

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
 Data File : BM018589.D
 Acq On : 16 Jan 2019 18:38
 Operator : JU/SJ
 Sample : K1149-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SW003-190114-01

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-BM010919.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	3.969	145	150	157	rBV	364149	545668	2.38%	0.459%
2	5.340	375	383	389	rBV	2634646	3917924	17.11%	3.296%
3	6.922	642	652	668	rBV2	1744216	3216368	14.05%	2.706%
4	7.281	705	713	724	rBV	5229411	8345369	36.46%	7.020%
5	7.745	784	792	799	rBV	1444526	2281827	9.97%	1.919%
6	8.063	839	846	852	rBV	4467477	7246370	31.65%	6.096%
7	8.110	852	854	862	rVB	251585	336815	1.47%	0.283%
8	8.192	862	868	874	rBV	224530	361760	1.58%	0.304%
9	8.275	874	882	891	rVB	335910	589403	2.57%	0.496%
10	8.522	917	924	930	rBV	348056	585114	2.56%	0.492%
11	8.916	983	991	1002	rBV	3724442	6117540	26.72%	5.146%
12	10.022	1174	1179	1185	rBV2	154995	243268	1.06%	0.205%
13	10.539	1259	1267	1271	rBV	1956742	3328754	14.54%	2.800%
14	10.586	1271	1275	1283	rVB	2332958	3751413	16.39%	3.156%
15	10.710	1288	1296	1304	rVB	208798	406309	1.77%	0.342%
16	11.939	1498	1505	1512	rBV	213559	365284	1.60%	0.307%
