

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
 Data File : BP003251.D
 Acq On : 10 Sep 2020 16:54
 Operator : CG/JU
 Sample : L3942-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 N35868

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_P\METHODS\8270-BP082420.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	4.522	252	278	287	rBV6	59748	484778	4.68%	0.693%
2	4.646	290	299	312	rVB2	105874	340156	3.28%	0.486%
3	5.258	397	403	411	rBV	497575	731115	7.06%	1.045%
4	6.840	663	672	685	rVB2	293783	562859	5.43%	0.804%
5	7.252	737	742	748	rBV	100753	158418	1.53%	0.226%
6	7.646	801	809	816	rBV	555019	869552	8.40%	1.242%
7	8.422	932	941	954	rBV2	417145	835155	8.06%	1.193%
8	8.793	995	1004	1016	rBV	1114196	1884856	18.20%	2.693%
9	8.981	1030	1036	1044	rBV2	69794	138626	1.34%	0.198%
10	9.734	1160	1164	1173	rVB2	69311	116972	1.13%	0.167%
11	10.216	1240	1246	1255	rBV	211335	360035	3.48%	0.514%
12	10.428	1274	1282	1291	rBV	716535	1331839	12.86%	1.903%
13	10.722	1325	1332	1338	rBV	156861	246642	2.38%	0.352%
14	10.787	1338	1343	1357	rVV	208685	443626	4.28%	0.634%
15	10.975	1367	1375	1378	rBV4	56414	121224	1.17%	0.173%
16	11.022	1378	1383	1398	rVB3	158202	454501	4.39%	0.649%
17	11.557	1466	1474	1483	rBV	93678	156215	1.51%	0.223%
18	11.746	1501	1506	1513	rBV3	48473	112947	1.09%	0.161%
19	11.828	1513	1520	1526	rVB2	109267	193962	1.87%	0.277%
20	12.146	1562	1574	1592	rBV	704457	1771027	17.10%	2.530%
21	12.651	1654	1660	1669	rBV	424282	641490	6.19%	0.916%
22	12.910	1697	1704	1719	rVB	3433092	5308210	51.25%	7.584%
23	13.140	1736	1743	1749	rBV	83922	143984	1.39%	0.206%
24	13.751	1840	1847	1857	rVB	715897	1077314	10.40%	1.539%
25	13.951	1877	1881	1893	rBV3	75914	136176	1.31%	0.195%
