

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053116\
 Data File : BF087607.D
 Acq On : 1 Jun 2016 6:02
 Operator : UM/SJ
 Sample : H3323-02
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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	4.696	270	272	292	rBV	89460	363975	9.41%	1.094%
2	5.347	327	329	357	rBV	1349617	3103735	80.22%	9.332%
3	7.016	472	475	480	rBV	1540552	2943469	76.08%	8.850%
4	7.096	480	482	502	rVB	1796369	3869023	100.00%	11.633%
5	7.450	511	513	528	rVB	437195	896744	23.18%	2.696%
6	7.679	531	533	545	rVV	1539852	2475803	63.99%	7.444%
7	8.365	591	593	621	rBV	1233403	2183051	56.42%	6.564%
8	9.473	689	690	705	rBV	455984	1134151	29.31%	3.410%
9	11.245	842	845	857	rBV	2511094	3443679	89.01%	10.354%
10	11.953	905	907	915	rBV	154119	319602	8.26%	0.961%
11	12.125	920	922	927	rVB2	20325	41150	1.06%	0.124%
12	12.296	935	937	942	rBV	808665	1114096	28.80%	3.350%
13	13.131	1007	1010	1012	rBV	56453	68380	1.77%	0.206%
14	13.485	1035	1041	1046	rBV2	25020	63983	1.65%	0.192%
15	13.599	1048	1051	1063	rBV	894010	1833822	47.40%	5.514%
16	13.897	1075	1077	1081	rBV	64784	132825	3.43%	0.399%
17	14.628	1138	1141	1143	rVB2	58232	78224	2.02%	0.235%
18	14.708	1146	1148	1151	rBV	593403	859174	22.21%	2.583%
19	14.765	1151	1153	1161	rVB	113585	285708	7.38%	0.859%
20	14.891	1162	1164	1166	rBV	21659	40079	1.04%	0.121%
21	15.302	1198	1200	1204	rVB2	30750	54894	1.42%	0.165%
22	15.542	1218	1221	1223	rBV	33772	51394	1.33%	0.155%