17	12.204	1543	1550	1557	rBV	175218	280886	1.23%	0.236%
18	12.421	1578	1587	1595	rVB	196740	370883	1.62%	0.312%
19	13.010	1680	1687	1695	rBV	10194393	15167188	66.26%	12.759%
20	14.398	1916	1923	1929	rBV2	2857194	4475168	19.55%	3.764%
21	14.457	1929	1933	1941	rVB	308410	469215	2.05%	0.395%
22	14.792	1985	1990	1998	rBV	197191	319343	1.40%	0.269%
23	15.445	2095	2101	2110	rBV	236572	344270	1.50%	0.290%
24	15.892	2170	2177	2189	rBV	9000802	12389662	54.12%	10.422%
25	16.127	2211	2217	2225	rVB4	180678	342377	1.50%	0.288%
26	17.145	2384	2390	2395	rBV2	3809721	5344478	23.35%	4.496%
27	17.186	2395	2397	2402	rVB	260038	308668	1.35%	0.260%
28	17.556	2455	2460	2465	rVB	258843	370385	1.62%	0.312%
29	17.903	2515	2519	2528	rBV3	125399	238503	1.04%	0.201%
30	18.033	2536	2541	2551	rBV	919280	1374941	6.01%	1.157%
31	19.203	2736	2740	2747	rVB2	196595	323707	1.41%	0.272%
32	19.315	2755	2759	2770	rBV2	591838	973233	4.25%	0.819%
33	19.780	2832	2838	2843	rBV	18550443	22891943	100.00%	19.257%
34	21.033	3048	3051	3055	rBV	258071	266833	1.17%	0.224%

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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	21.339	3098	3103	3111	rBV	4346612	5396827	23.58%	4.540%