26	14.104	1900	1907	1912	rBV	375275	615746	5.95%	0.880%
27	14.292	1930	1939	1949	rBV	1204357	1897421	18.32%	2.711%
28	15.063	2060	2070	2071	rBV3	110682	293179	2.83%	0.419%
29	15.122	2076	2080	2085	rVV	116046	173398	1.67%	0.248%
30	15.251	2098	2102	2110	rBV4	46562	107171	1.03%	0.153%
31	15.663	2167	2172	2178	rBV2	112066	167639	1.62%	0.240%
32	15.787	2187	2193	2201	rBV	1720832	2649345	25.58%	3.785%
33	15.939	2213	2219	2225	rBV4	72530	149896	1.45%	0.214%
34	16.828	2367	2370	2378	rVB4	79906	131928	1.27%	0.188%

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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	17.045	2401	2407	2416	rBV	1527656	2108866	20.36%	3.013%
36	17.316	2449	2453	2456	rBV2	129257	179515	1.73%	0.256%
37	17.357	2456	2460	2468	rVB	596428	928603	8.97%	1.327%
38	17.969	2559	2564	2570	rBV2	532954	809688	7.82%	1.157%
39	18.792	2700	2704	2712	rBV	235867	326520	3.15%	0.466%
40	19.204	2771	2774	2779	rBV2	144559	183253	1.77%	0.262%
41	19.622	2840	2845	2851	rBV	6222921	8052217	77.75%	11.504%
42	20.869	3053	3057	3063	rBV	690557	861222	8.32%	1.230%
43	20.922	3063	3066	3073	rVB	280488	322222	3.11%	0.460%
44	21.139	3099	3103	3108	rBV	1914853	2460752	23.76%	3.516%
45	21.304	3128	3131	3140	rVB	182592	238183	2.30%	0.340%
46	22.198	3280	3283	3289	rVB	242672	317563	3.07%	0.454%
47	22.327	3300	3305	3316	rVB	514078	818215	7.90%	1.169%
48	22.710	3366	3370	3375	rBV	414703	597482	5.77%	0.854%
49	23.098	3432	3436	3441	rBV2	336926	546000	5.27%	0.780%
50	23.286	3463	3468	3475	rVV	372575	634934	6.13%	0.907%
51	23.380	3478	3484	3496	rVB	1472161	2713790	26.20%	3.877%
52	23.939	3576	3579	3587	rVB	290524	529358	5.11%	0.756%
53	24.410	3651	3659	3681	rVB2	2990664	7925014	76.52%	11.322%