23	15.588	1223	1225	1230	rVB	30556	48891	1.26%	0.147%
24	15.691	1231	1234	1237	rBV2	71068	149909	3.87%	0.451%
25	16.537	1306	1308	1316	rBV	236133	445758	11.52%	1.340%
26	16.834	1332	1334	1338	rBV	246139	448316	11.59%	1.348%
27	16.903	1338	1340	1343	rVB	345206	398796	10.31%	1.199%
28	16.971	1343	1346	1347	rBV	49461	71184	1.84%	0.214%
29	17.005	1347	1349	1351	rBV	58346	70759	1.83%	0.213%
30	17.063	1351	1354	1360	rVB	1704524	2358098	60.95%	7.090%
31	17.177	1362	1364	1367	rBV2	23004	47685	1.23%	0.143%
32	17.325	1376	1377	1380	rVB	31784	43084	1.11%	0.130%
33	17.577	1396	1399	1400	rBV2	27470	56585	1.46%	0.170%
34	17.725	1409	1412	1414	rBV	181318	233153	6.03%	0.701%

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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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35	17.828	1419	1421	1423	rBV	219746	248093	6.41%	0.746%
36	17.885	1424	1426	1428	rBV	59040	57611	1.49%	0.173%
37	18.148	1447	1449	1452	rVB3	31421	42020	1.09%	0.126%
38	18.308	1461	1463	1471	rBV3	80605	186038	4.81%	0.559%
39	18.423	1471	1473	1481	rBV	533597	1191643	30.80%	3.583%
40	18.708	1496	1498	1502	rBV	76704	112837	2.92%	0.339%
41	19.086	1529	1531	1533	rBV2	66504	111313	2.88%	0.335%
42	19.428	1559	1561	1563	rBV2	106161	172063	4.45%	0.517%
43	19.726	1585	1587	1589	rBV	116793	197446	5.10%	0.594%
44	19.817	1593	1595	1597	rVB	120791	146403	3.78%	0.440%
45	20.080	1616	1618	1619	rBV	114246	159908	4.13%	0.481%
