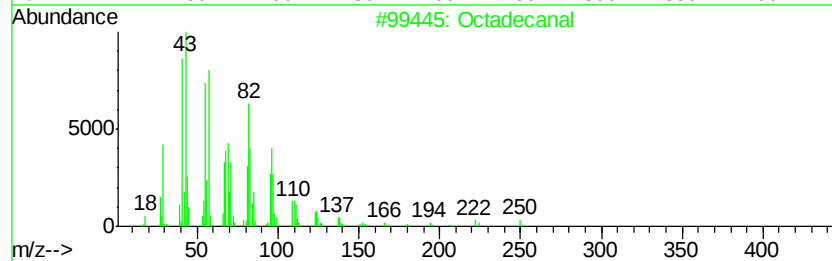
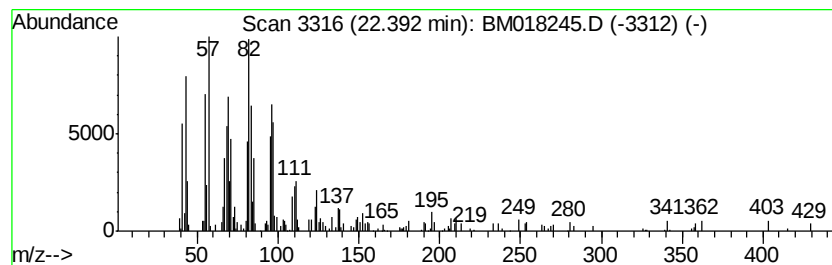
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanal Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	2.19 ng	164006	Perylene-d12	23.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanal	268 C18H36O	000638-66-4	93
2	Oxirane, hexadecyl-	268 C18H36O	007390-81-0	92
3	E-11(13-Methyl)tetradecen-1-ol a...	268 C17H32O2	1000130-80-4	78
4	E-8-Hexadecen-1-ol acetate	282 C18H34O2	1000131-01-1	70
5	Oleyl Alcohol	268 C18H36O	000143-28-2	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121718\
Data File : BM018245.D
Acq On : 17 Dec 2018 12:46
Operator : JU/SJ
Sample : J6388-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

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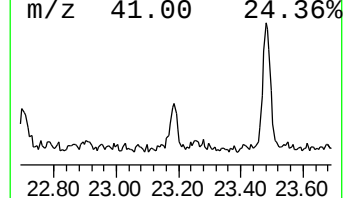
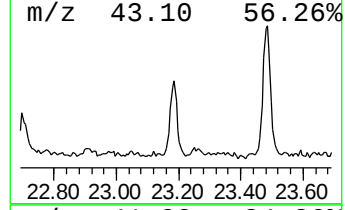
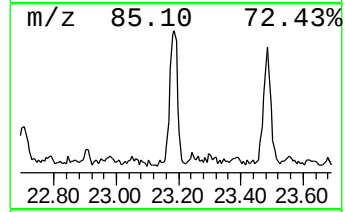
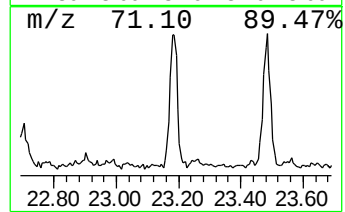
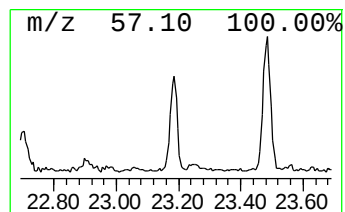
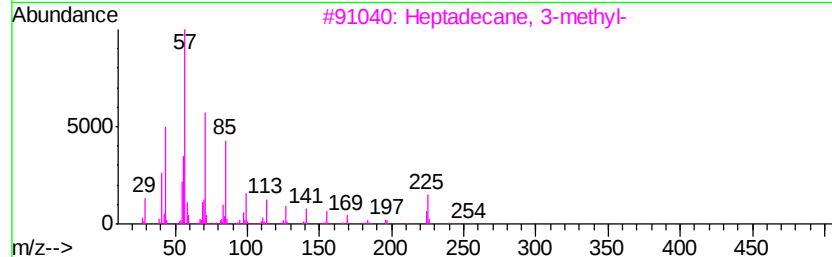
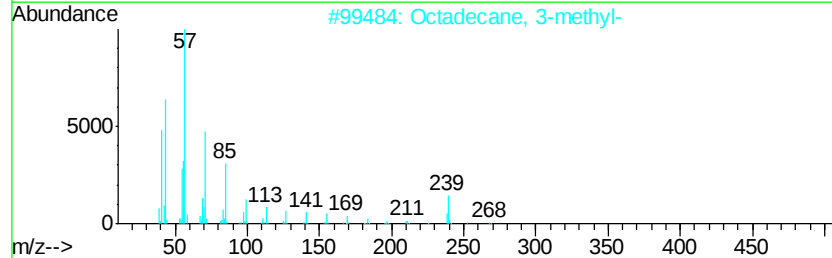
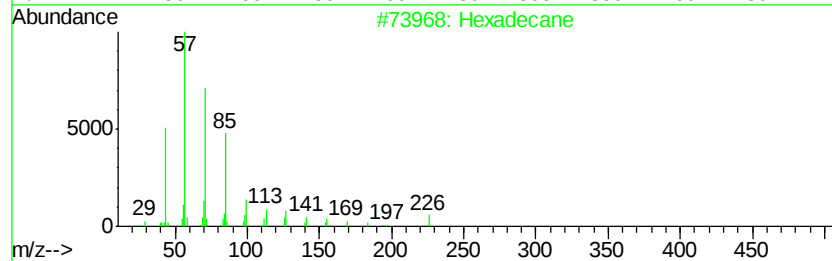