54	24.692	3698	3707	3722	rBV5	3298796	10357179	100.00%	14.797%
55	26.115	3943	3949	3967	rVB2	535154	1732965	16.73%	2.476%
56	26.480	4003	4011	4031	rVB4	735006	2543090	24.55%	3.633%

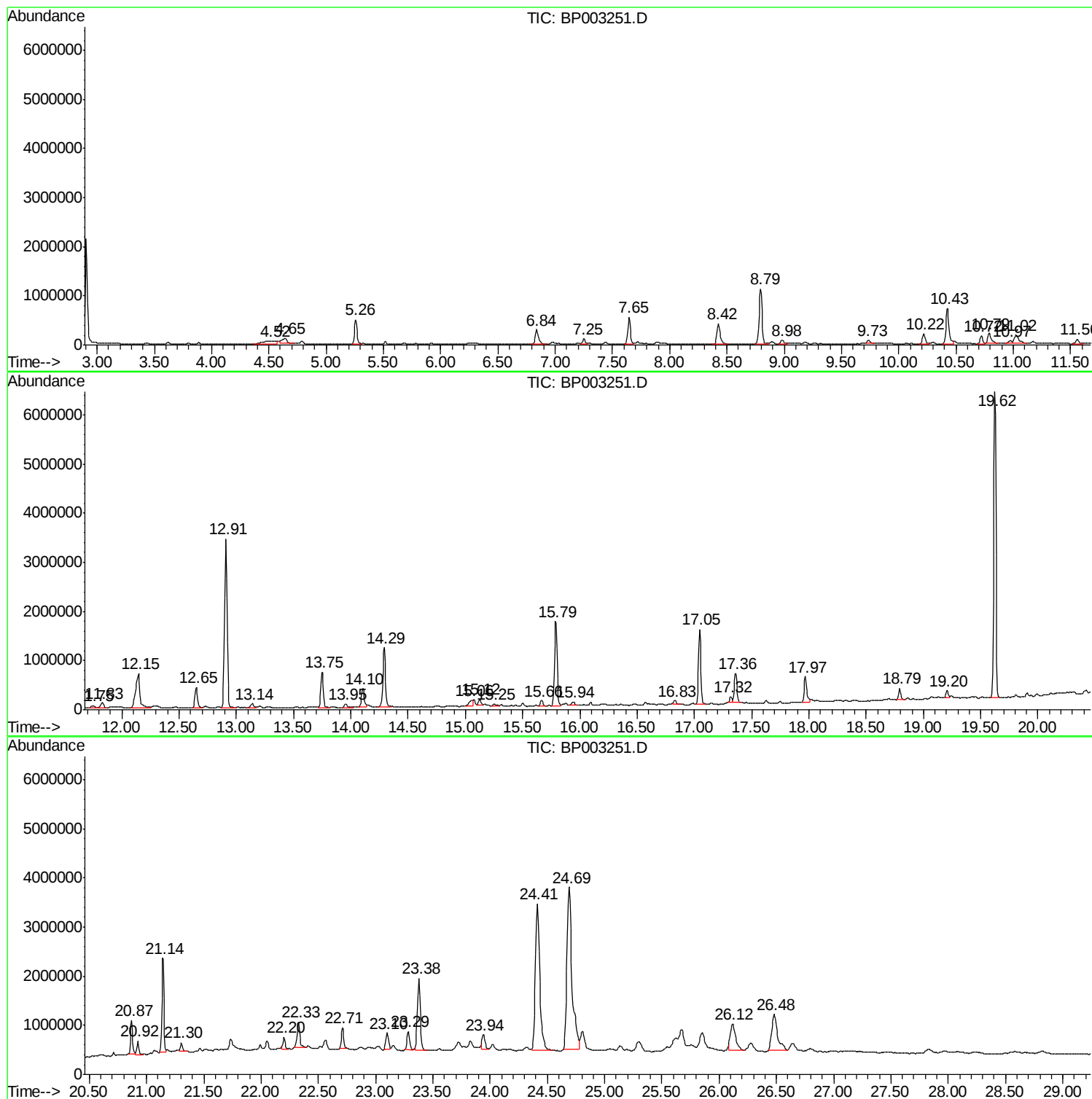
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP082420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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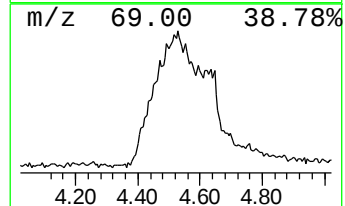
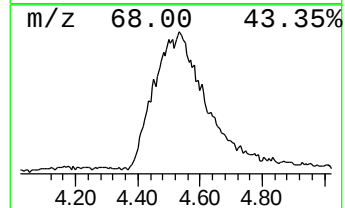
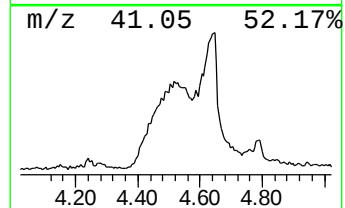
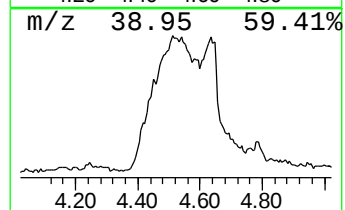
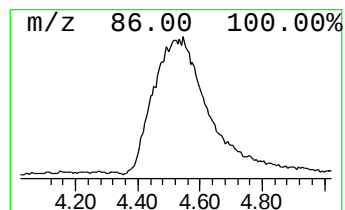
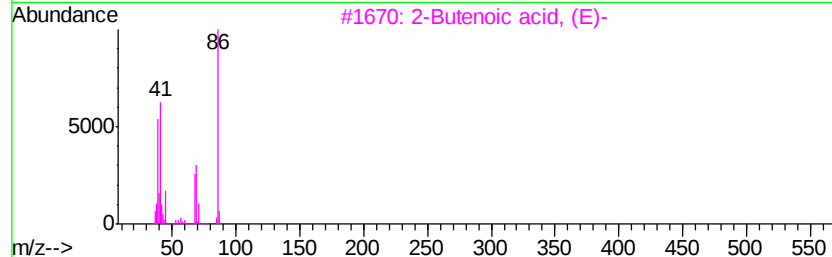
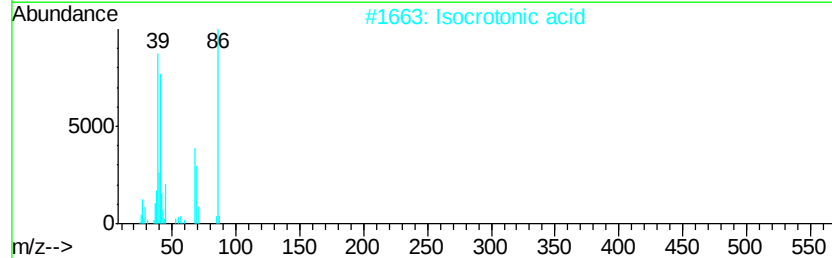
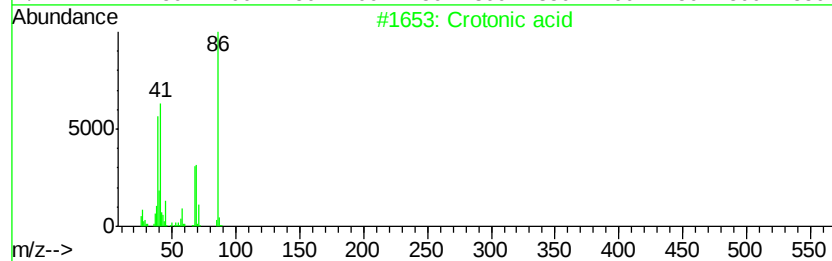
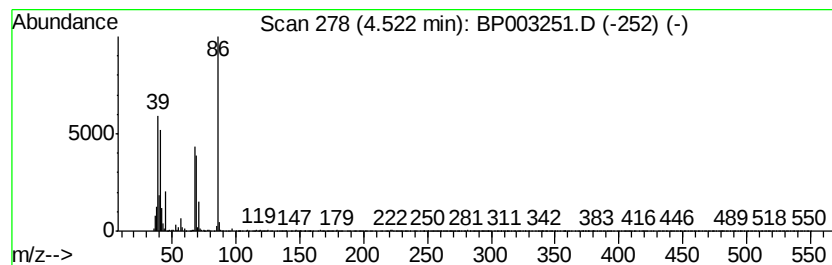
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Crotonic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	11.15 ng	484778	1,4-Dichlorobenzene-d4	7.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Crotonic acid	86	C4H6O2	003724-65-0	91
2		Isocrotonic acid	86	C4H6O2	000503-64-0	91
3		2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	91
4		2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	64
5		cis-4-Hydroxy-L-proline	131	C5H9NO3	000618-27-9	40



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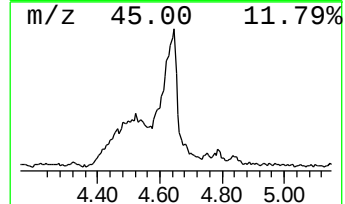
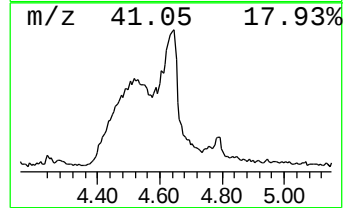
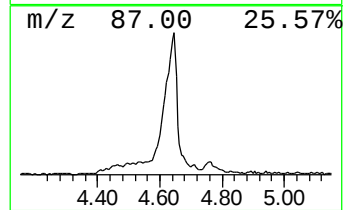
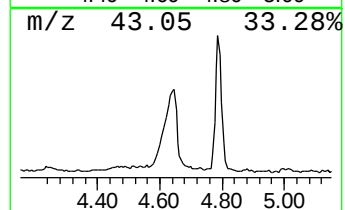
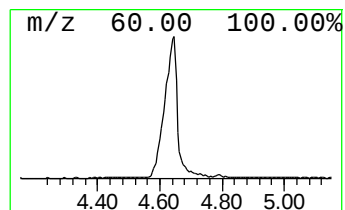
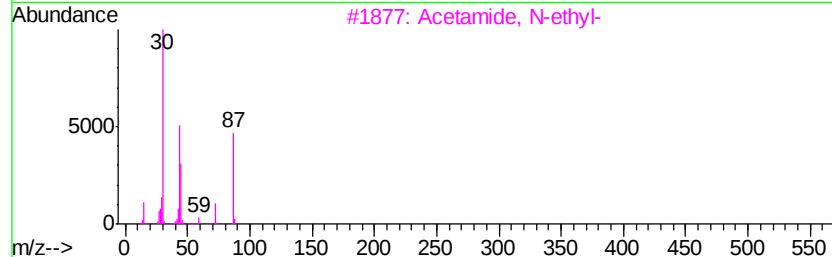
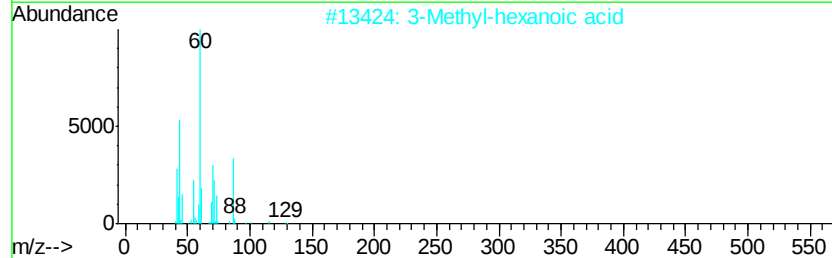
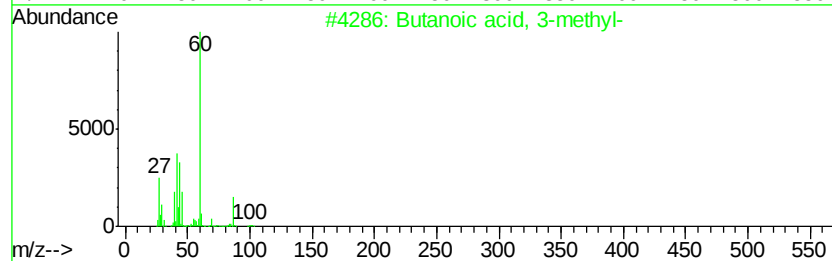
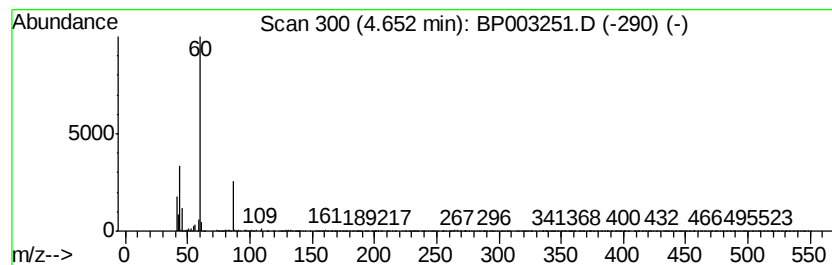