46	20.114	1619	1621	1623	rBV	296132	415377	10.74%	1.249%
47	20.594	1661	1663	1667	rVB2	167796	272173	7.03%	0.818%
48	20.926	1690	1692	1696	rVB2	127836	217331	5.62%	0.653%

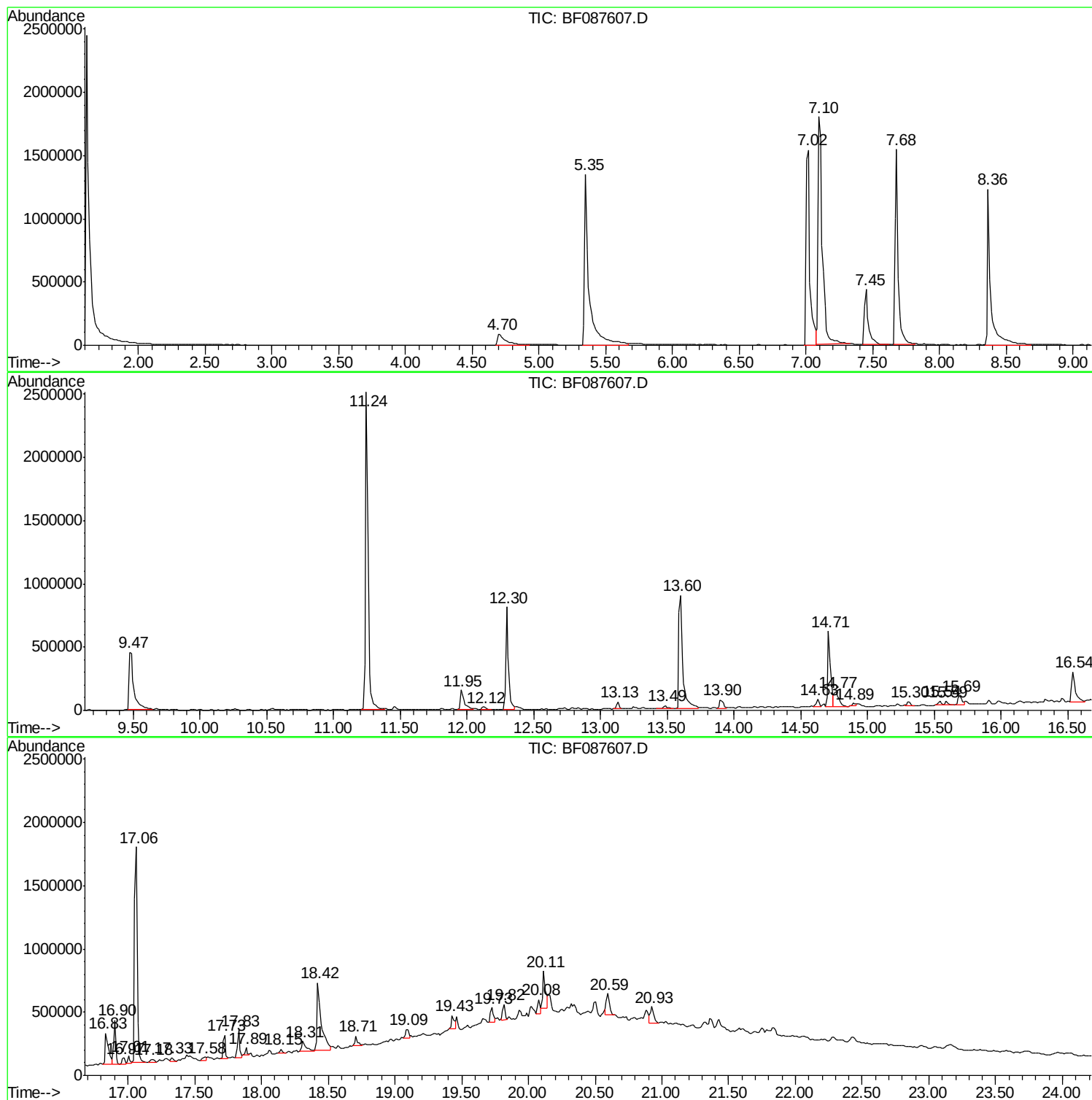
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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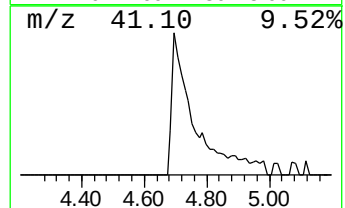
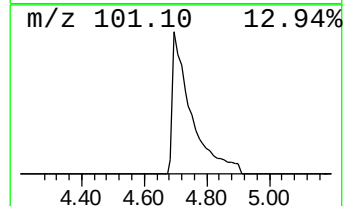
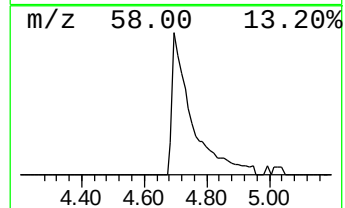
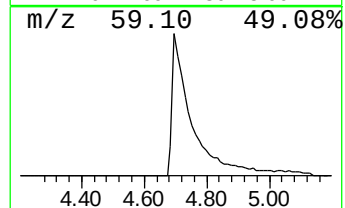
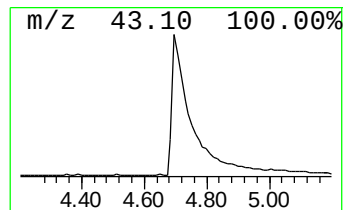
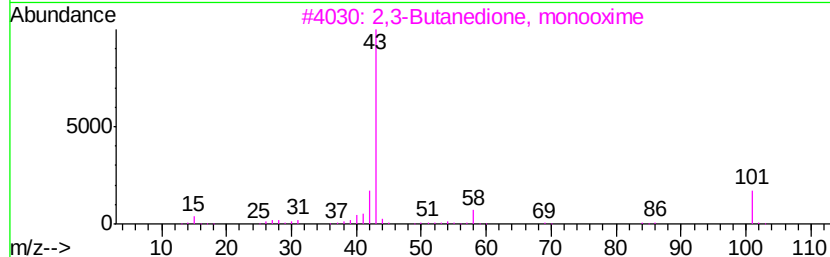
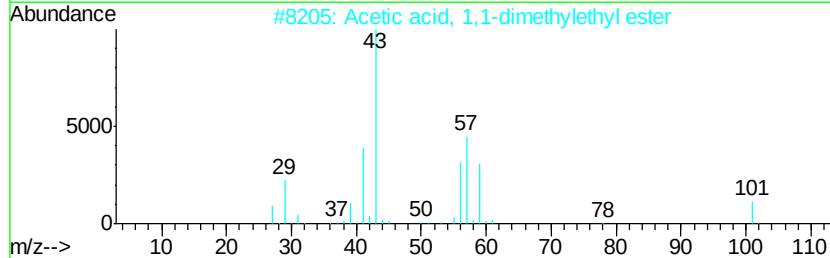
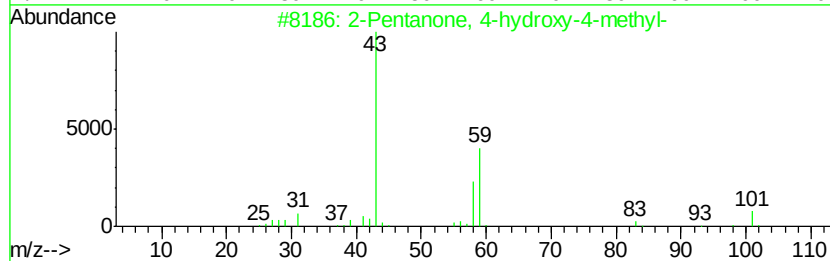
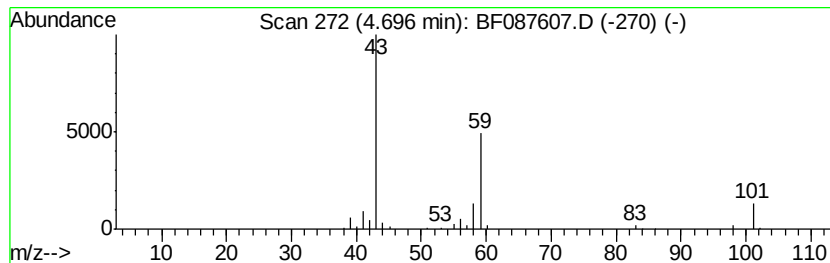
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.70	8.12 ng	363975	1,4-Dichlorobenzene-d4	7.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		Butanoic acid, 4-amino-3-hydroxy...	119	C4H9NO3	000924-49-2	9



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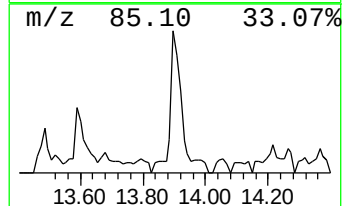
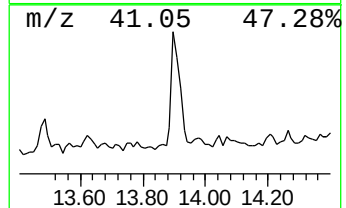
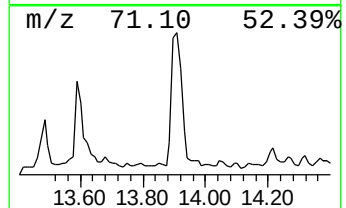
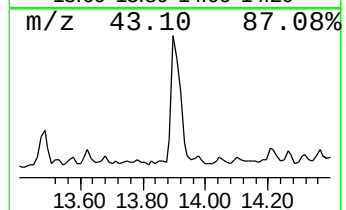
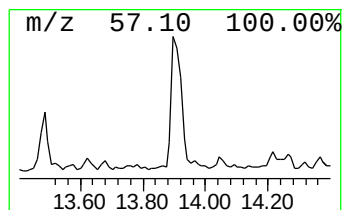
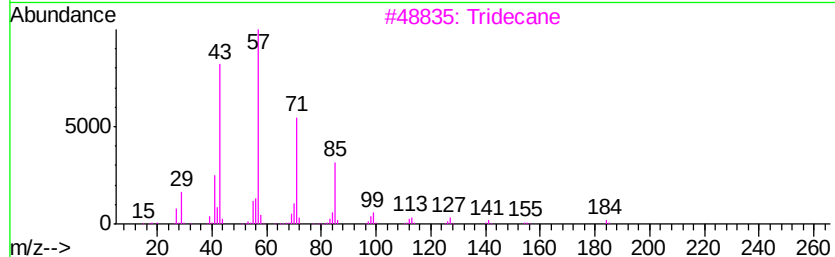
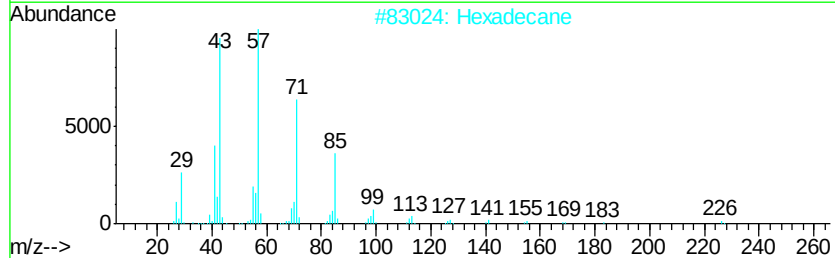
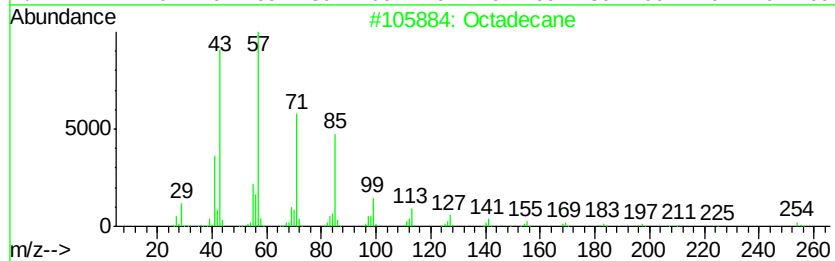
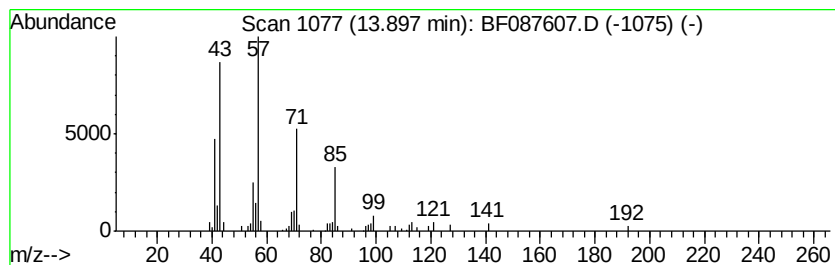
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Octadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	3.09 ng	132825	Phenanthrene-d10	14.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Heptadecane	240	C17H36	000629-78-7	80