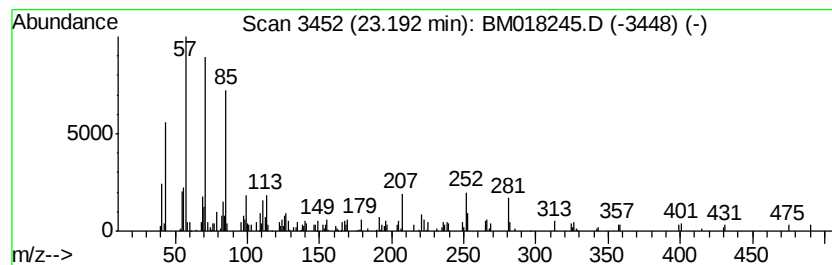
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	2.34 ng	175860	Perylene-d12	23.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	89
2		Octadecane, 3-methyl-	268	C19H40	006561-44-0	87
3		Heptadecane, 3-methyl-	254	C18H38	006418-44-6	83
4		Heneicosane	296	C21H44	000629-94-7	83
5		Tetratriacontane	479	C34H70	014167-59-0	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121718\
Data File : BM018245.D
Acq On : 17 Dec 2018 12:46
Operator : JU/SJ
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Instrument :
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ClientSampleId :
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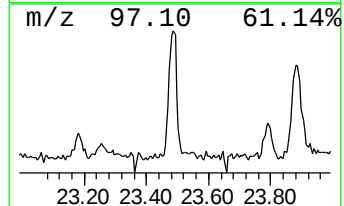
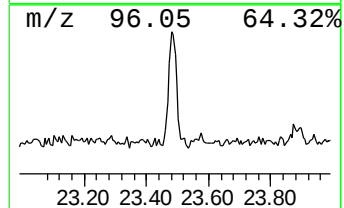
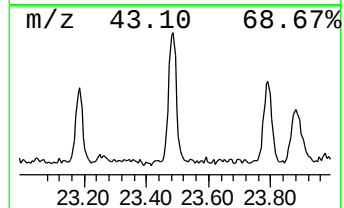
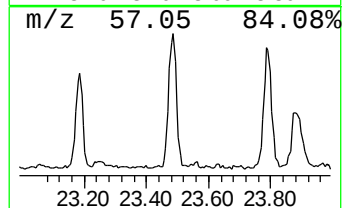
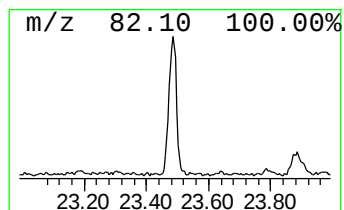
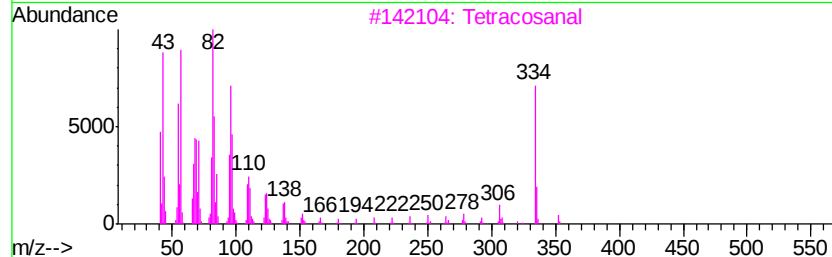
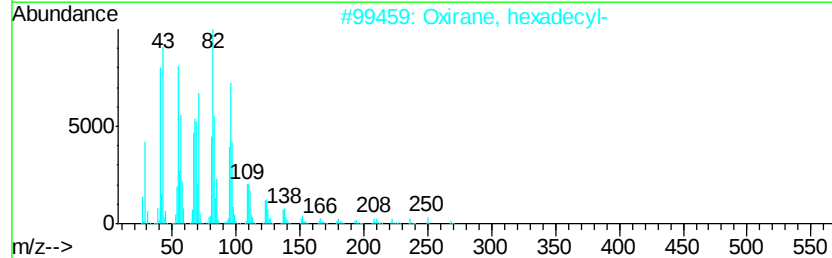
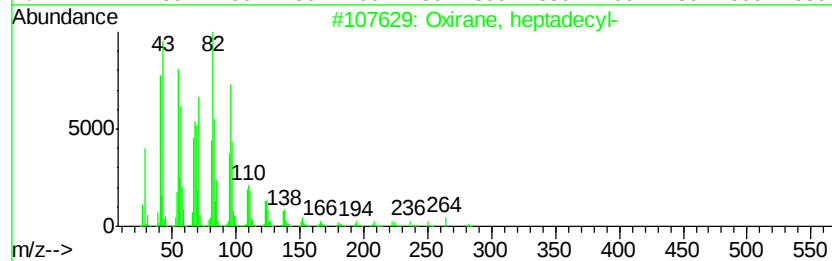
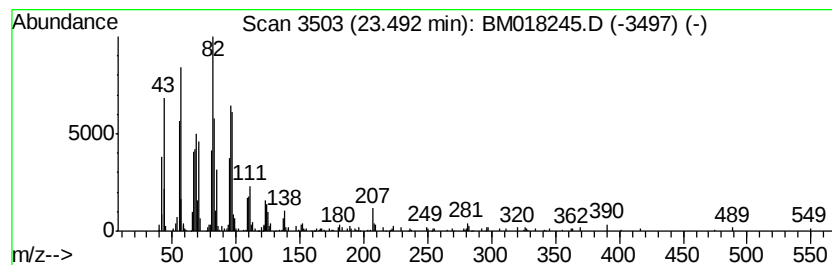
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Oxirane, heptadecyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.49	9.25 ng	693978	Perylene-d12	23.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3		Tetracosanal	352	C24H48O	057866-08-7	91
4		Pentadecanal-	226	C15H30O	002765-11-9	83
5		1,19-Eicosadiene	278	C20H38	014811-95-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM121718\
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ALS Vial : 7 Sample Multiplier: 1

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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
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n-Hexadecanoic acid	17.83	3.6	ng	239674	4	16.92	1346510	20.0
1,1'-Biphenyl, 2,...	19.85	2.6	ng	210178	5	21.14	1625710	20.0
1,1'-Biphenyl, 2,...	20.45	2.7	ng	216236	5	21.14	1625710	20.0
9-Tricosene, (Z)-	20.86	4.6	ng	373106	5	21.14	1625710	20.0
Heneicosane	21.72	4.6	ng	372740	5	21.14	1625710	20.0
Heptadecane	22.17	2.3	ng	187635	5	21.14	1625710	20.0
Octadecanal	22.39	2.2	ng	164006	6	23.30	1501090	20.0
Hexadecane	23.19	2.3	ng	175860	6	23.30	1501090	20.0
Oxirane, heptadecyl-	23.49	9.3	ng	693978	6	23.30	1501090	20.0