

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
 Data File : BM018931.D
 Acq On : 26 Feb 2019 16:09
 Operator : JU/SJ
 Sample : K1597-15
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-23

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-BM021119.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	5.287	368	374	391	rBV	5754996	8224022	91.08%	9.775%
2	6.363	551	557	563	rVB	262966	390323	4.32%	0.464%
3	6.875	636	644	660	rBV	5235469	8964752	99.29%	10.656%
4	7.228	697	704	719	rBV	5802978	9029303	100.00%	10.732%
5	7.692	777	783	791	rBV	1023279	1570170	17.39%	1.866%
6	8.010	830	837	848	rVB	4066673	6366252	70.51%	7.567%
7	8.863	974	982	996	rBV	3132762	5194050	57.52%	6.174%
8	10.480	1250	1257	1264	rBV	1137470	1902371	21.07%	2.261%
9	11.516	1428	1433	1447	rVB2	79418	176667	1.96%	0.210%
10	12.957	1671	1678	1690	rBV	5482172	7855510	87.00%	9.337%
11	13.286	1728	1734	1739	rBV2	45827	97648	1.08%	0.116%
12	13.592	1778	1786	1793	rVB	362129	525324	5.82%	0.624%
13	13.804	1817	1822	1835	rVB	324764	487906	5.40%	0.580%
14	14.345	1907	1914	1921	rVB2	1436208	2129587	23.59%	2.531%
15	15.839	2159	2168	2182	rBV	4317502	6298052	69.75%	7.486%
16	17.098	2376	2382	2386	rBV	1576951	2240008	24.81%	2.662%
17	17.139	2386	2389	2394	rVB	222979	292997	3.24%	0.348%
18	17.986	2527	2533	2543	rBV2	683940	1115530	12.35%	1.326%
19	18.892	2684	2687	2694	rVB3	45911	96512	1.07%	0.115%
20	19.162	2728	2733	2740	rVB	394774	539357	5.97%	0.641%