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80



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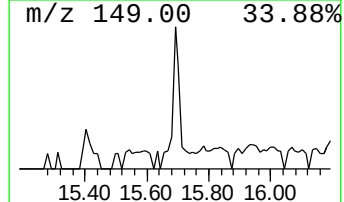
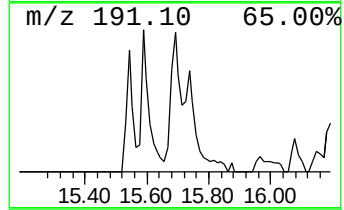
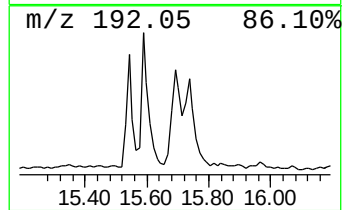
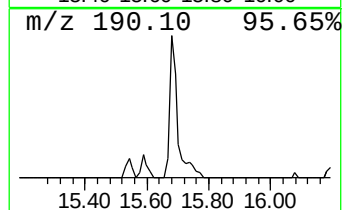
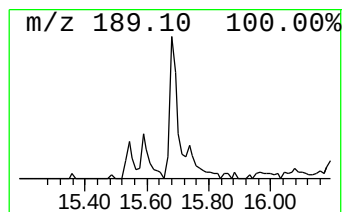
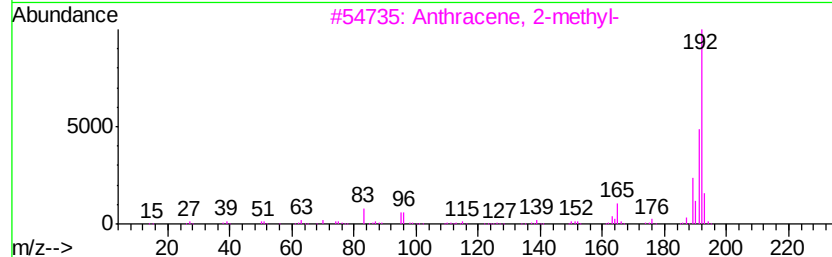
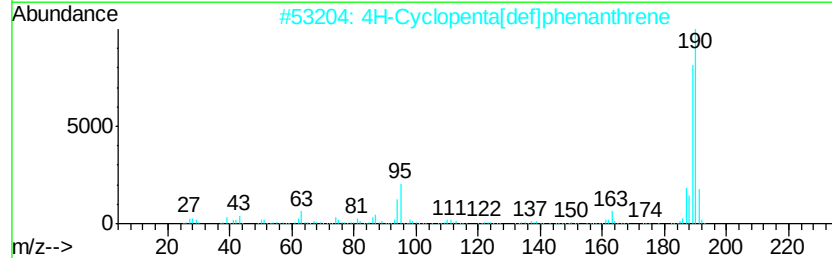
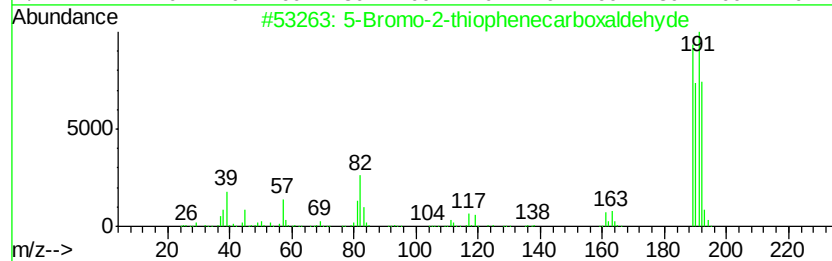
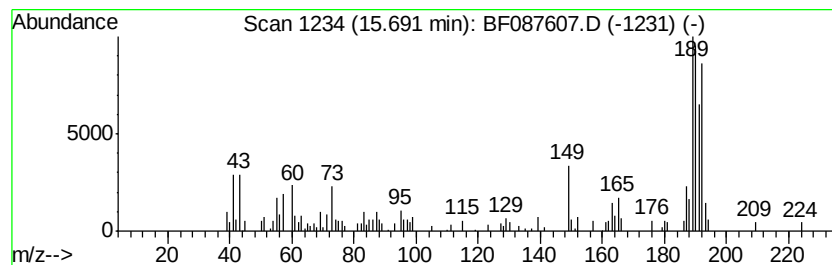
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Bromo-2-thiophenecarboxal... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	3.49 ng	149909	Phenanthrene-d10	14.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	53
2		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	38
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	38
4		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	30
5		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30



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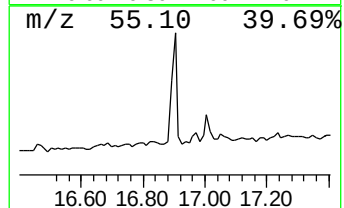
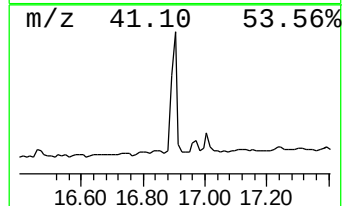
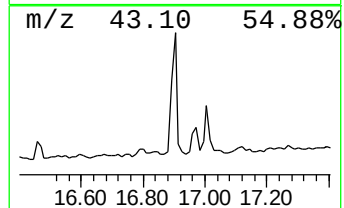
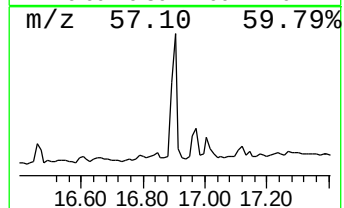
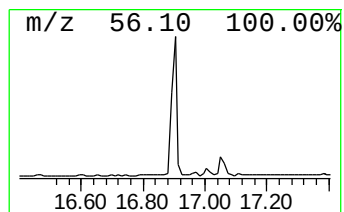
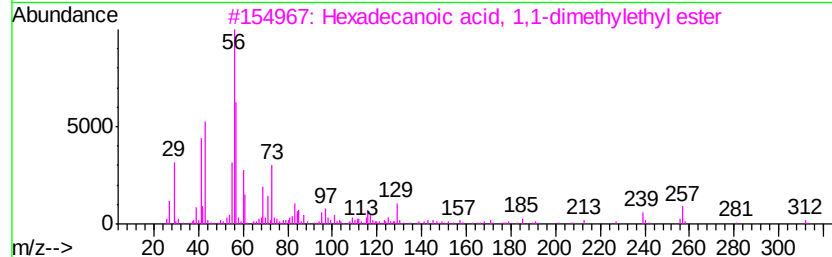
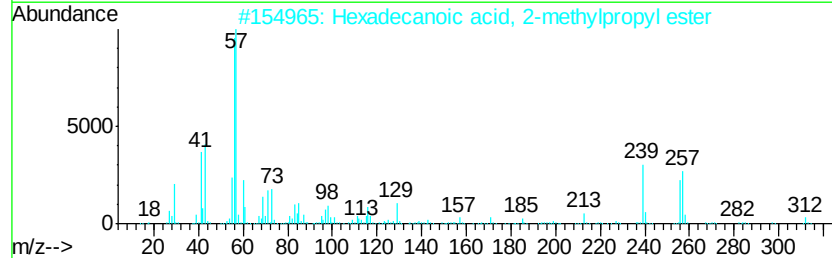
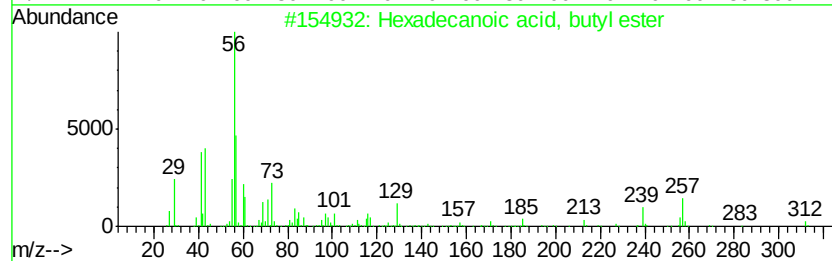
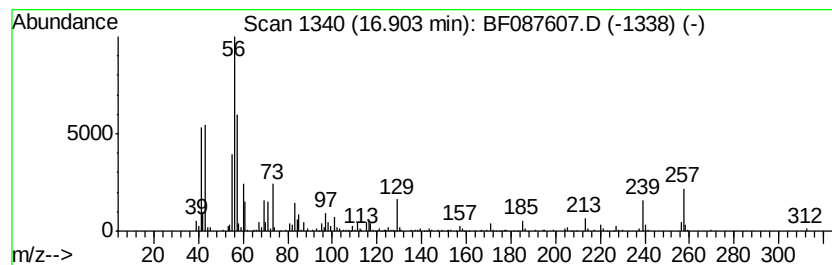