36	22.386	3279	3281	3289	rVB2	302312	416909	1.82%	0.351%
37	22.509	3298	3302	3308	rVB	783253	1023039	4.47%	0.861%
38	23.615	3484	3490	3498	rVB	2186136	4150747	18.13%	3.492%

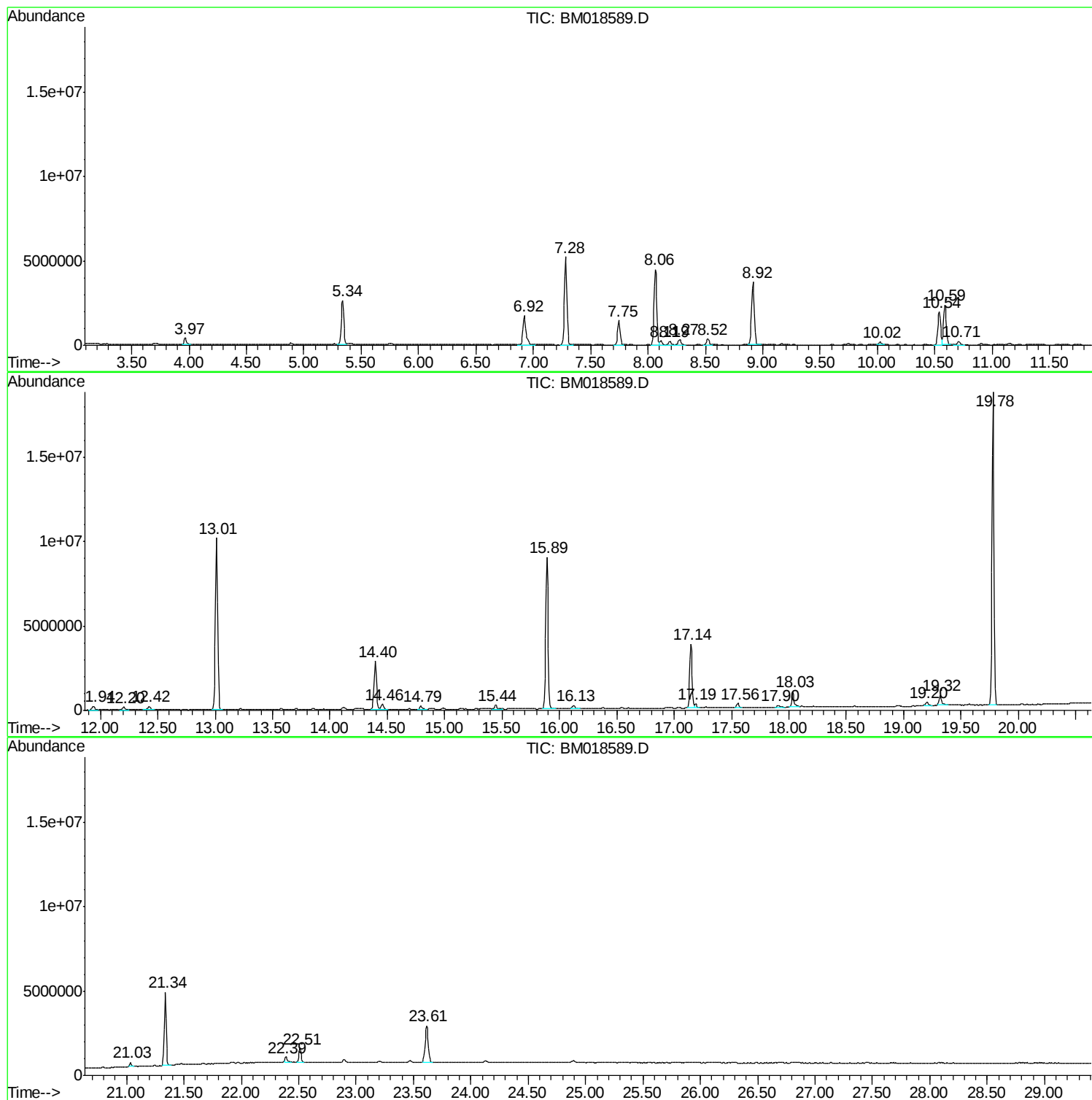
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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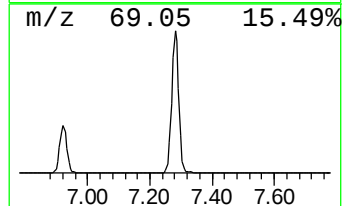
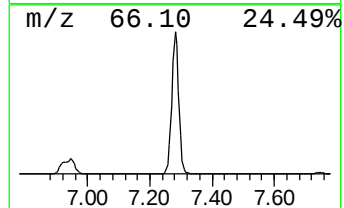
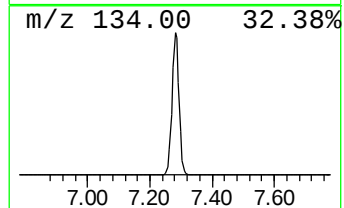
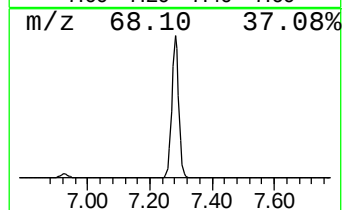
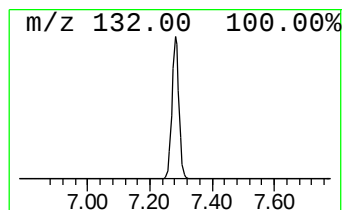
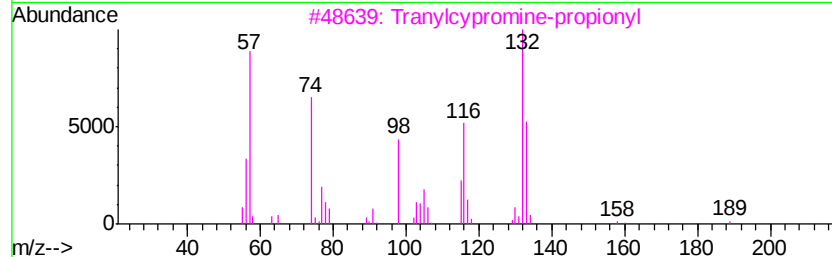
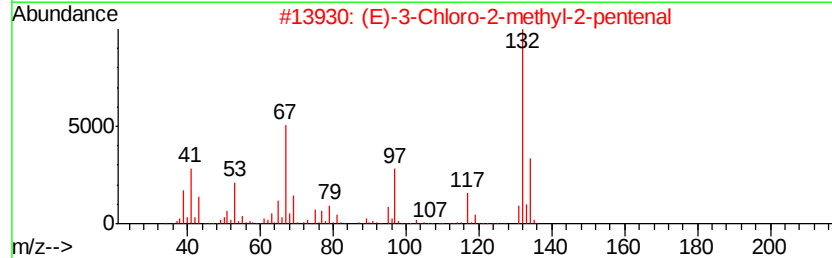
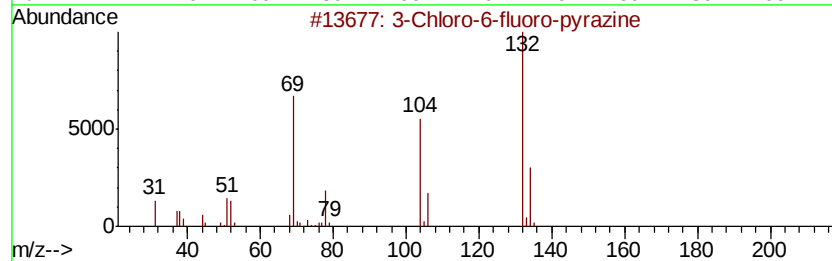
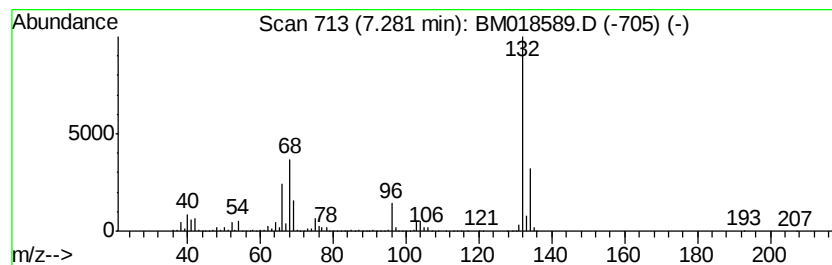
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	73.15 ng	8345370	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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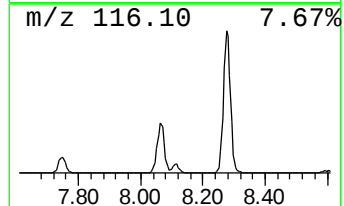
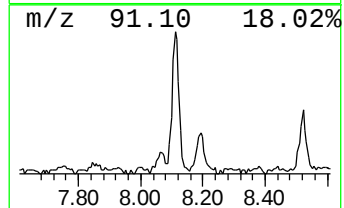
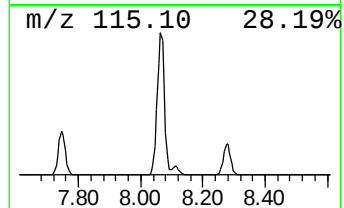
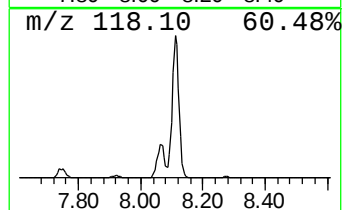
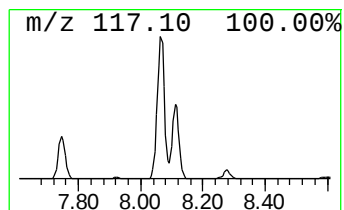
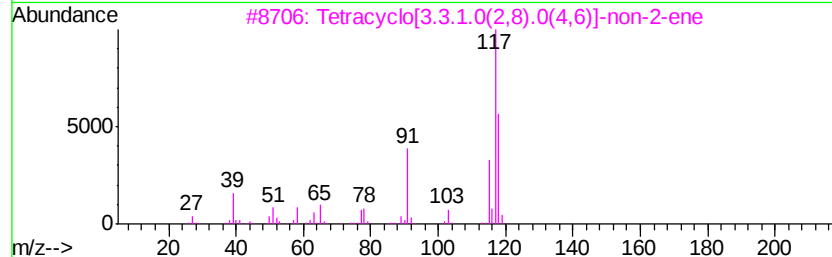