21	19.274	2747	2752	2763	rBV2	285105	516524	5.72%	0.614%
22	19.527	2791	2795	2802	rVB	375263	505940	5.60%	0.601%
23	19.733	2824	2830	2835	rBV	7061596	8361393	92.60%	9.938%
24	19.862	2849	2852	2856	rVB2	139138	172310	1.91%	0.205%
25	20.368	2934	2938	2945	rBV2	232153	361227	4.00%	0.429%
26	20.474	2952	2956	2959	rBV	186885	229597	2.54%	0.273%
27	20.992	3040	3044	3055	rBV2	736136	1053874	11.67%	1.253%
28	21.292	3090	3095	3099	rBV	2283067	2988596	33.10%	3.552%
29	21.862	3189	3192	3194	rBV	287915	325290	3.60%	0.387%
30	22.327	3267	3271	3279	rVB	448963	630726	6.99%	0.750%
31	22.827	3353	3356	3361	rBV	479967	698041	7.73%	0.830%
32	23.397	3450	3453	3458	rVB	554997	781704	8.66%	0.929%
33	23.544	3473	3478	3486	rVB	1579232	2807819	31.10%	3.337%
34	24.044	3559	3563	3572	rVB	642217	1203101	13.32%	1.430%

LSC Area Percent Report

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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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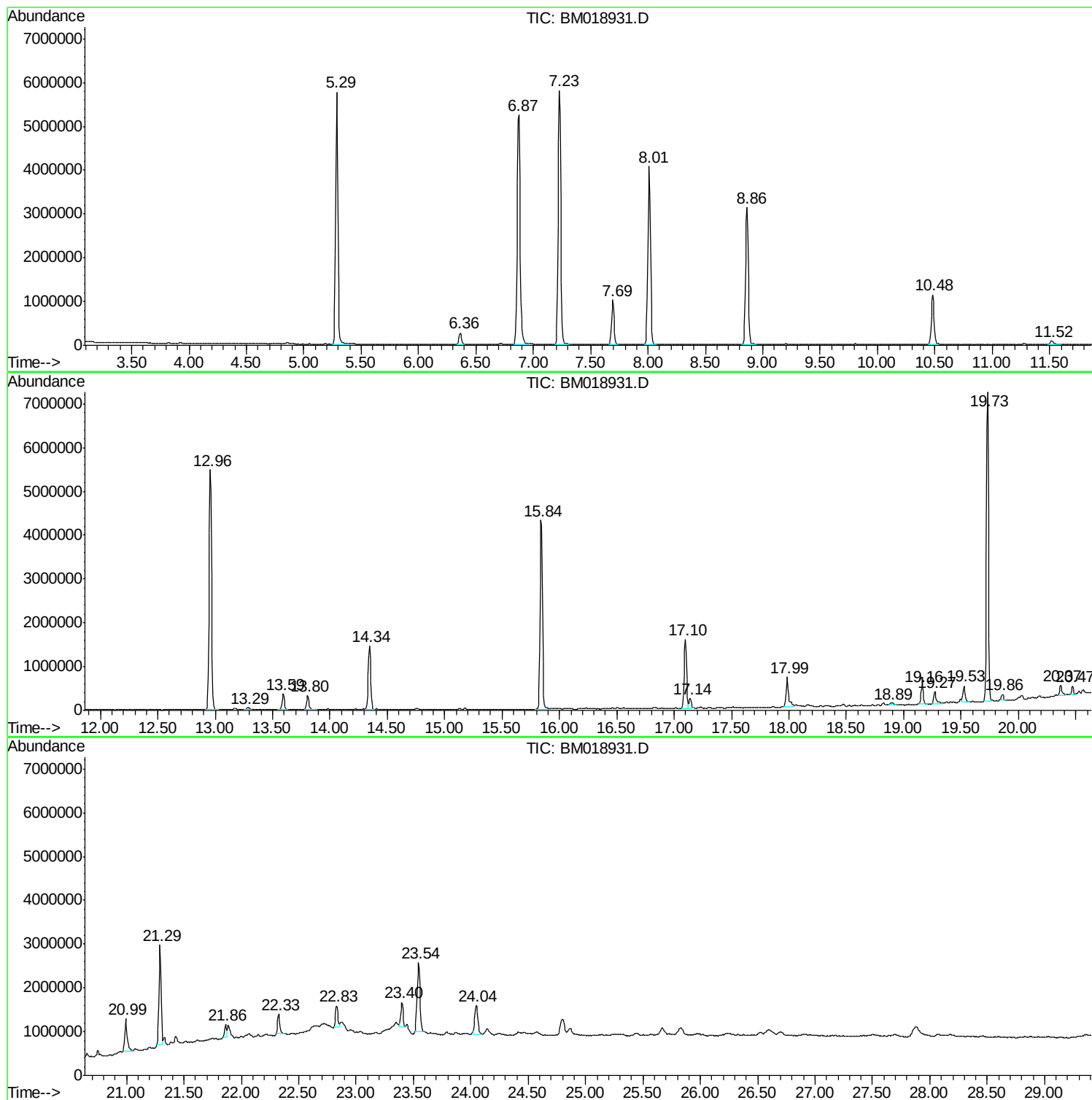
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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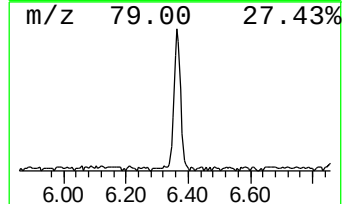
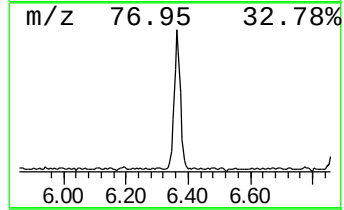
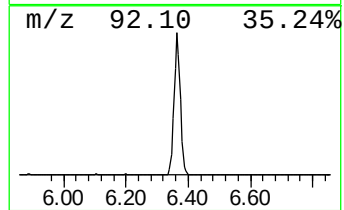
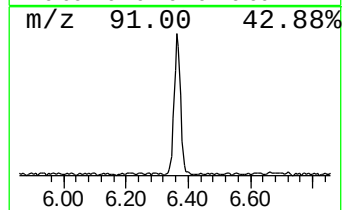
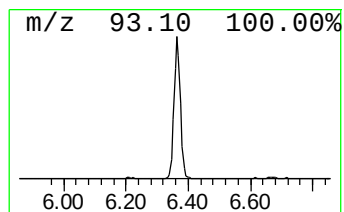
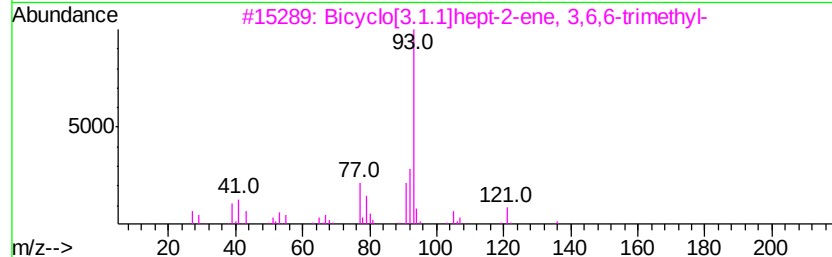