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.90	6.69 ng	398796	Chrysene-d12	18.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	38
4		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35
5		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



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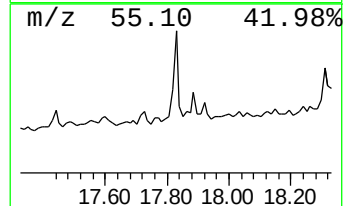
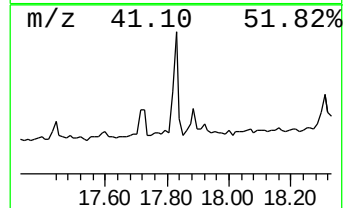
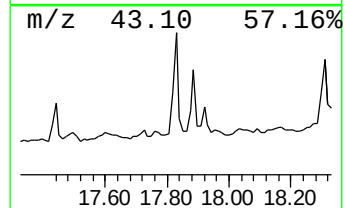
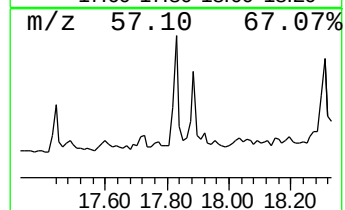
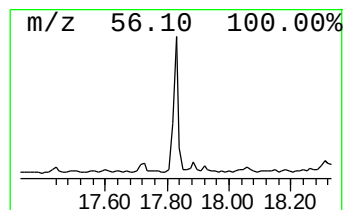
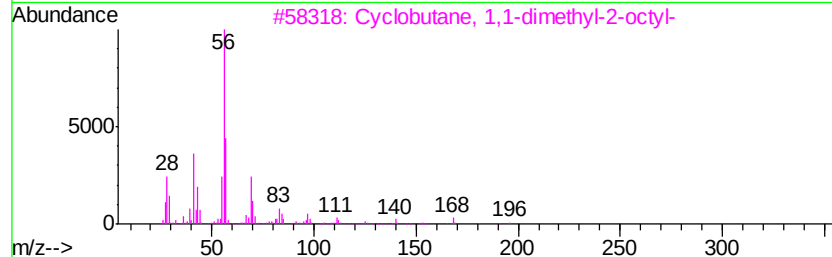
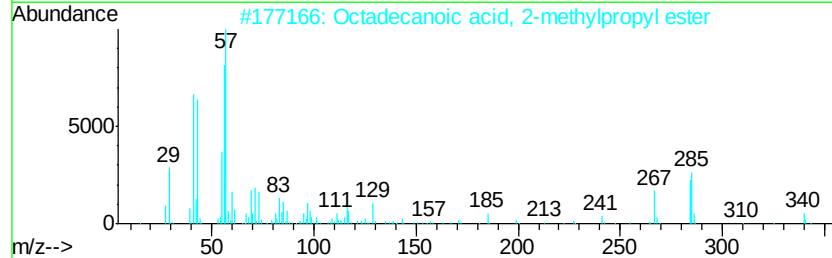
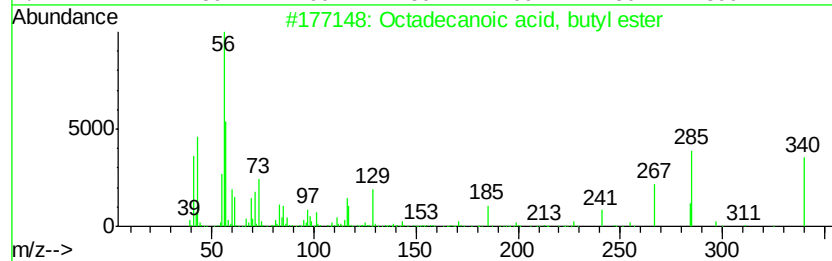
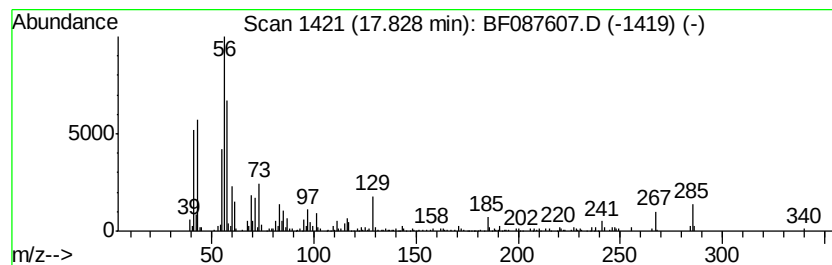
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	4.16 ng	248093	Chrysene-d12	18.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	60
2		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	38
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	35



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Acq On : 1 Jun 2016 6:02
Operator : UM/SJ
Sample : H3323-02
Misc :
ALS Vial : 22 Sample Multiplier: 1

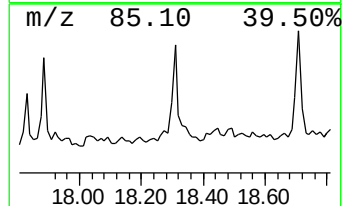
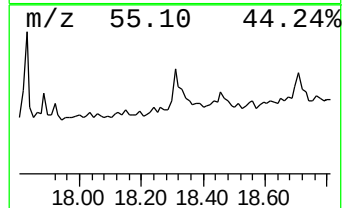
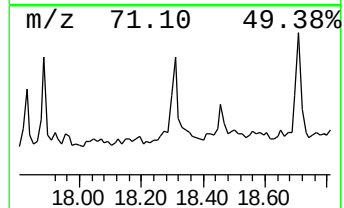
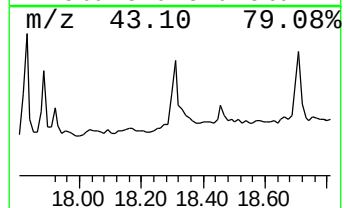
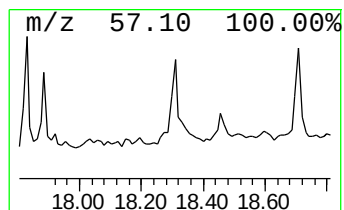
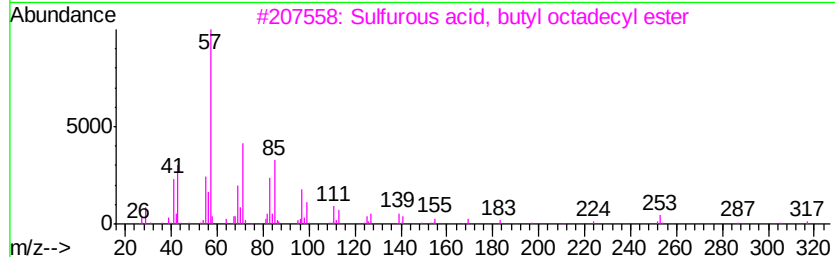
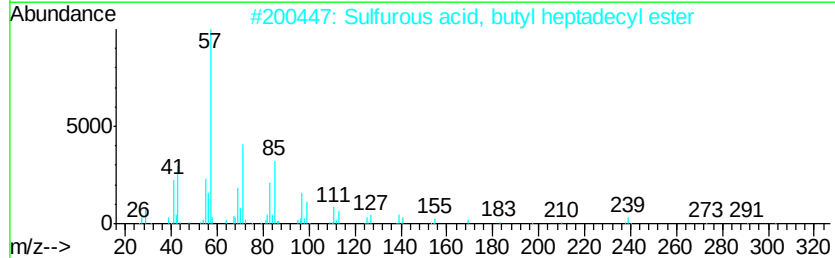
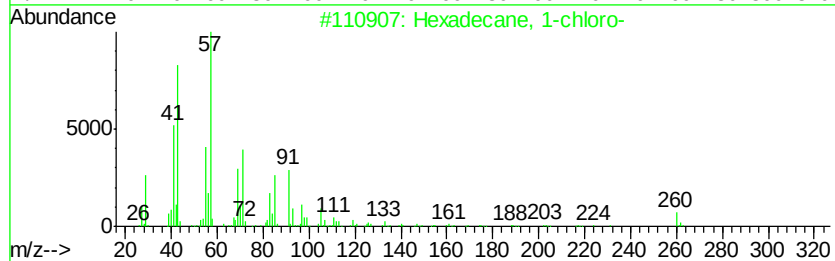
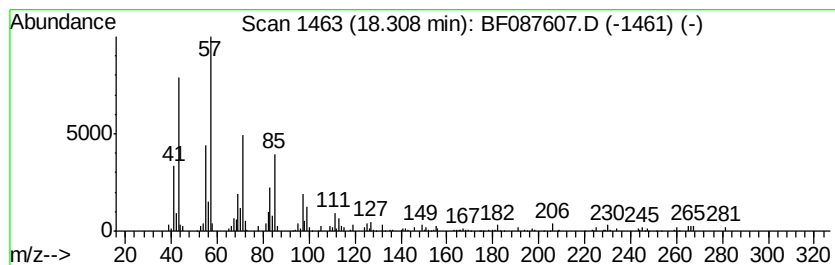