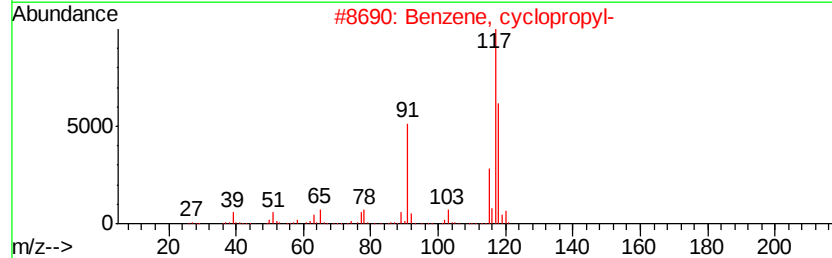
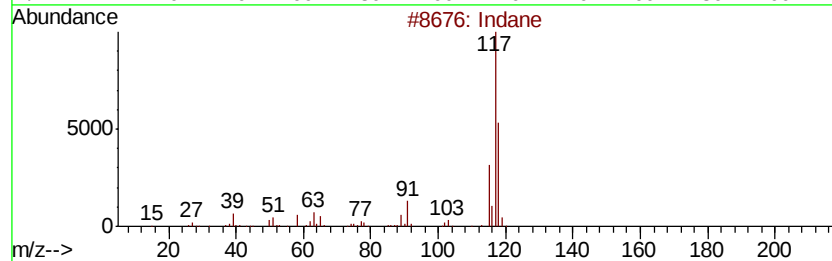
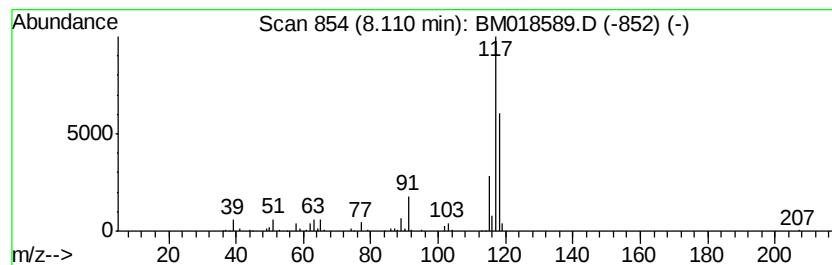
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.11	2.95 ng	336815	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indane	118	C9H10	000496-11-7	83
2		Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
3		Tetracyclo[3.3.1.0(2,8).0(4,6)]-	118	C9H10	1000191-13-7	64
4		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
5		Benzene, (chloromethyl)ethenyl-	152	C9H9Cl	030030-25-2	59



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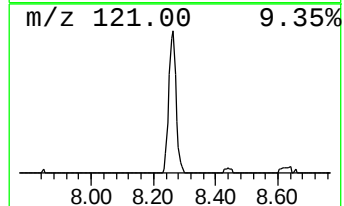
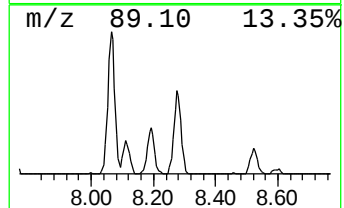
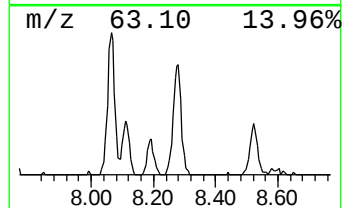
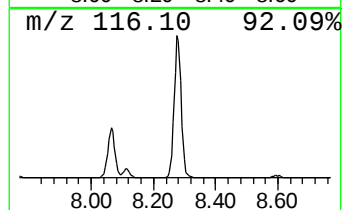
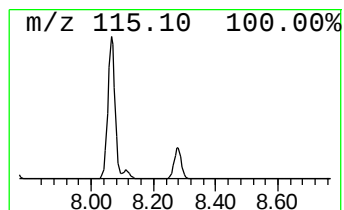
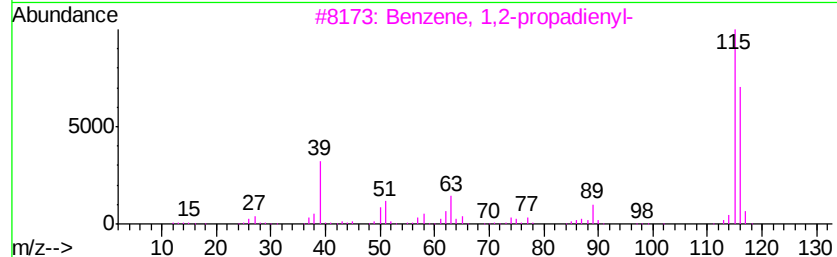
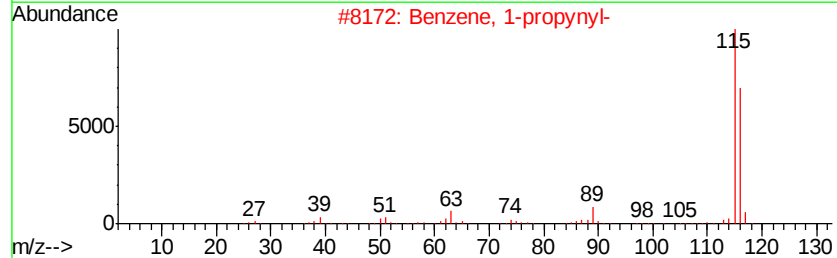
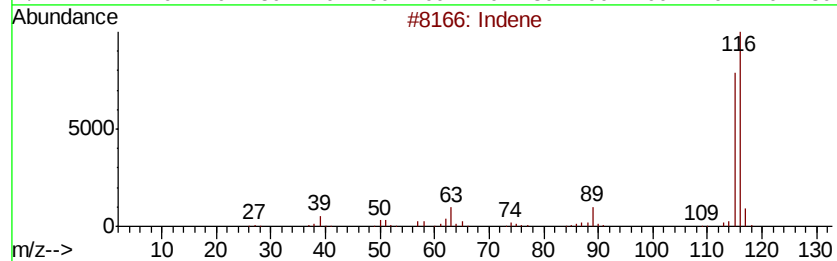
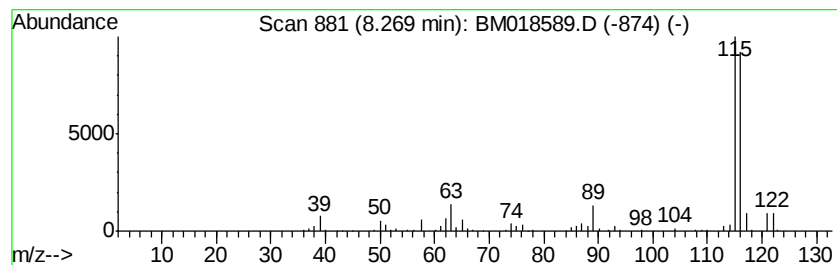
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.27	5.17 ng	589403	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indene	116	C9H8	000095-13-6	97
2		Benzene, 1-propynyl-	116	C9H8	000673-32-5	95