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanoic acid, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	7.82 ng	340156	1,4-Dichlorobenzene-d4	7.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	56
2			3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4			Formic acid hydrazide	60	CH4N2O	000624-84-0	9
5			2-Thiazoline-2-carboxylic acid, ...	159	C6H9NO2S	082677-98-3	9



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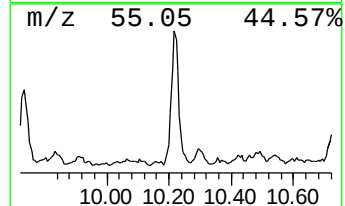
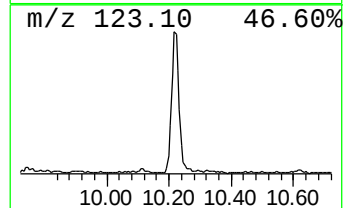
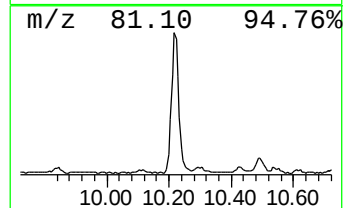
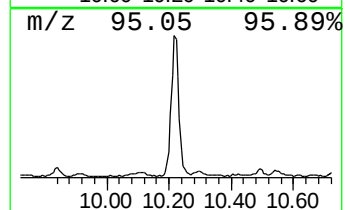
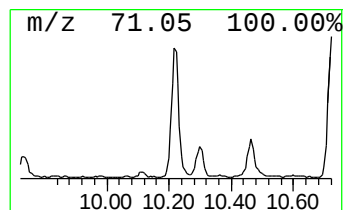
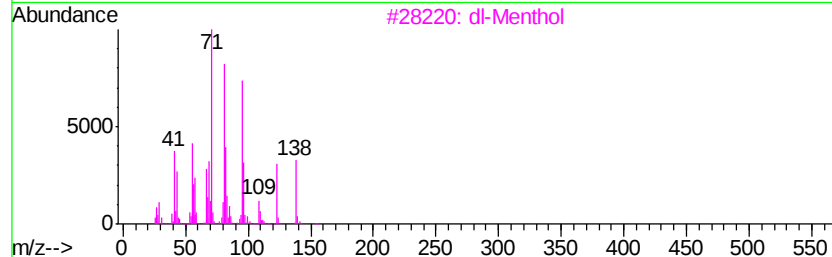
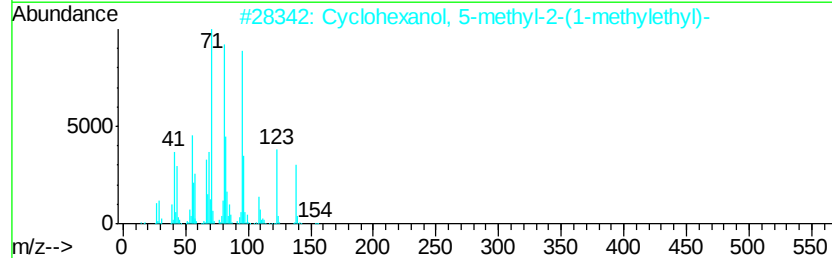
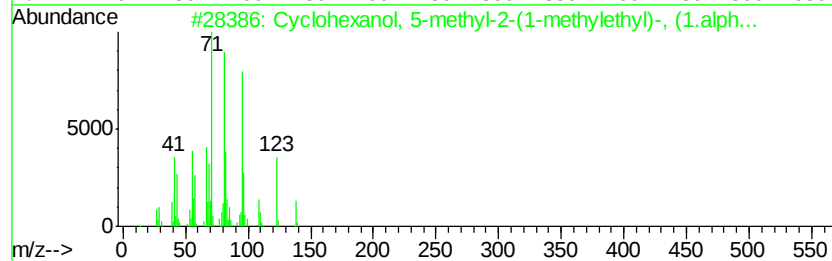
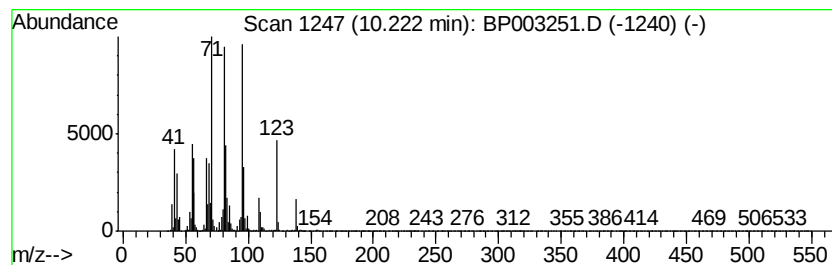
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.22	5.41 ng	360035	Naphthalene-d8	10.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	91
2		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	91
3		dl-Menthol	156	C10H20O	000089-78-1	91
4		Levomenthol	156	C10H20O	002216-51-5	91
5		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	023283-97-8	90



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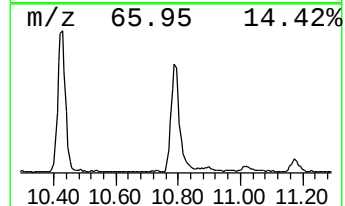
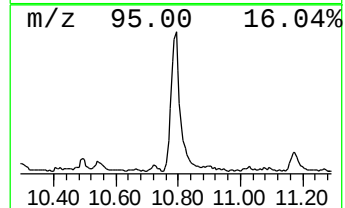
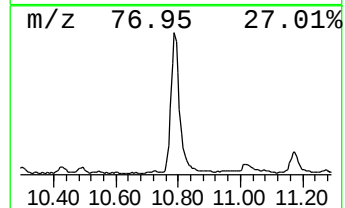
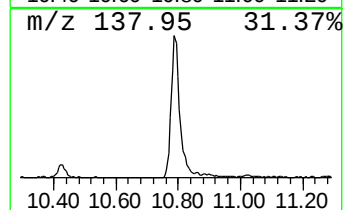
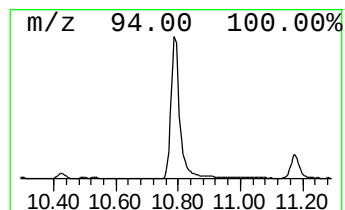
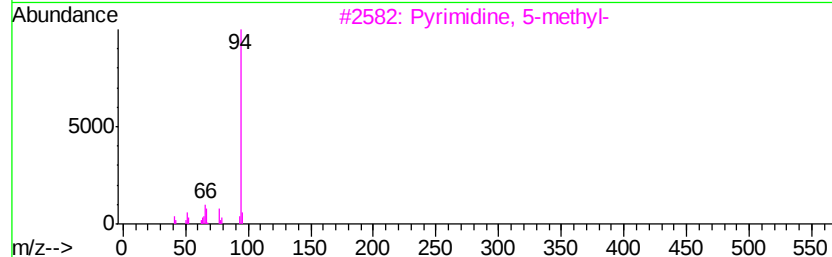
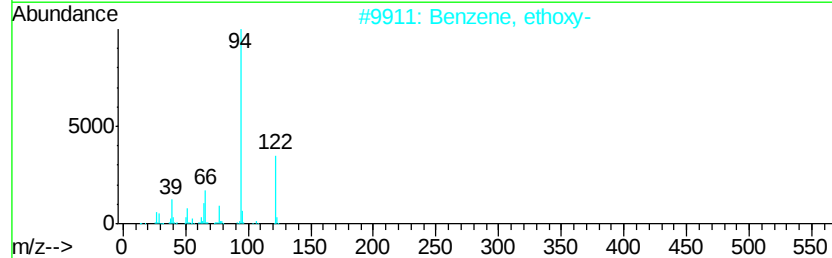
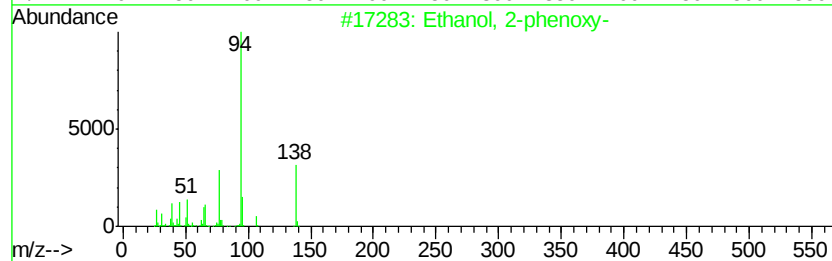
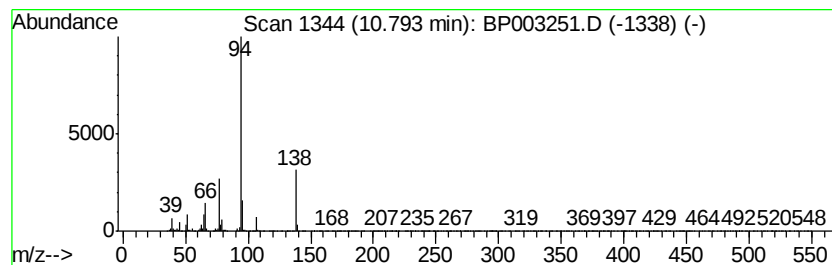
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Ethanol, 2-phenoxy- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	6.66 ng	443626	Naphthalene-d8	10.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	94