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane, 1-chloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	3.12 ng	186038	Chrysene-d12	18.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane, 1-chloro-	260 C16H33Cl	004860-03-1	93
2	Sulfurous acid, butyl heptadecyl...	376 C21H44O3S	1000309-18-4	87
3	Sulfurous acid, butyl octadecyl ...	390 C22H46O3S	1000309-18-5	87
4	Tritetracontane	605 C43H88	007098-21-7	86
5	Sulfurous acid, 2-propyl tridecy...	306 C16H34O3S	1000309-12-4	86



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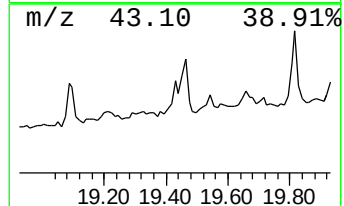
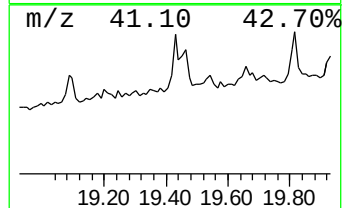
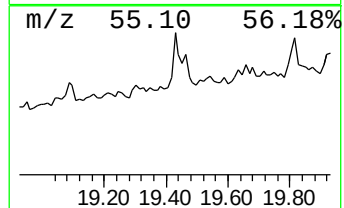
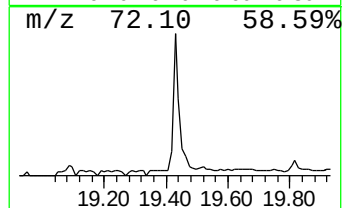
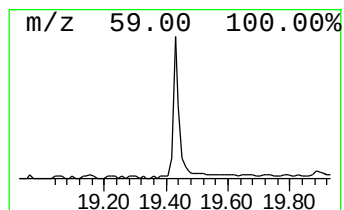
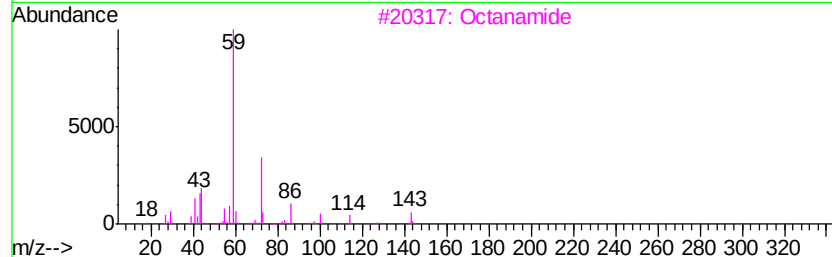
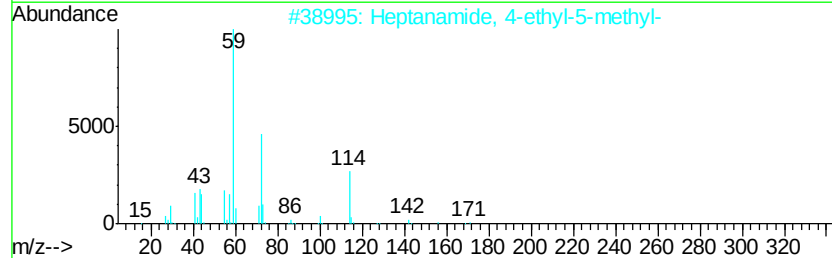
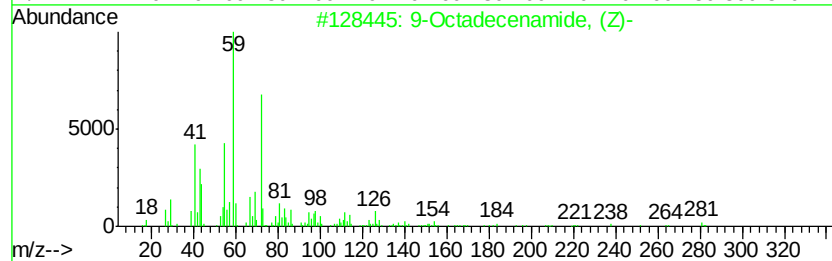
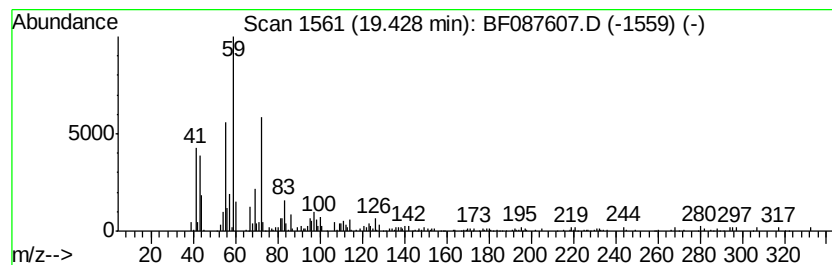
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	8.28 ng	172063	Perylene-d12	20.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
3		Octanamide	143	C8H17NO	000629-01-6	53
4		Nonanamide	157	C9H19NO	001120-07-6	53
5		Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	43



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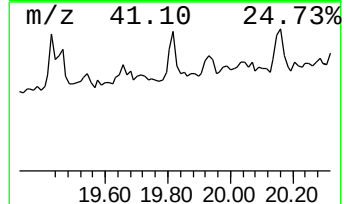
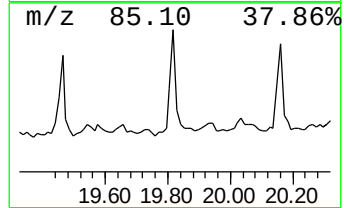
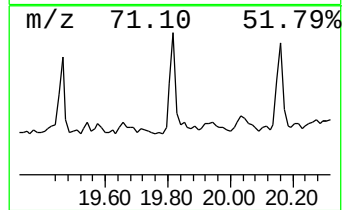
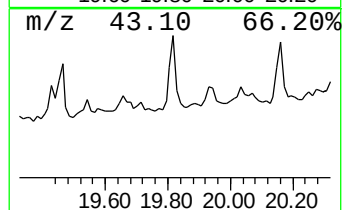
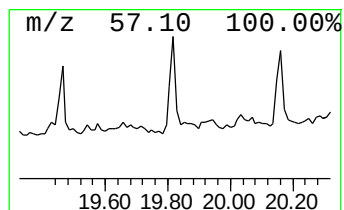