3		Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
4		Benzene, 1-ethynyl-2-methyl-	116	C9H8	000766-47-2	90
5		Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90



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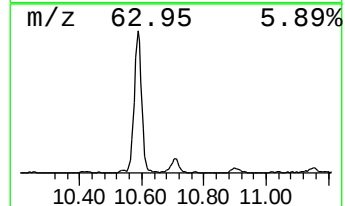
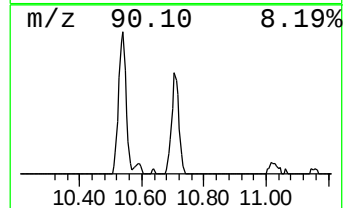
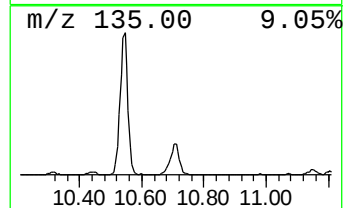
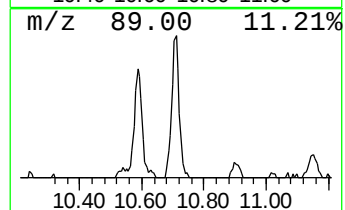
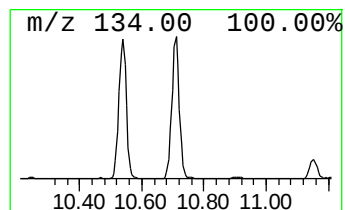
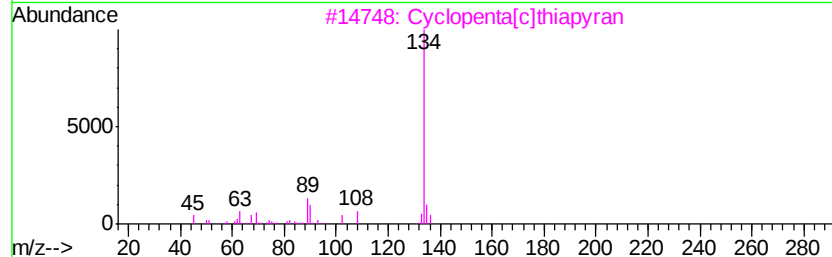
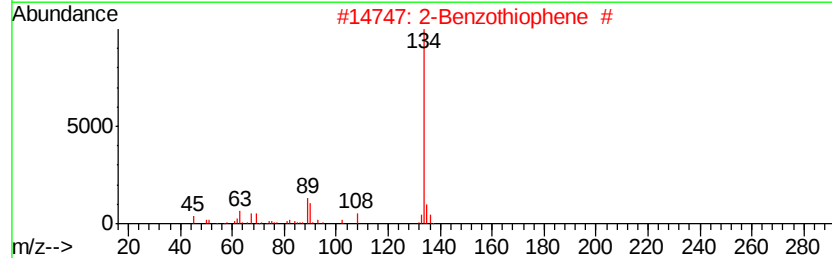
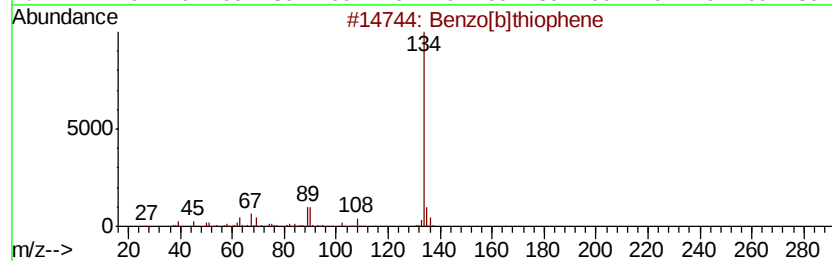
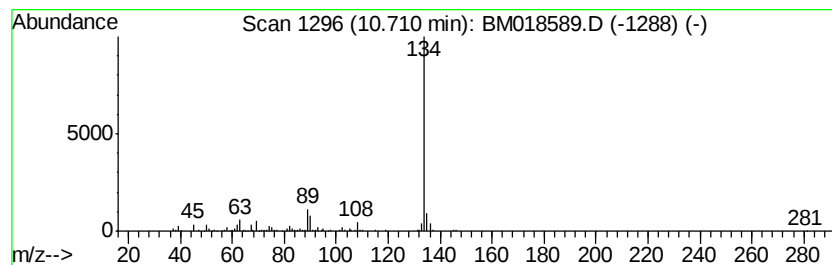
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[b]thiophene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	2.44 ng	406309	Naphthalene-d8	10.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[b]thiophene	134	C8H6S	000095-15-8	94
2		2-Benzothiophene #	134	C8H6S	000270-82-6	91
3		Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
4		Cyclopenta[b]thiapyran	134	C8H6S	000271-17-0	87
5		Thiepineo[3,2-e]isobenzofuran-1,3...	260	C14H12O3S	055044-57-0	72



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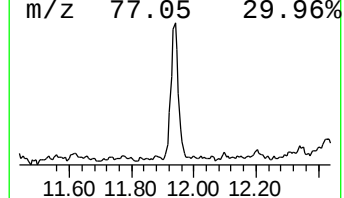
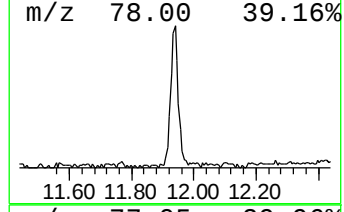