2		Benzene, ethoxy-	122	C8H10O	000103-73-1	53
3		Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	53
4		Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	50
5		Acetic acid, phenyl ester	136	C8H8O2	000122-79-2	50



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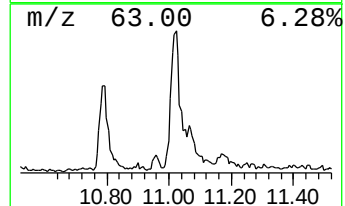
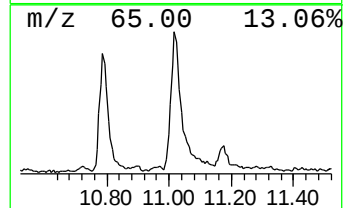
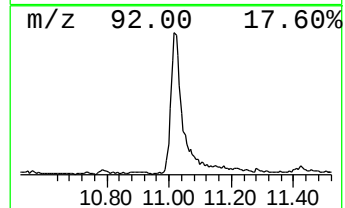
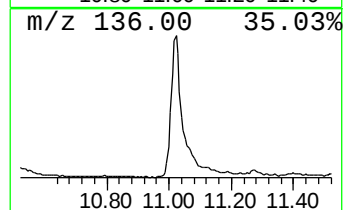
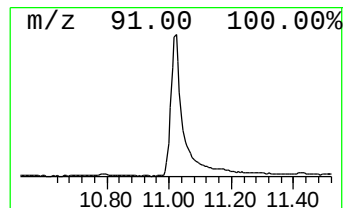
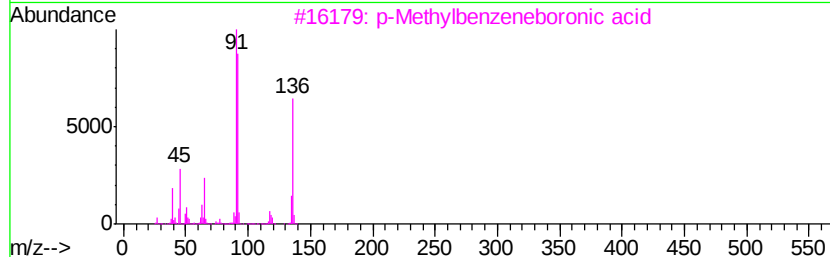
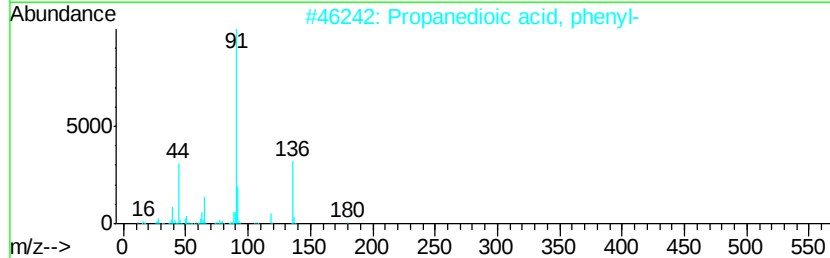
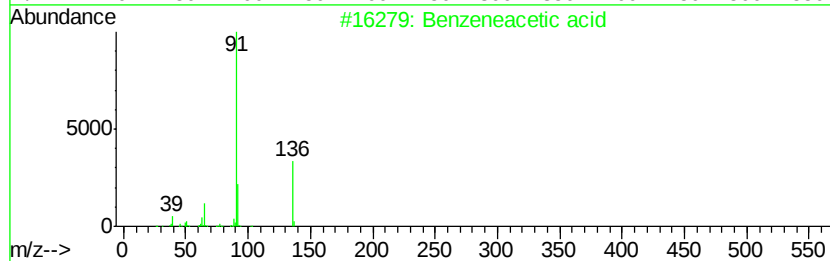
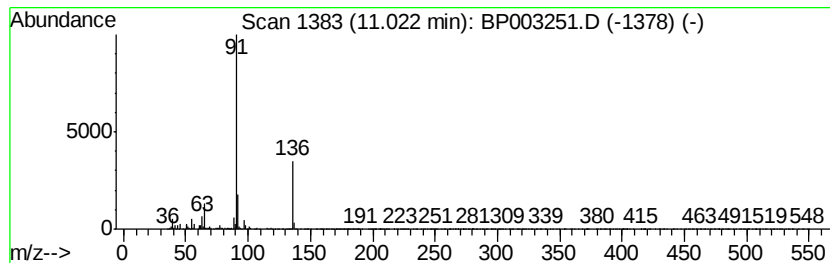
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzeneacetic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	6.83 ng	454501	Naphthalene-d8	10.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzeneacetic acid	136	C8H8O2	000103-82-2	93
2		Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	72
3		p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	59
4		Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	50
5		5-(Benzylsulfonyl)dihydro-1,3,5-...	243	C10H13NO4S	081763-18-0	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
Operator : CG/JU
Sample : L3942-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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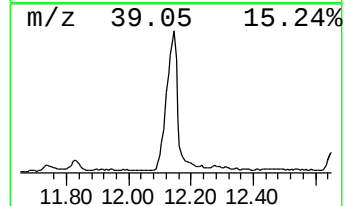
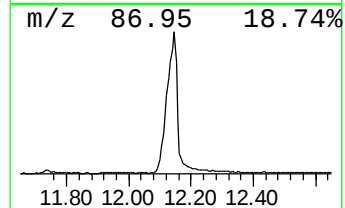
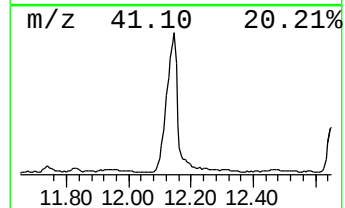
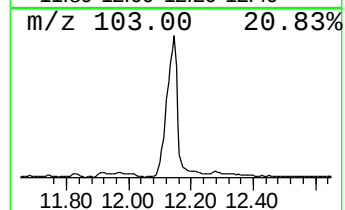
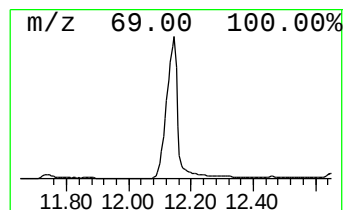
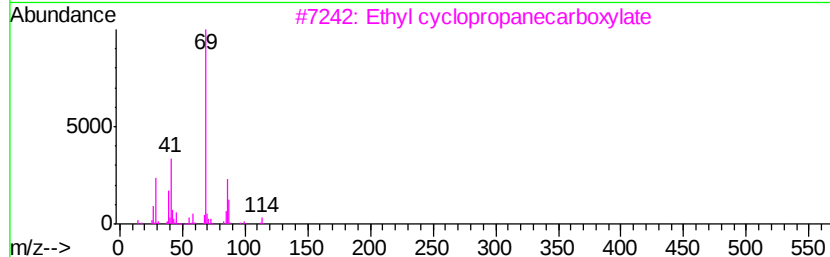
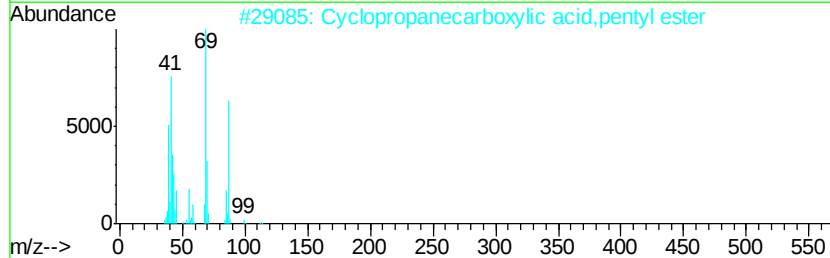