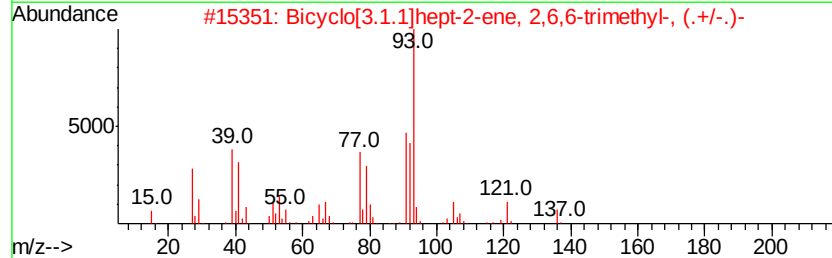
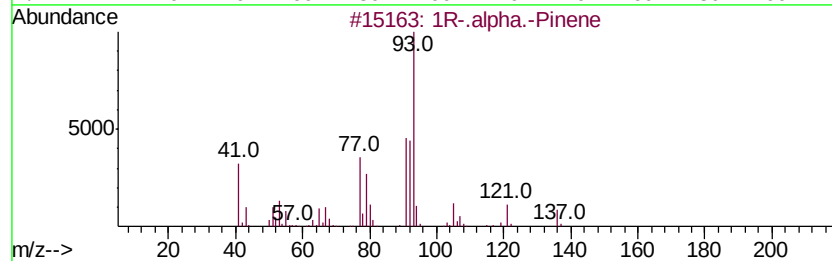
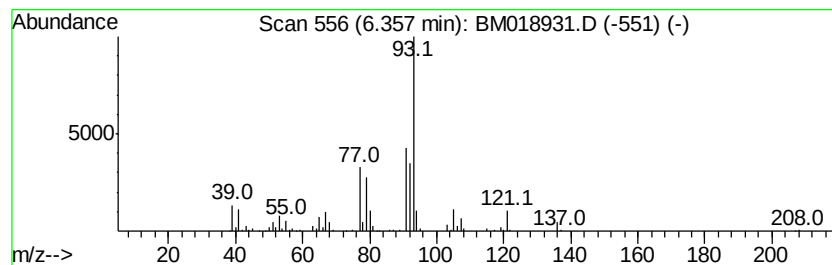
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1R-.alpha.-Pinene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	4.97 ng	390323	1,4-Dichlorobenzene-d4	7.69
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1R-.alpha.-Pinene	136 C10H16	007785-70-8 95
2		Bicyclo[3.1.1]hept-2-ene, 2,6,6-...	136 C10H16	002437-95-8 95
3		Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136 C10H16	004889-83-2 94
4		Bicyclo[4.1.0]hept-3-ene, 3,7,7-...	136 C10H16	000498-15-7 91
5		1,4-Cyclohexadiene, 1-methyl-4-(...	136 C10H16	000099-85-4 91



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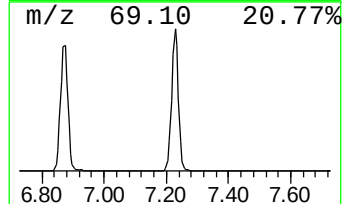
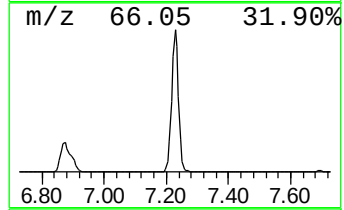
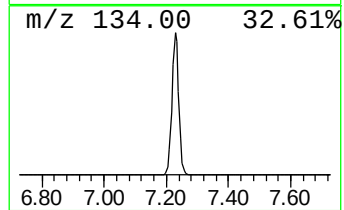
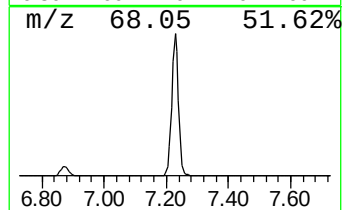
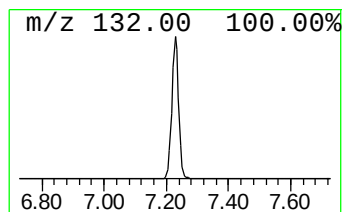
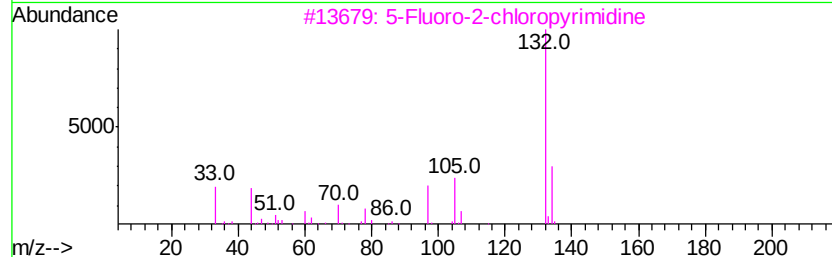
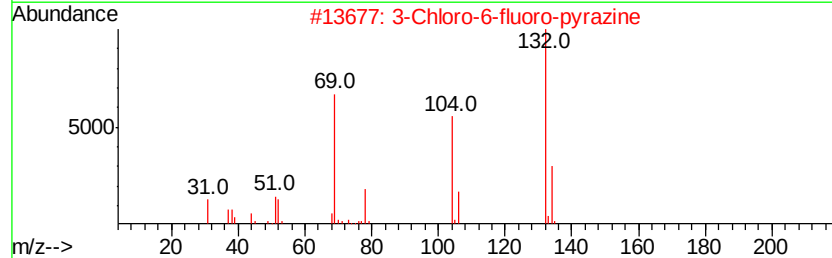
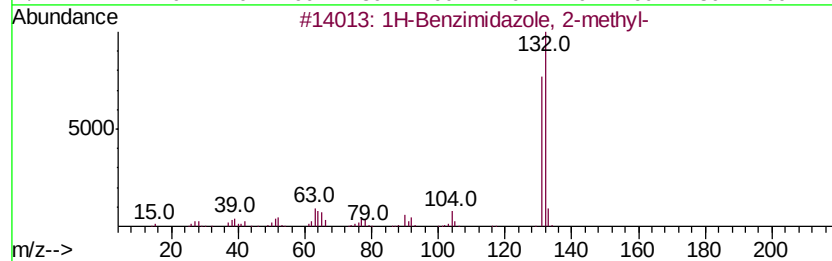
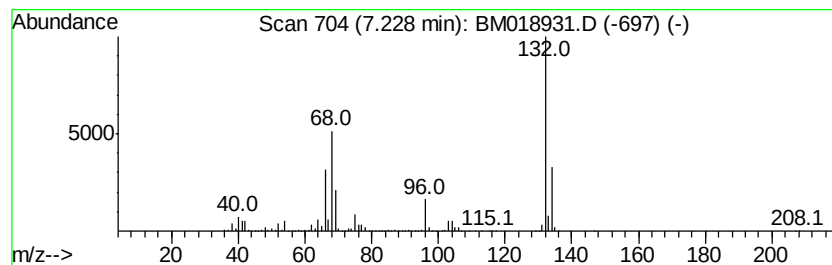
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	115.01 ng	9029300	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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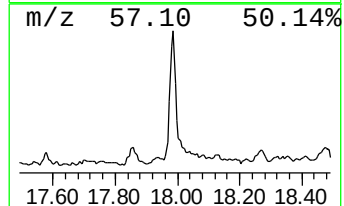
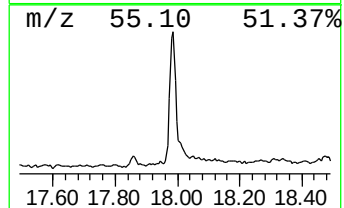
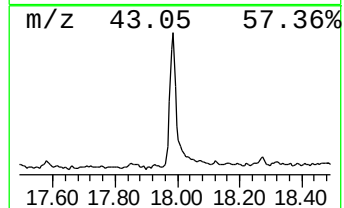
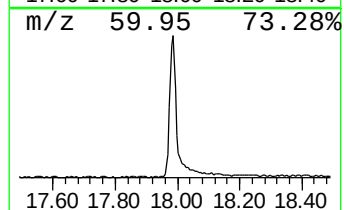