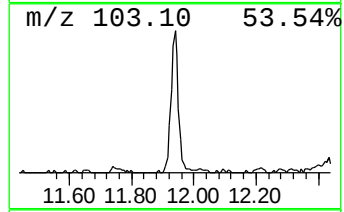
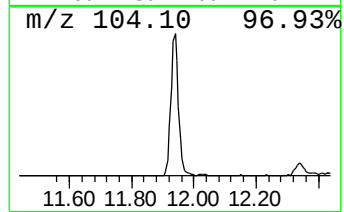
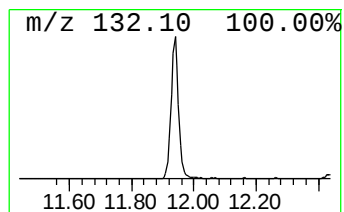
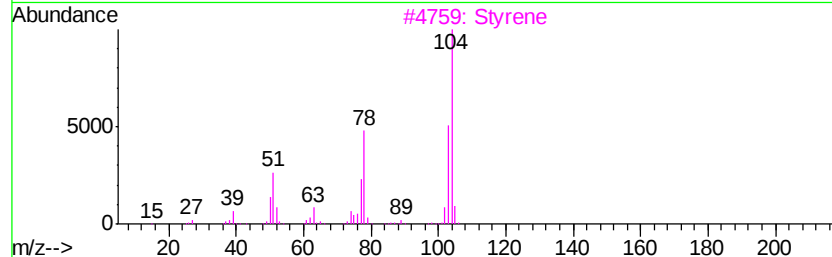
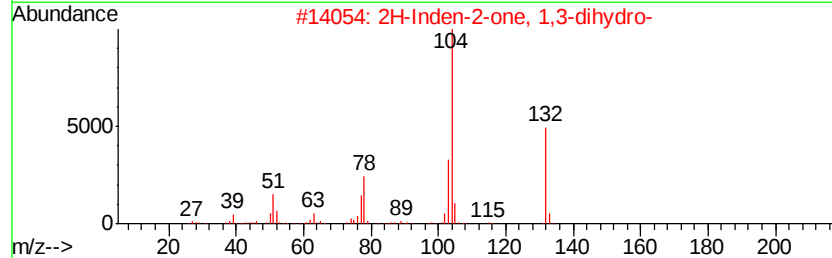
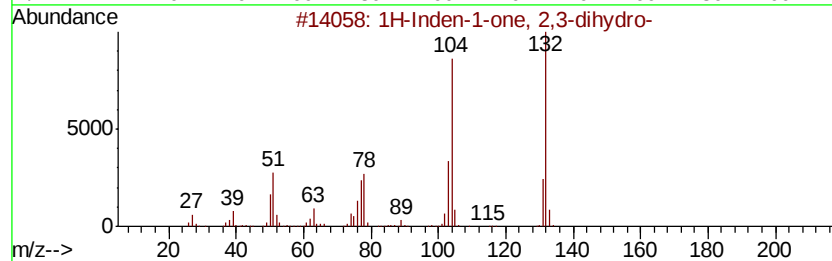
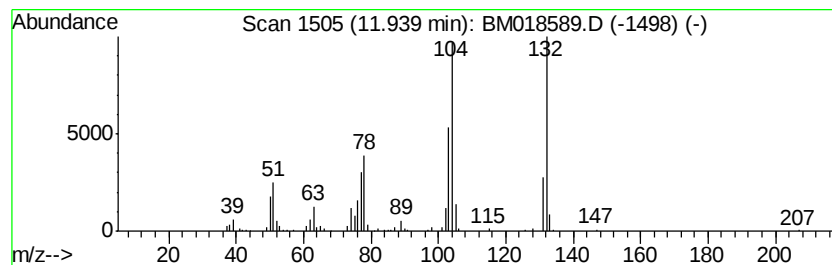
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.19 ng	365284	Napthalene-d8	10.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1H-Inden-1-one, 2,3-dihydro-	132 C9H8O	000083-33-0 96
2		2H-Inden-2-one, 1,3-dihydro-	132 C9H8O	000615-13-4 64
3		Styrene	104 C8H8	000100-42-5 60
4		Bicyclo[4.2.0]octa-1,3,5-triene	104 C8H8	000694-87-1 53
5		2H-Cyclopenta[d]pyridazine, 2-me...	132 C8H8N2	022291-85-6 52



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Data File : BM018589.D
Acq On : 16 Jan 2019 18:38
Operator : JU/SJ
Sample : K1149-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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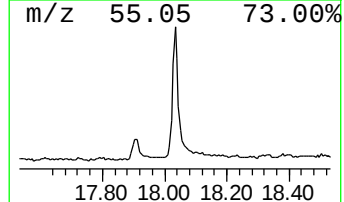
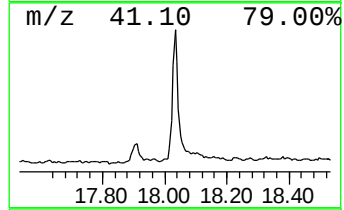
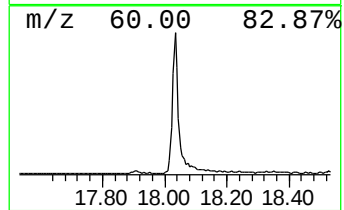
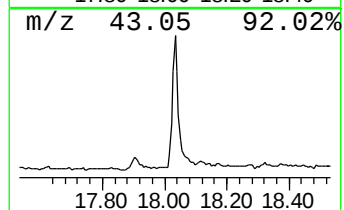
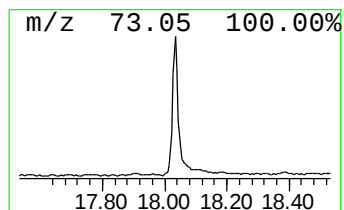
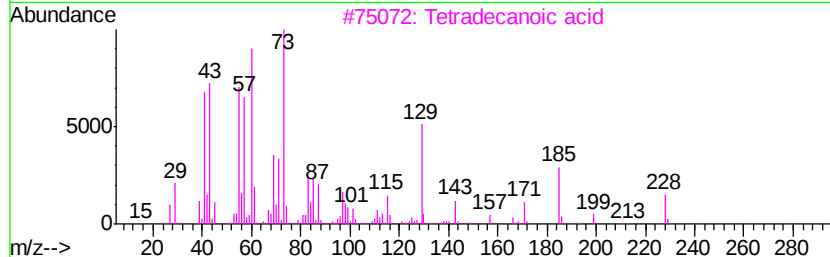