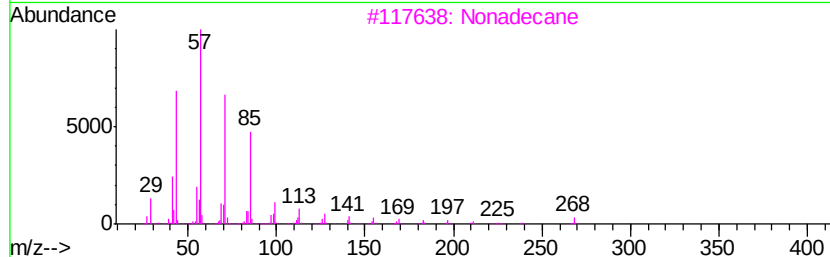
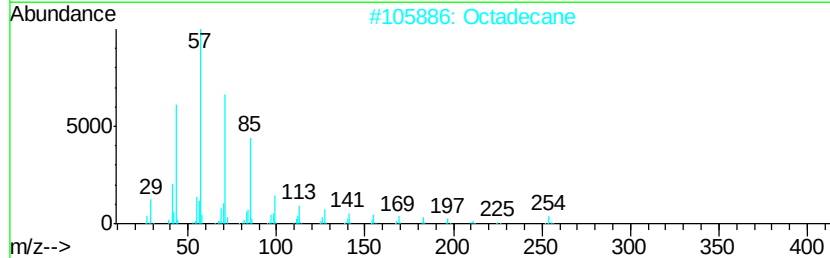
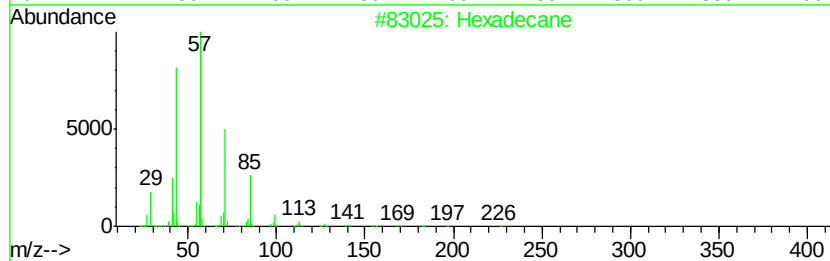
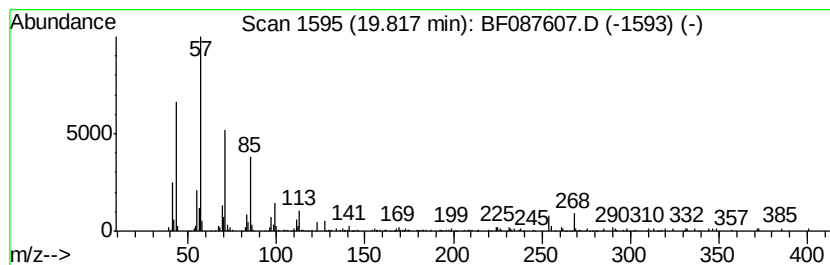
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.82	7.05 ng	146403	Perylene-d12	20.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Octadecane	254	C18H38	000593-45-3	91
3		Nonadecane	268	C19H40	000629-92-5	91
4		Tricosane	324	C23H48	000638-67-5	81
5		Hexatriacontane	507	C36H74	000630-06-8	74



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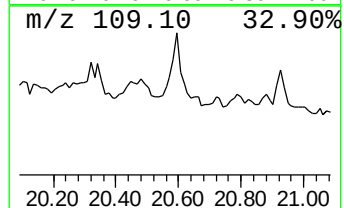
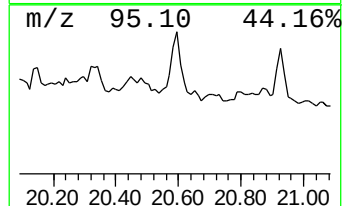
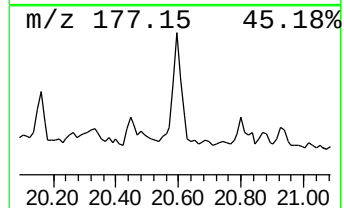
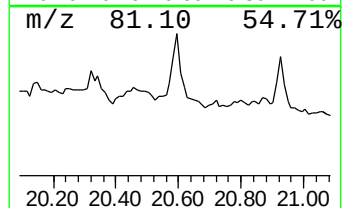
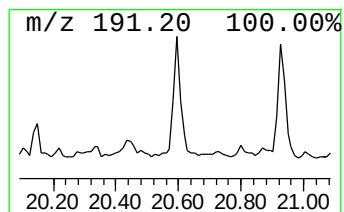
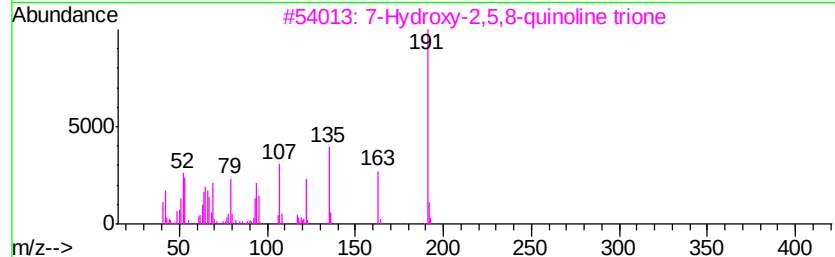
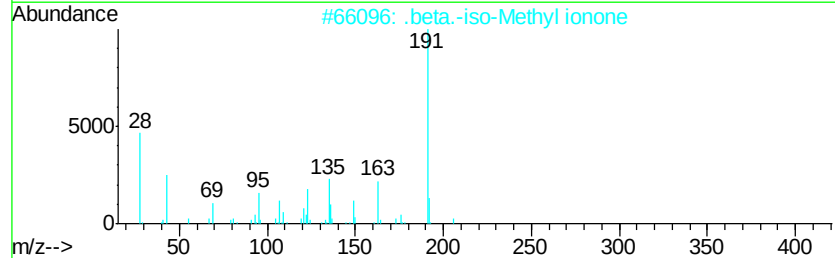
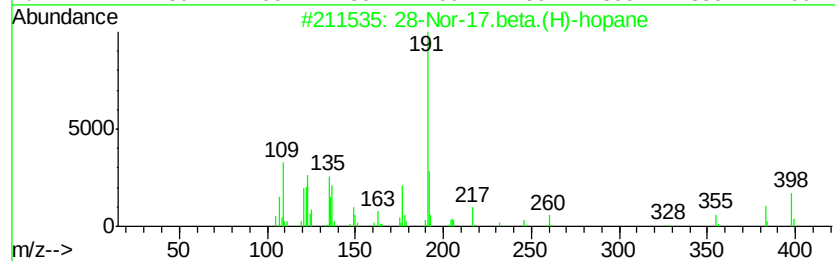
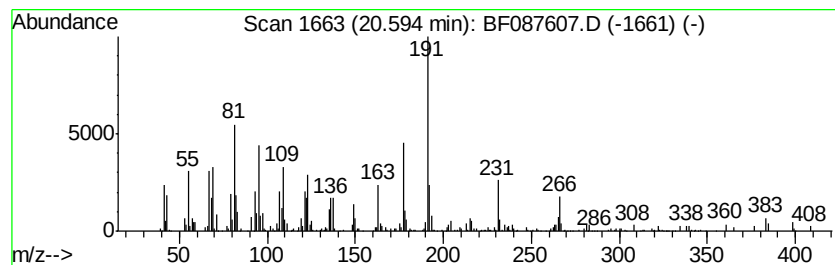
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 28-Nor-17.beta.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.59	13.10 ng	272173	Perylene-d12	20.11
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		28-Nor-17.beta.(H)-hopane	398 C29H50	036728-72-0 78
2		.beta.-iso-Methyl ionone	206 C14H22O	1000285-40-2 38
3		7-Hydroxy-2,5,8-quinoline trione	191 C9H5NO4	015544-54-4 35
4		Anthracene, 9-butyltetradecahydro-	248 C18H32	055133-89-6 27
5		1-Penten-3-one, 1-(2,6,6-trimeth...	206 C14H22O	000127-43-5 27