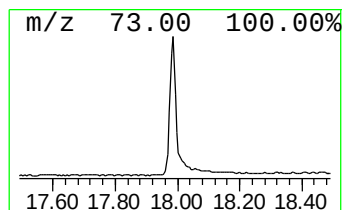
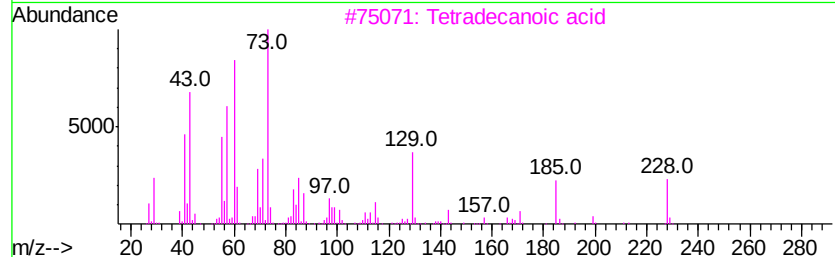
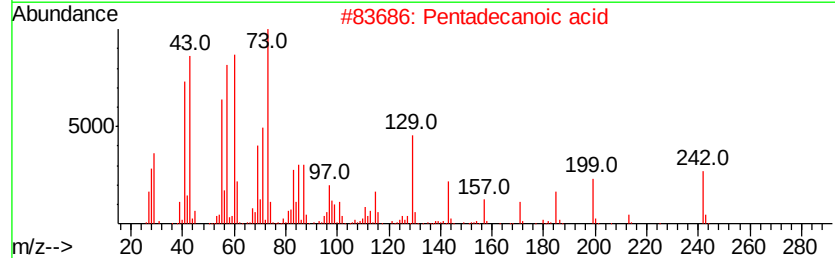
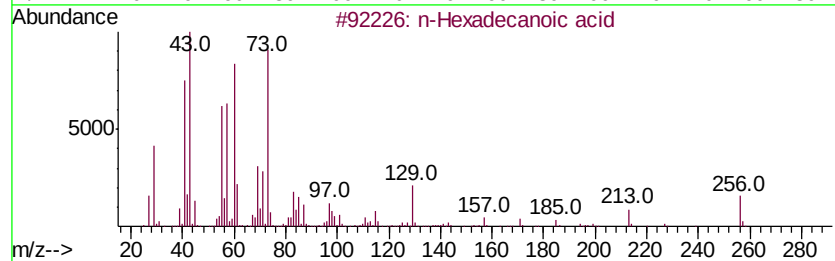
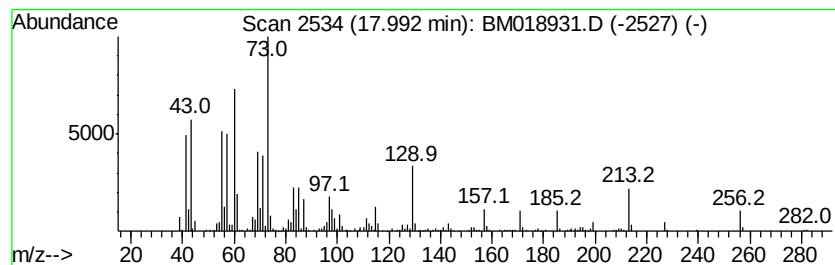
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.99	9.96 ng	1115530	Phenanthrene-d10		17.10
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	43
5	Tridecanoic acid	214	C13H26O2	000638-53-9	40



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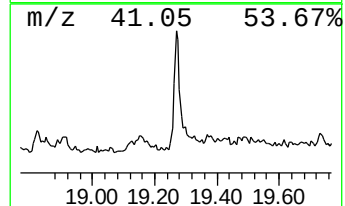
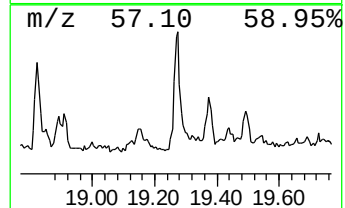
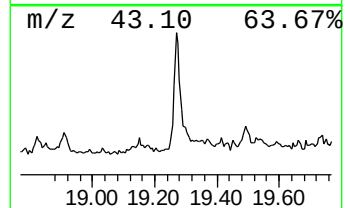
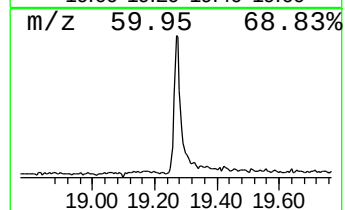
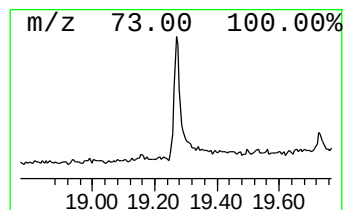
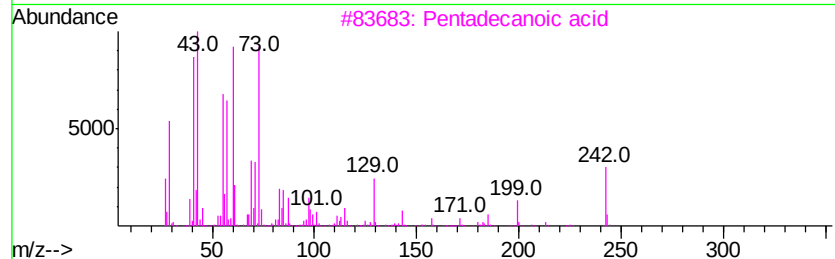
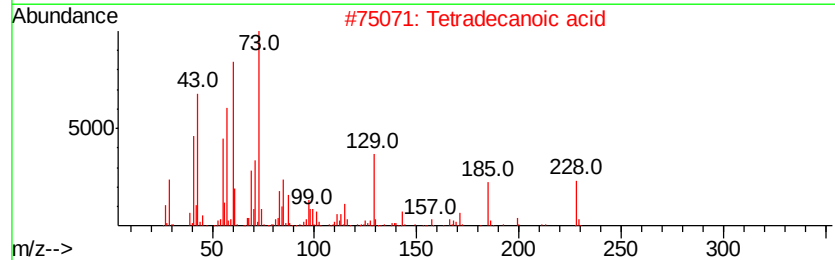
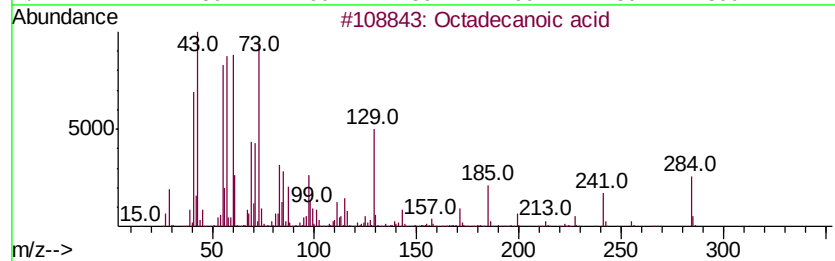
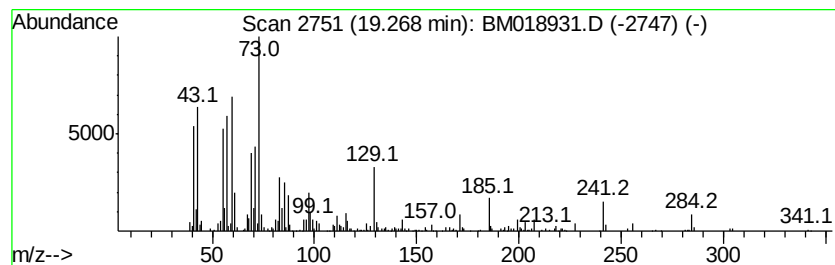
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.27	3.46 ng	516524	Chrysene-d12	21.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	30



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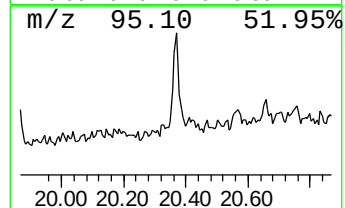
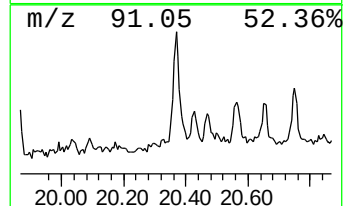
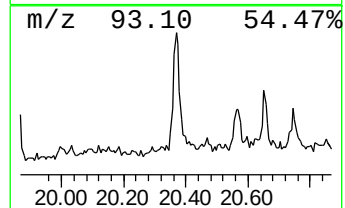
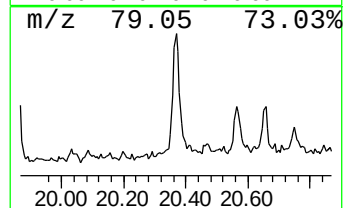
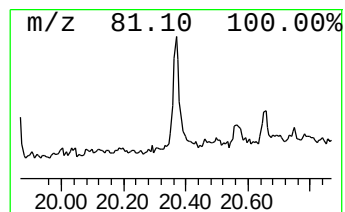
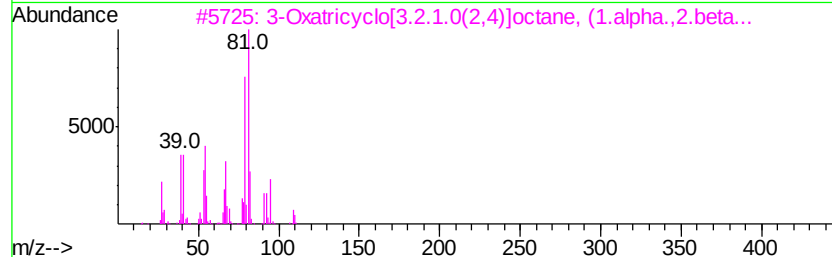
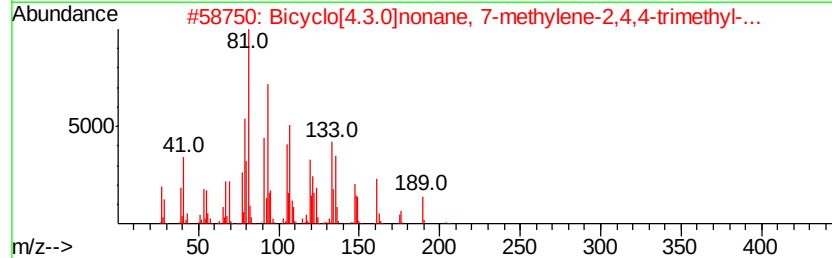
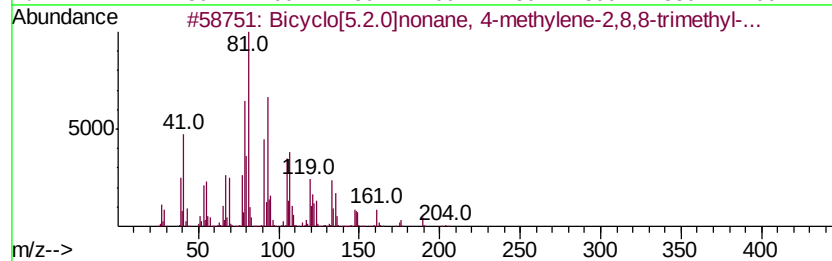
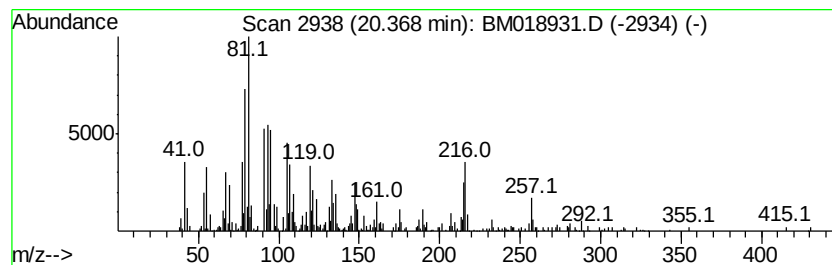