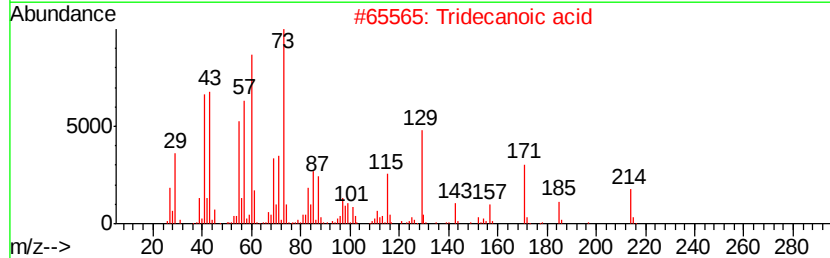
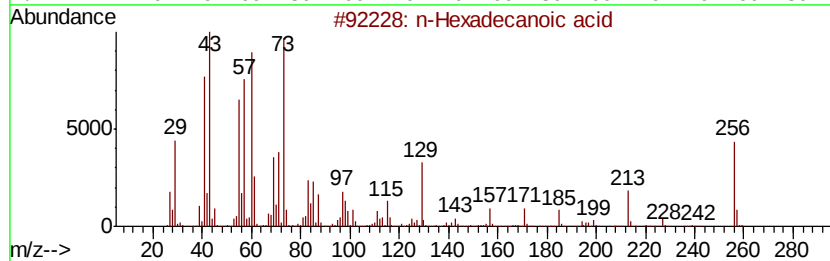
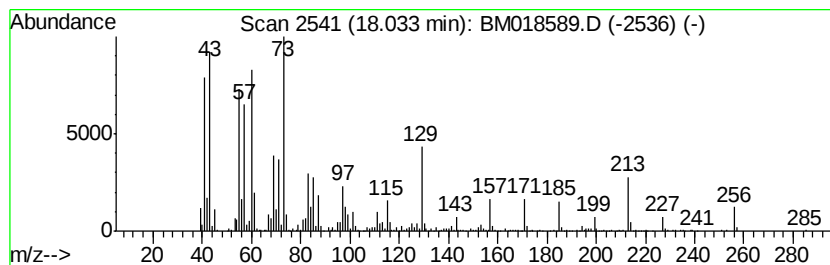
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	5.15 ng	1374940	Phenanthrene-d10	17.14

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	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018589.D
Acq On : 16 Jan 2019 18:38
Operator : JU/SJ
Sample : K1149-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW003-190114-01

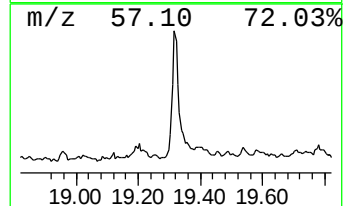
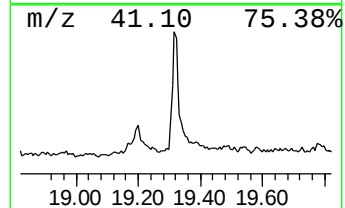
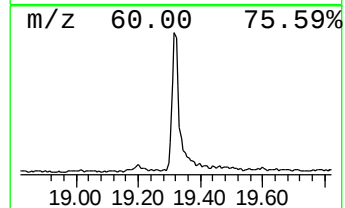
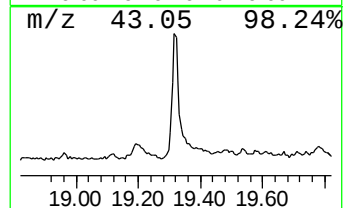
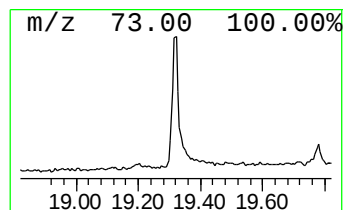
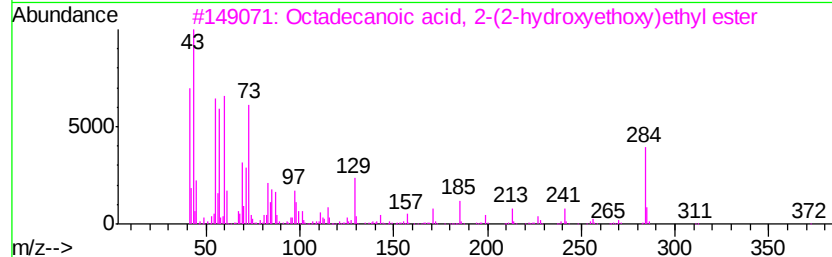
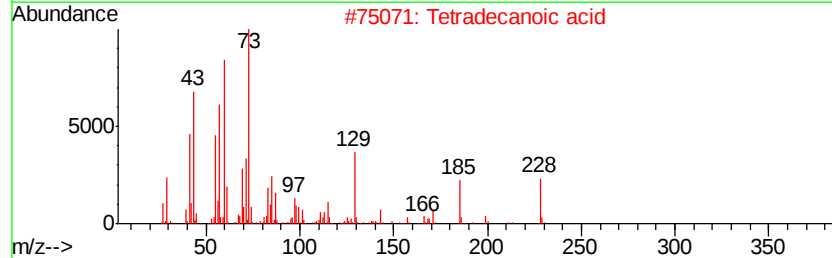
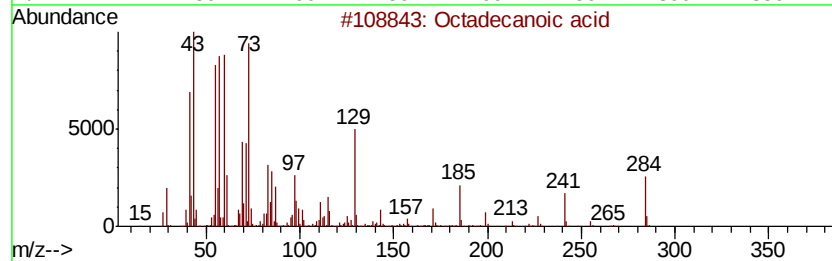
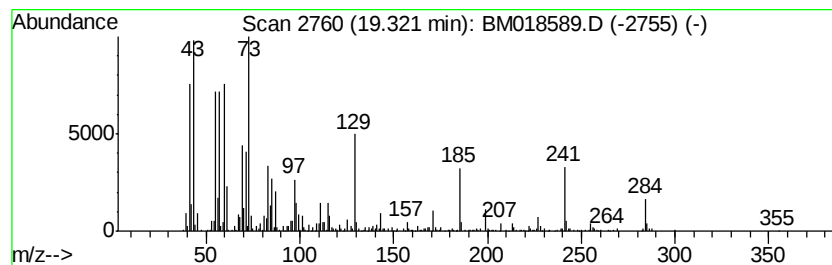
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	3.61 ng	973233	Chrysene-d12	21.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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Sample : K1149-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId :
SW003-190114-01

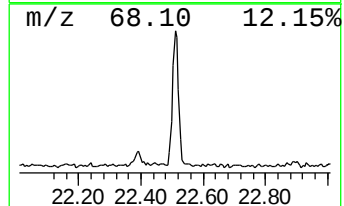