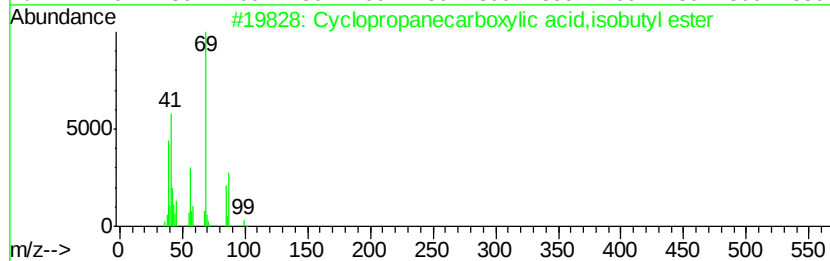
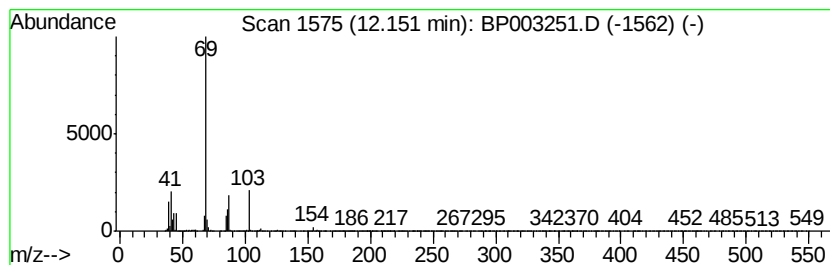
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.15 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	26.60 ng	1771030	Napthalene-d8	10.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropanecarboxylic acid, isob...	142	C8H14O2	064969-79-5	45
2		Cyclopropanecarboxylic acid, pent...	156	C9H16O2	060128-02-1	45
3		Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
4		2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	11
5		Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
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Sample : L3942-01
Misc :
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Instrument :
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ClientSampleId :
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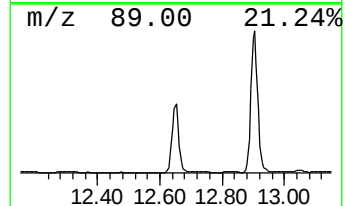
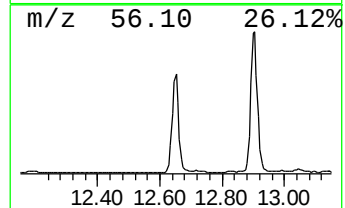
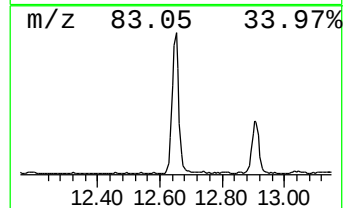
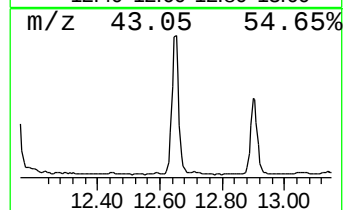
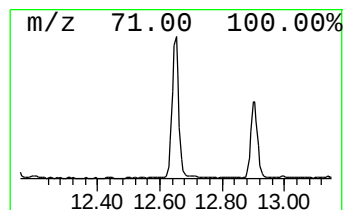
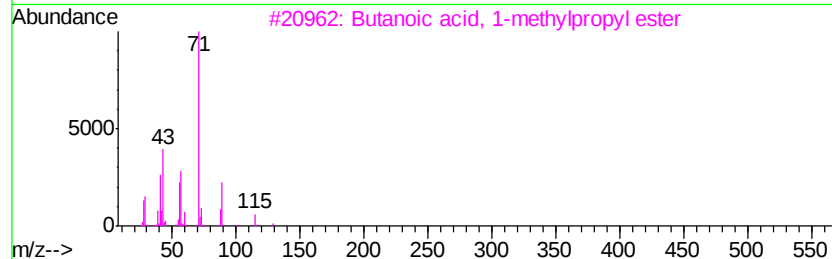
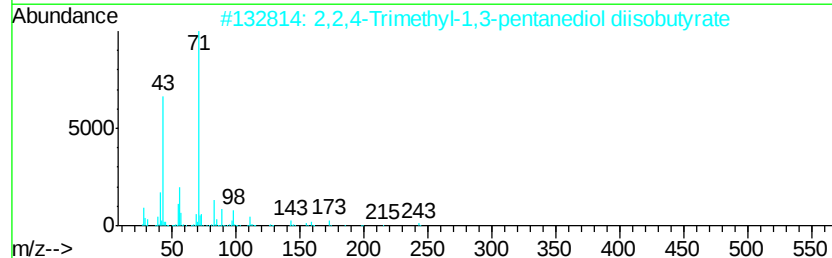
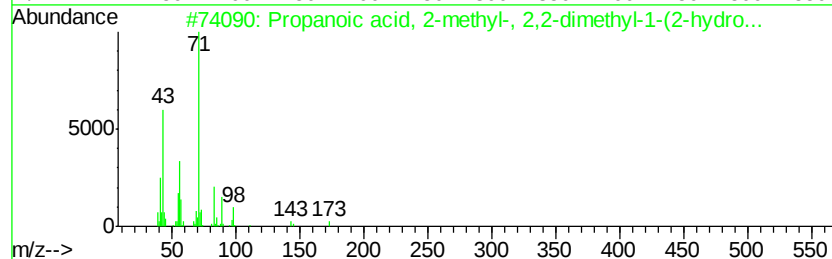
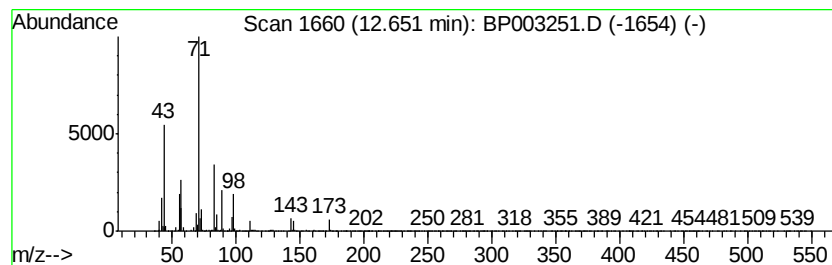
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Propanoic acid, 2-methyl-, ... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	6.76 ng	641490	Acenaphthene-d10	14.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	59
2		2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	53
3		Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	50
4		Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	40
5		Butyric acid, 3-tridecyl ester	270	C17H34O2	1000280-56-8	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