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Bicyclo[5.2.0]nonane, 4-met... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.37	2.42 ng	361227	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[5.2.0]nonane, 4-methylen...	204	C15H24	1000159-38-2	70
2		Bicyclo[4.3.0]nonane, 7-methylen...	204	C15H24	1000156-11-9	51
3		3-Oxatricyclo[3.2.1.0(2,4)]octan...	110	C7H10O	003146-39-2	38
4		2-Pentadecen-4-yne, (Z)-	206	C15H26	074646-33-6	25
5		3-Tetradecen-5-yne, (Z)-	192	C14H24	074663-68-6	25



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Sample : K1597-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-23

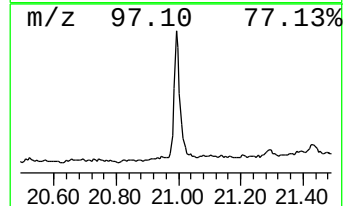
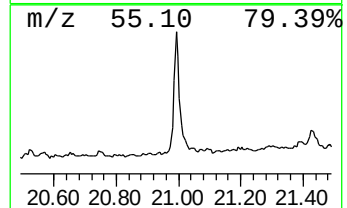
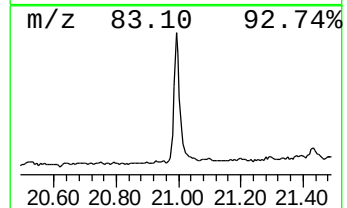
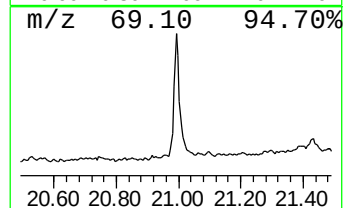
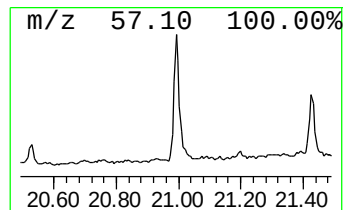
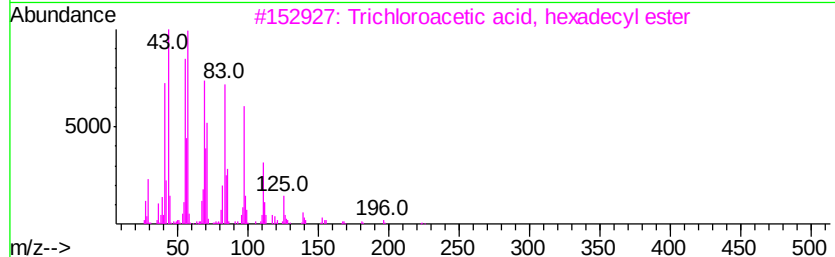
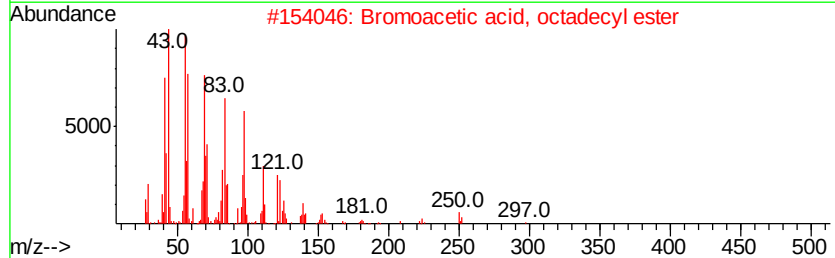
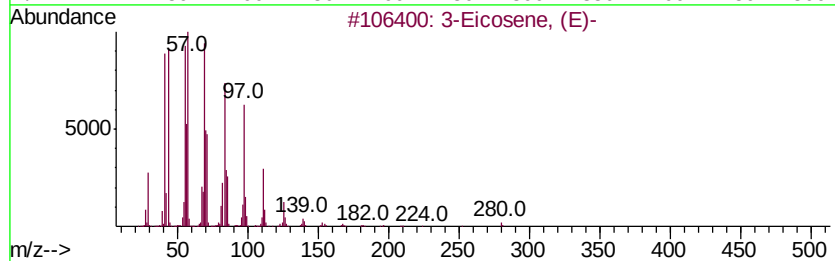
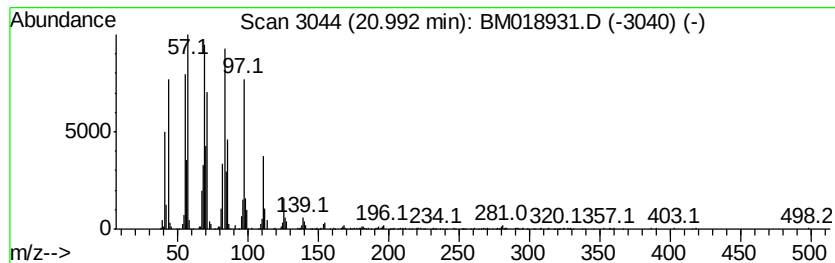
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.99	7.05 ng	1053870	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018931.D
Acq On : 26 Feb 2019 16:09
Operator : JU/SJ
Sample : K1597-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

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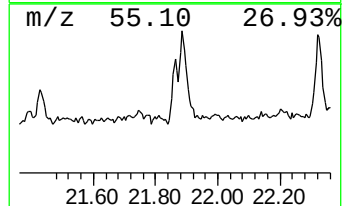
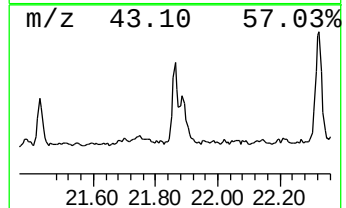
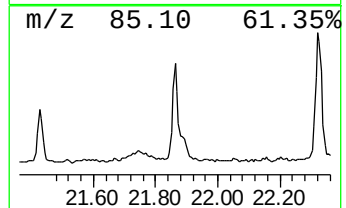