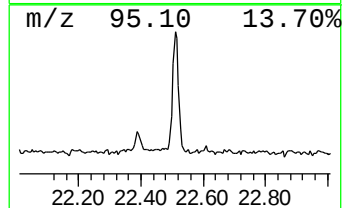
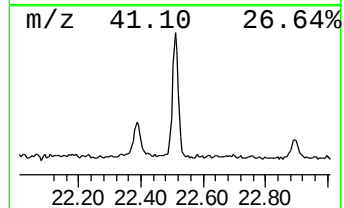
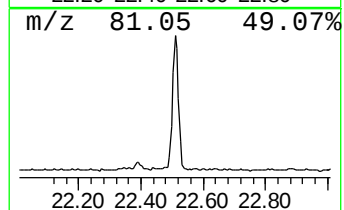
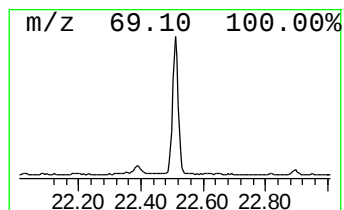
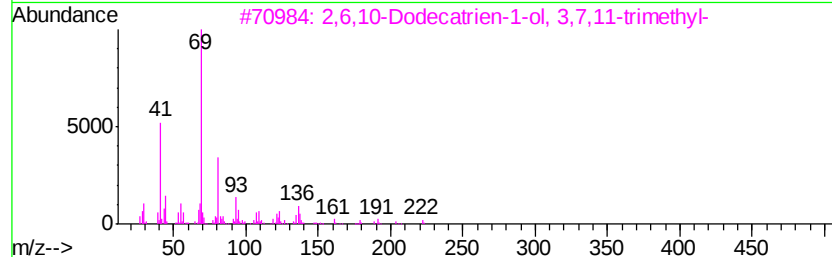
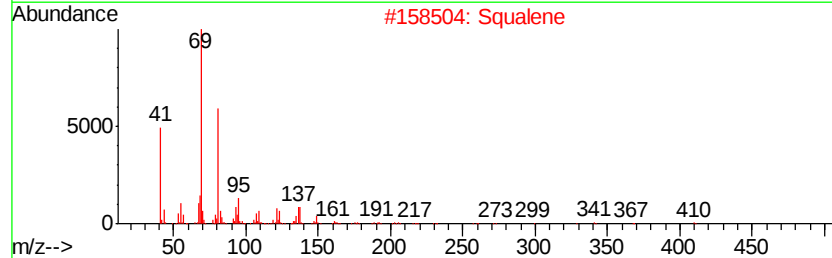
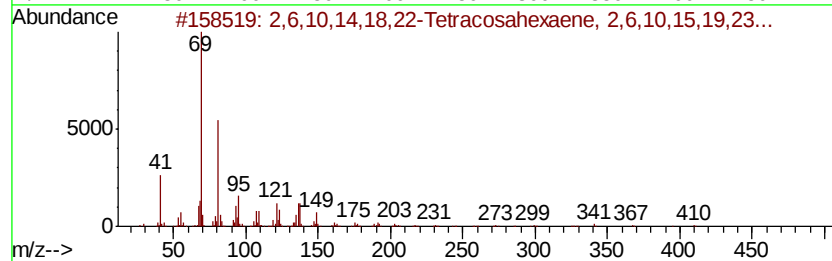
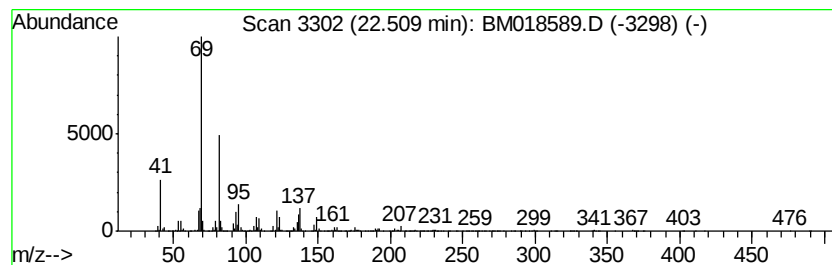
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	4.93 ng	1023040	Perylene-d12	23.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
2		Squalene	410	C30H50	007683-64-9	91
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52



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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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
unknown7.28	7.28	73.2	ng	8345370	1	7.75	2281830	20.0
Indane	8.11	3.0	ng	336815	1	7.75	2281830	20.0
Indene	8.27	5.2	ng	589403	1	7.75	2281830	20.0
Benzo[b]thiophene	10.71	2.4	ng	406309	2	10.54	3328750	20.0
1H-Inden-1-one, 2...	11.94	2.2	ng	365284	2	10.54	3328750	20.0
n-Hexadecanoic acid	18.03	5.2	ng	1374940	4	17.14	5344480	20.0
Octadecanoic acid	19.32	3.6	ng	973233	5	21.34	5396830	20.0
2,6,10,14,18,22-T...	22.51	4.9	ng	1023040	6	23.61	4150750	20.0