Operator : CG/JU
Sample : L3942-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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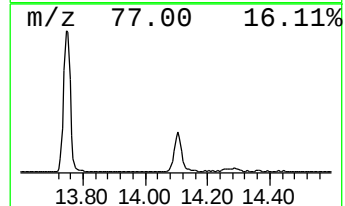
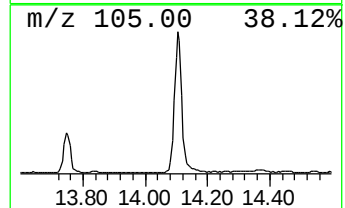
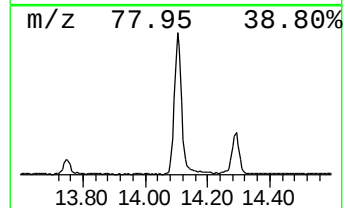
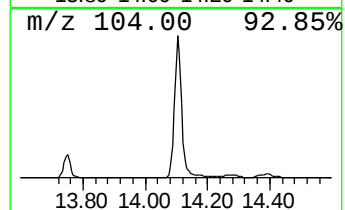
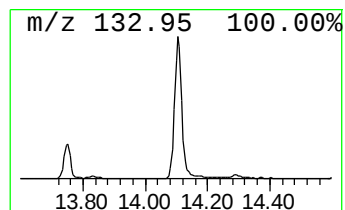
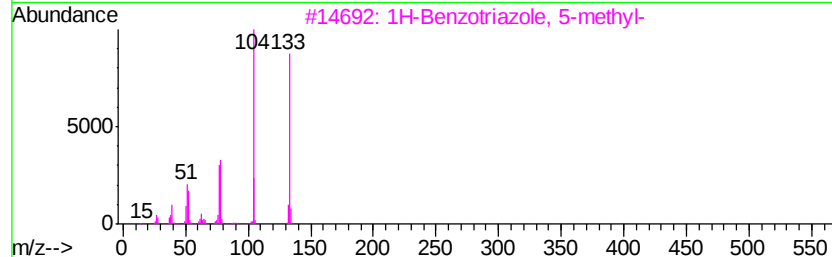
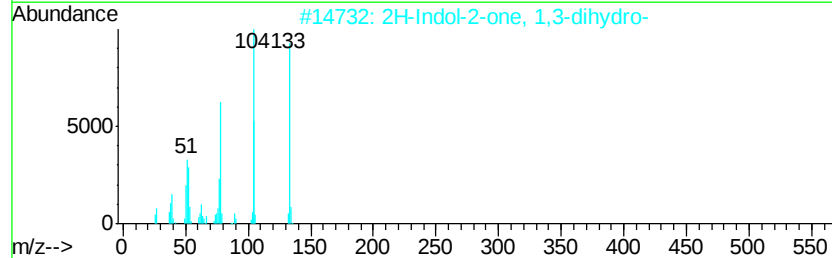
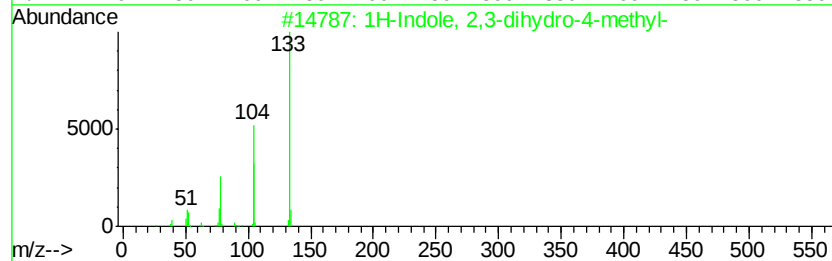
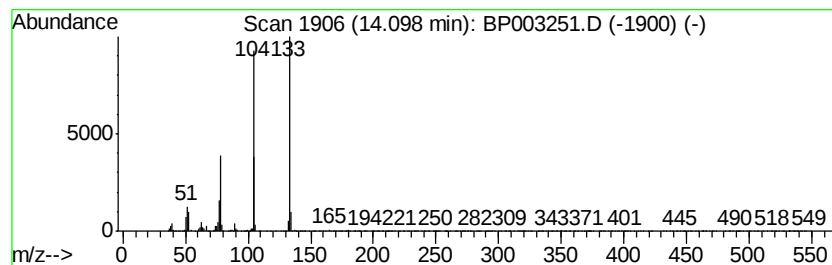
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1H-Indole, 2,3-dihydro-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	6.49 ng	615746	Acenaphthene-d10	14.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indole, 2,3-dihydro-4-methyl-	133	C9H11N	062108-16-1	95
2		2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	94
3		1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	91
4		1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	90
5		Benzene, 1-isocyanato-2-methyl-	133	C8H7NO	000614-68-6	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
Operator : CG/JU
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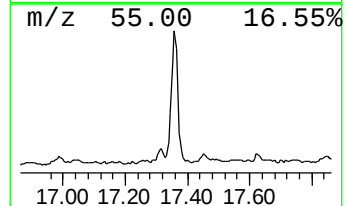
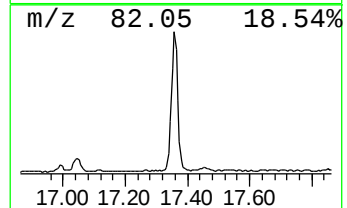
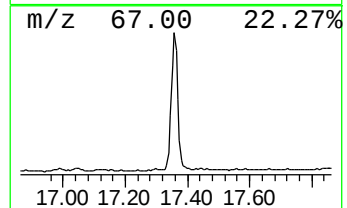
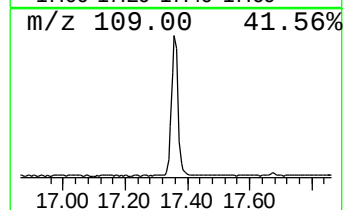
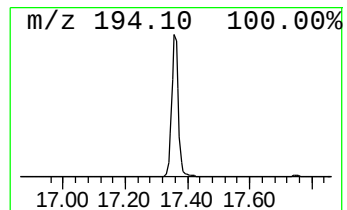
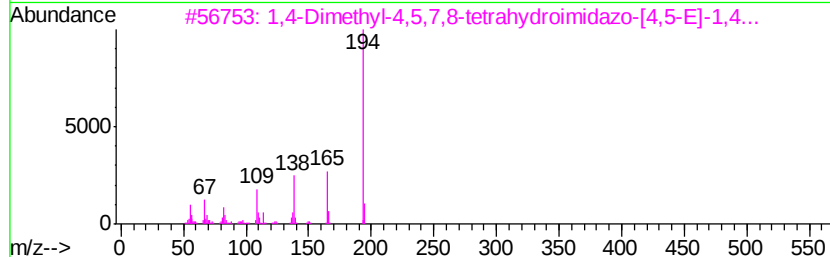
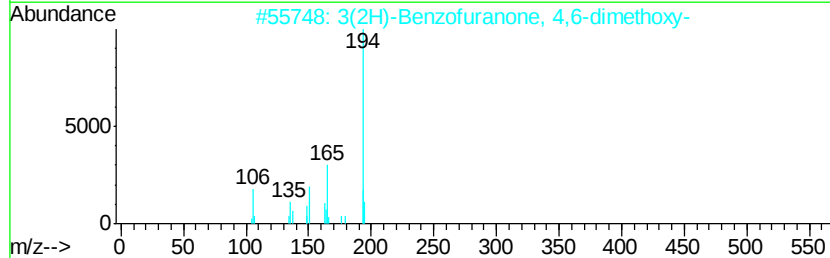
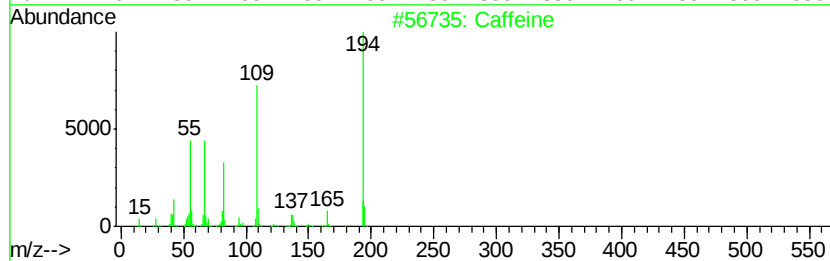
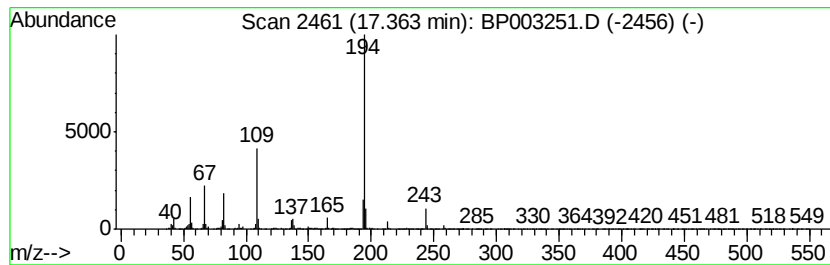
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP082420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Caffeine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.36	8.81 ng	928603	Phenanthrene-d10		17.05	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Caffeine	194	C8H10N4O2	000058-08-2	97