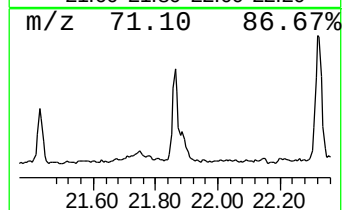
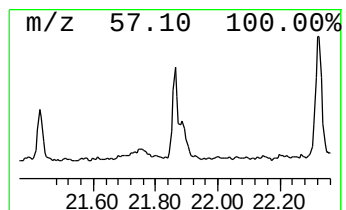
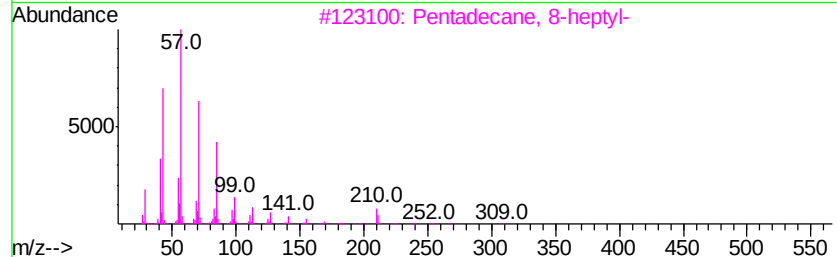
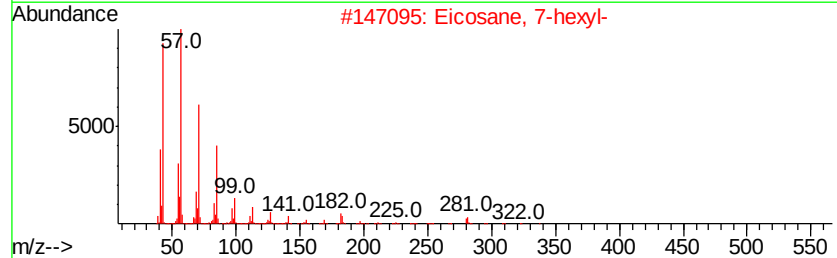
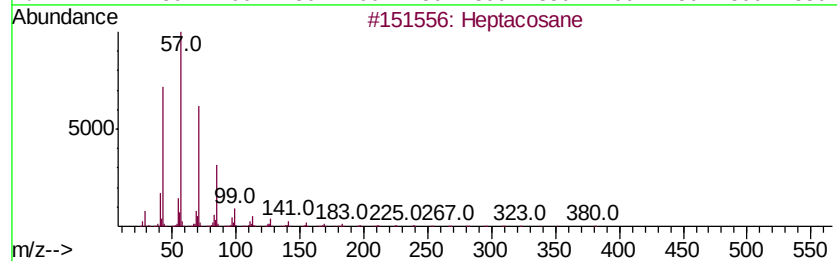
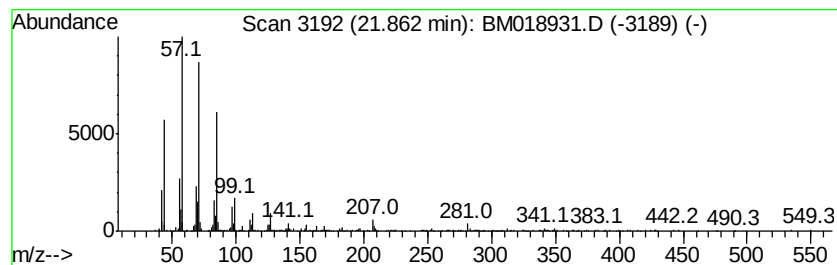
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	2.18 ng	325290	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	90
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
4		Eicosane	282	C20H42	000112-95-8	86
5		Docosane, 9-butyl-	366	C26H54	055282-14-9	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
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Sample : K1597-15
Misc :
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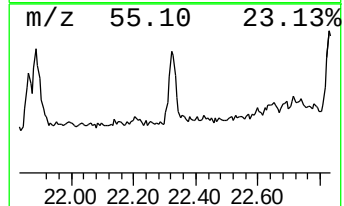
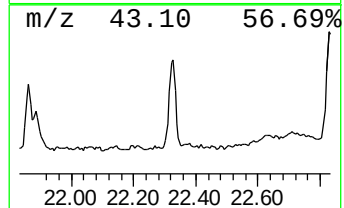
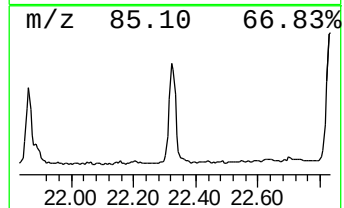
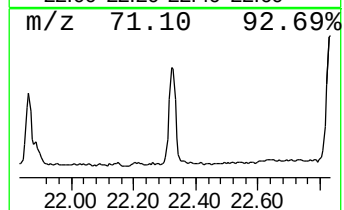
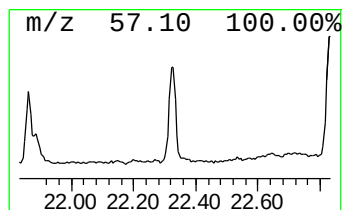
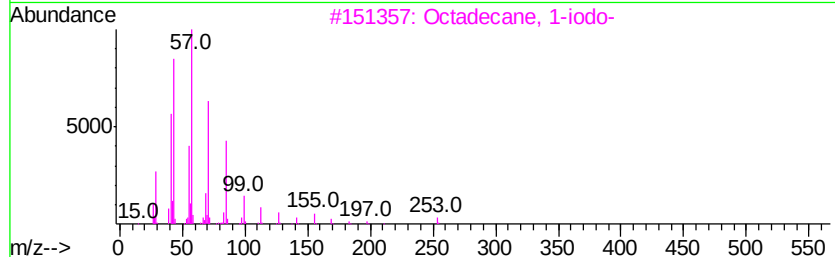
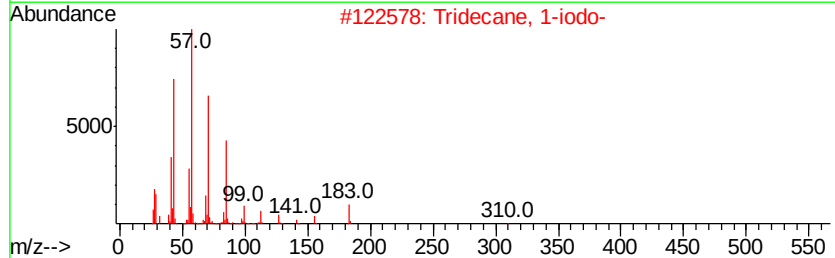
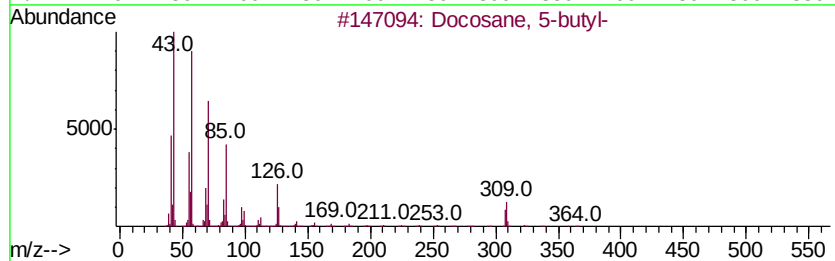
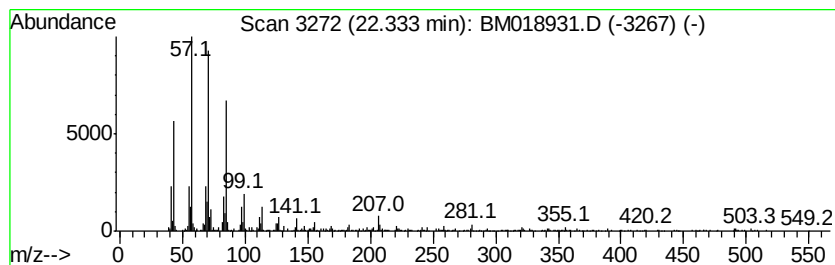
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane, 5-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	4.22 ng	630726	Chrysene-d12	21.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Docosane, 5-butyl-	366 C26H54	055282-16-1 93
2		Tridecane, 1-iodo-	310 C13H27I	035599-77-0 90
3		Octadecane, 1-iodo-	380 C18H37I	000629-93-6 87