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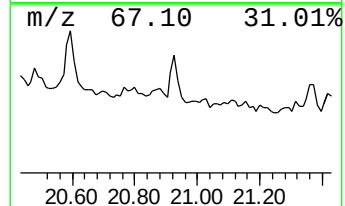
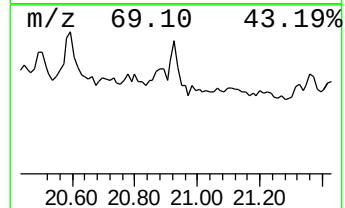
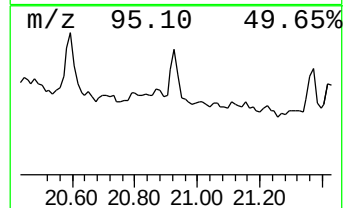
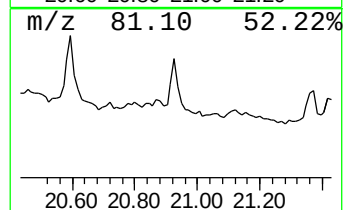
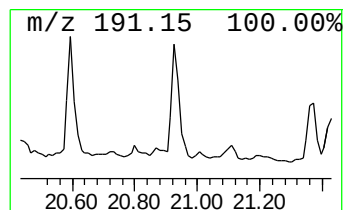
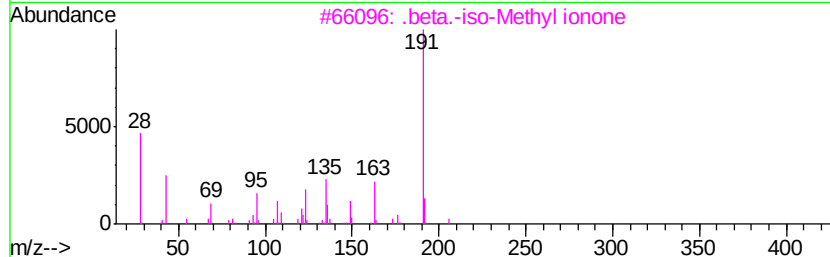
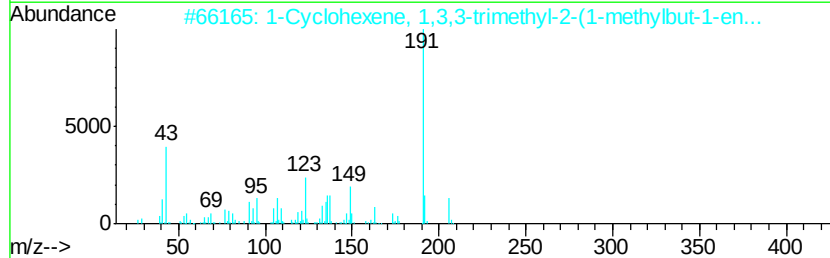
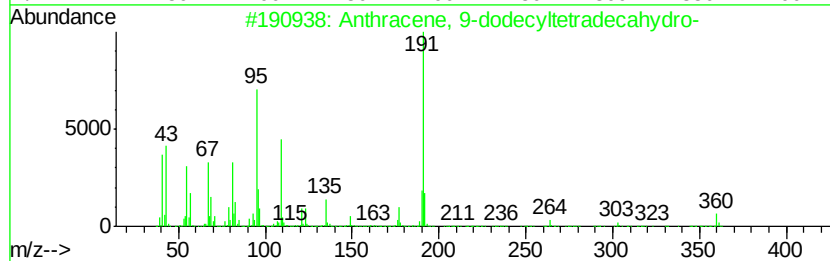
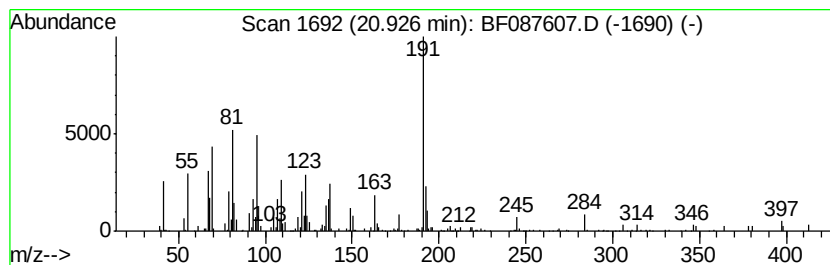
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown10.46 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	10.46 ng	217331	Perylene-d12	20.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	38
2		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
3		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	37
4		Benzoic acid, 4-[3-(3,4-dimethox...	397	C23H27NO5	1000317-25-8	35
5		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	35



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.70	8.1 ng		363975	1	7.45	896744	20.0
Octadecane	13.90	3.1 ng		132825	4	14.71	859174	20.0
5-Bromo-2-thiophe...	15.69	3.5 ng		149909	4	14.71	859174	20.0
Hexadecanoic acid...	16.90	6.7 ng		398796	5	18.42	1191640	20.0
Octadecanoic acid...	17.83	4.2 ng		248093	5	18.42	1191640	20.0
Hexadecane, 1-chl...	18.31	3.1 ng		186038	5	18.42	1191640	20.0
9-Octadecenamide,...	19.43	8.3 ng		172063	6	20.11	415377	20.0
Hexadecane	19.82	7.0 ng		146403	6	20.11	415377	20.0
28-Nor-17.beta.(H...	20.59	13.1 ng		272173	6	20.11	415377	20.0
unknown10.46	20.93	10.5 ng		217331	6	20.11	415377	20.0