4		Heneicosane, 11-(1-ethylpropyl)-	366 C26H54	055282-11-6 87
5		Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6 86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
Data File : BM018931.D
Acq On : 26 Feb 2019 16:09
Operator : JU/SJ
Sample : K1597-15
Misc :
ALS Vial : 5 Sample Multiplier: 1

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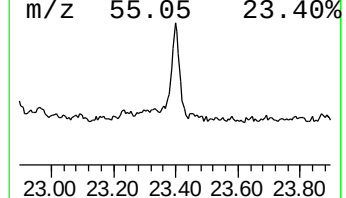
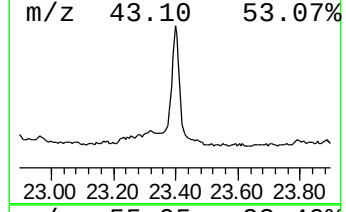
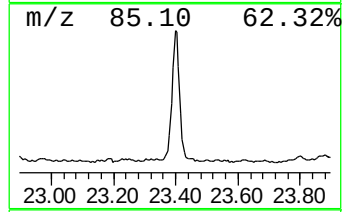
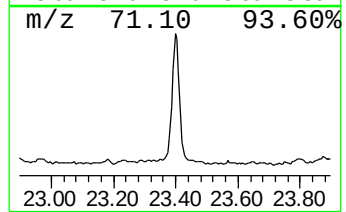
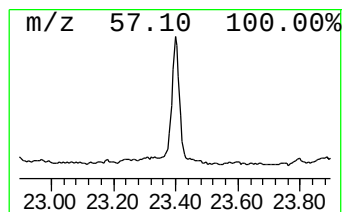
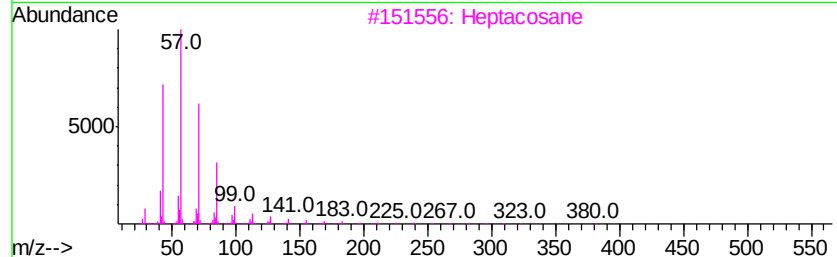
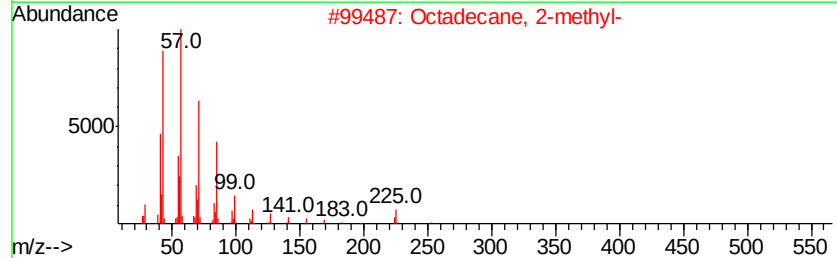
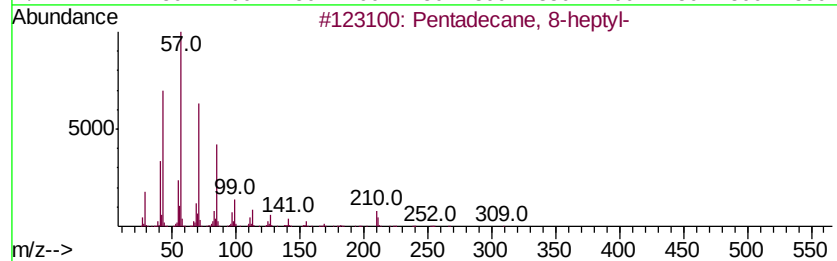
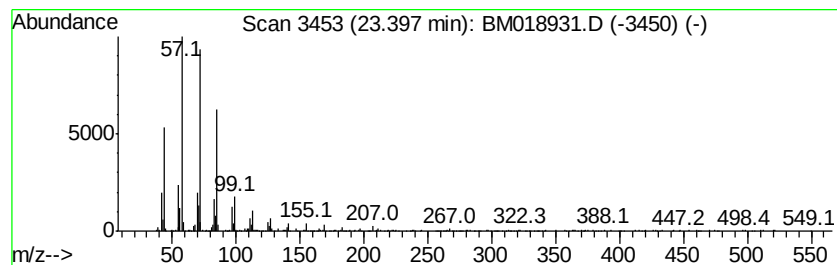
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Pentadecane, 8-heptyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.40	5.57 ng	781704	Perylene-d12	23.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
3		Heptacosane	380	C27H56	000593-49-7	74
4		Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72
5		Tetracosane, 3-ethyl-	366	C26H54	055282-17-2	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022619\
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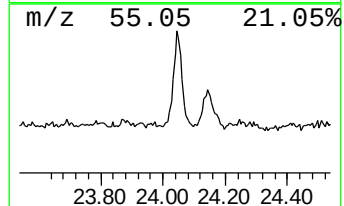
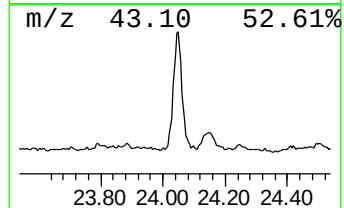
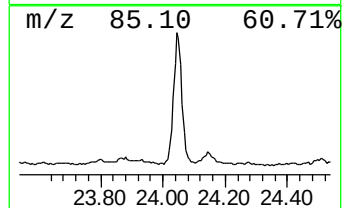
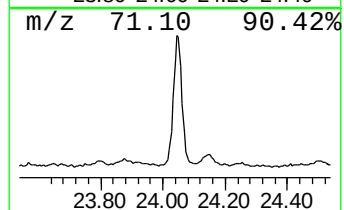
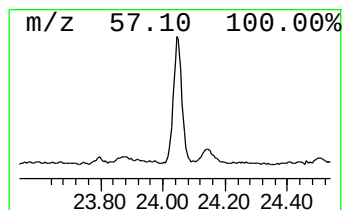
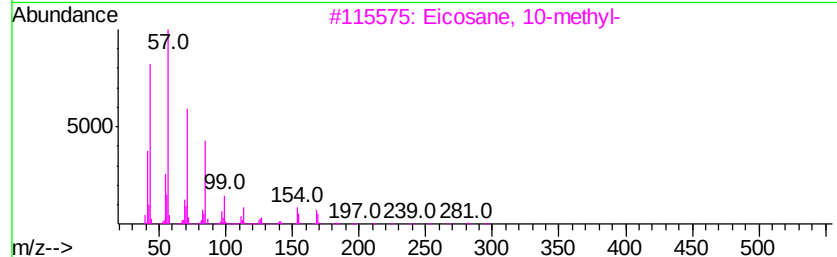
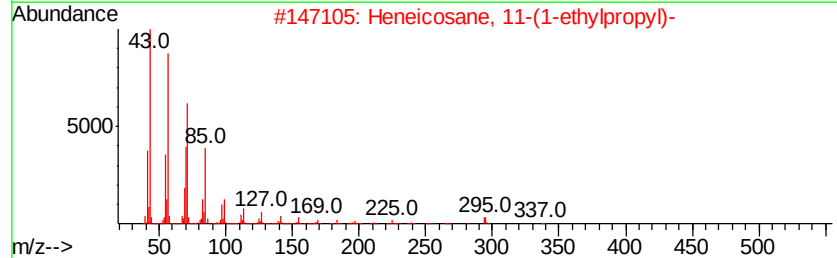
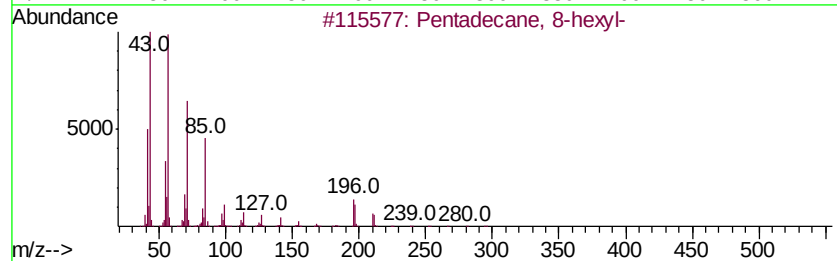
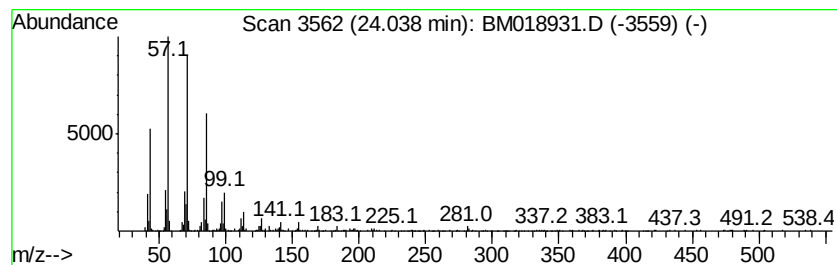
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentadecane, 8-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.04	8.57 ng	1203100	Perylene-d12	23.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3		Eicosane, 10-methyl-	296	C21H44	054833-23-7	87
4		Heptacosane	380	C27H56	000593-49-7	87
5		Hexadecane	226	C16H34	000544-76-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM022619\
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Acq On : 26 Feb 2019 16:09
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ALS Vial : 5 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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unknown7.23	7.23	115.0	ng	9029300	1	7.69	1570170	20.0
1,4-Methanoazulen...	13.59	4.9	ng	525324	3	14.34	2129590	20.0
n-Hexadecanoic acid	17.99	10.0	ng	1115530	4	17.10	2240010	20.0
Octadecanoic acid	19.27	3.5	ng	516524	5	21.29	2988600	20.0
Bicyclo[5.2.0]non...	20.37	2.4	ng	361227	5	21.29	2988600	20.0
3-Eicosene, (E)-	20.99	7.0	ng	1053870	5	21.29	2988600	20.0
Heptacosane	21.86	2.2	ng	325290	5	21.29	2988600	20.0
Docosane, 5-butyl-	22.33	4.2	ng	630726	5	21.29	2988600	20.0
Pentadecane, 8-he...	23.40	5.6	ng	781704	6	23.54	2807820	20.0
Pentadecane, 8-he...	24.04	8.6	ng	1203100	6	23.54	2807820	20.0