2		3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	50
3		1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	43
4		5-[5-Ethyl-2-furyl]hydantoin	194	C9H10N2O3	1000214-65-8	35
5		2H-Pyrazol-3-ol, 5-(2,5-dimethyl...	194	C9H10N2O5	1000304-22-5	32



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
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Sample : L3942-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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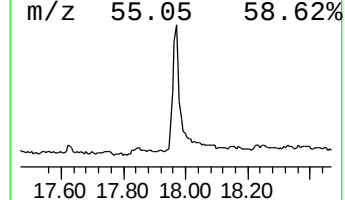
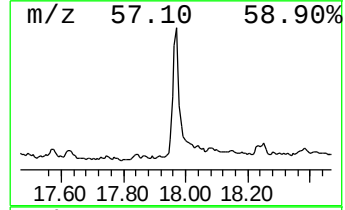
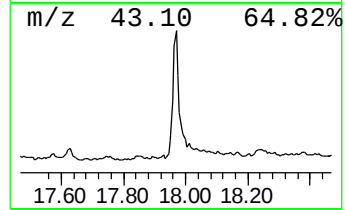
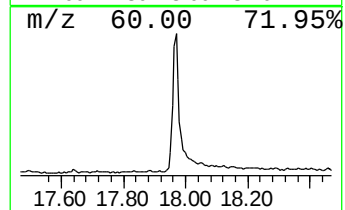
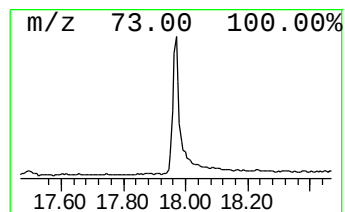
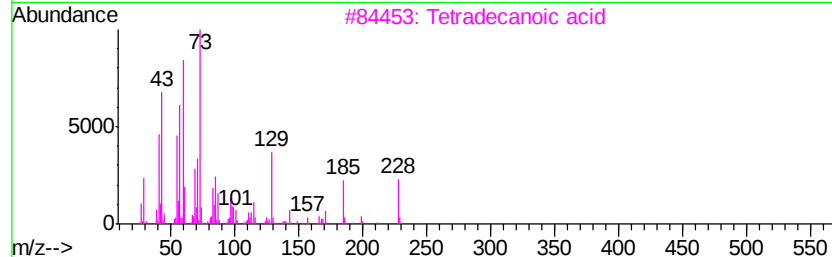
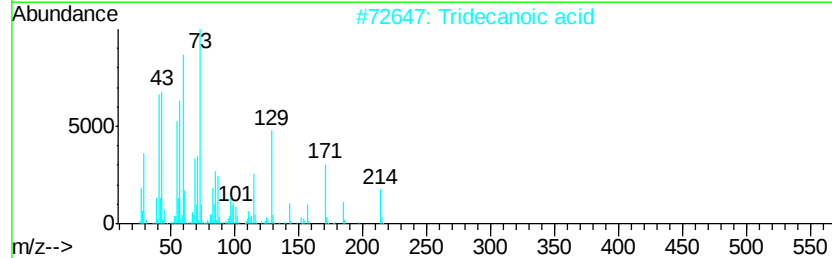
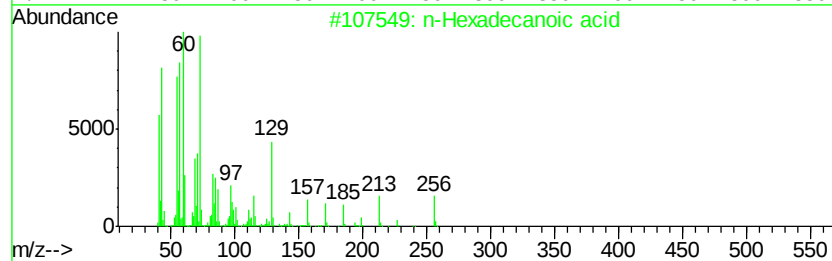
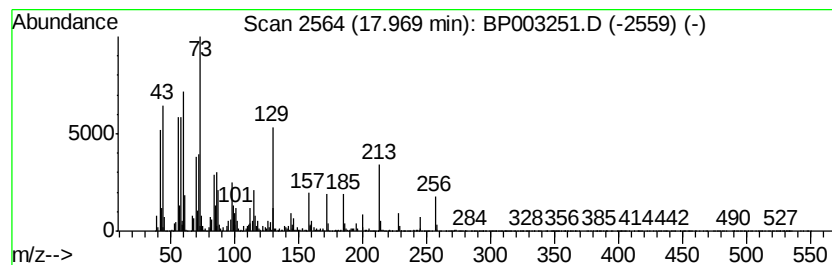
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	7.68 ng	809688	Phenanthrene-d10	17.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4		n-Decanoic acid	172	C10H20O2	000334-48-5	78
5		Undecanoic acid	186	C11H22O2	000112-37-8	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
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ALS Vial : 5 Sample Multiplier: 1

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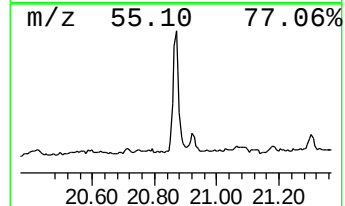
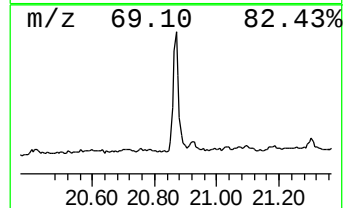
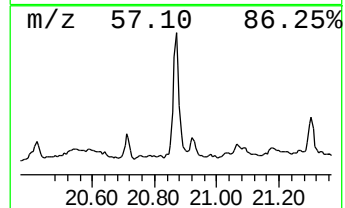
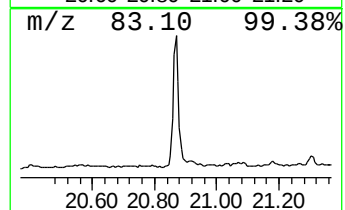
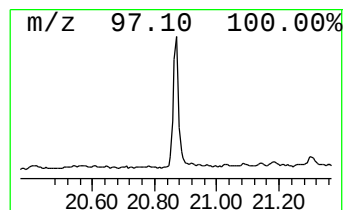
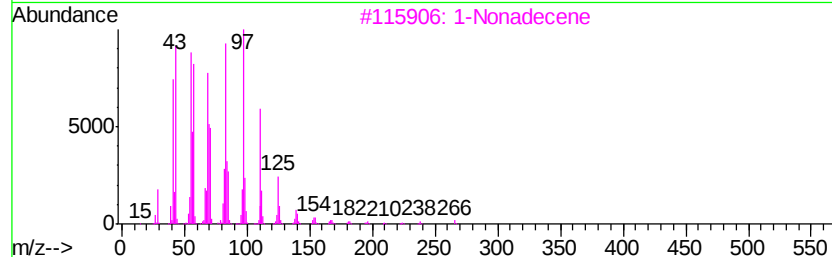
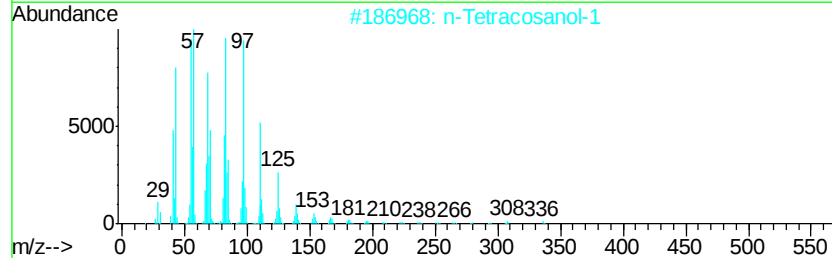
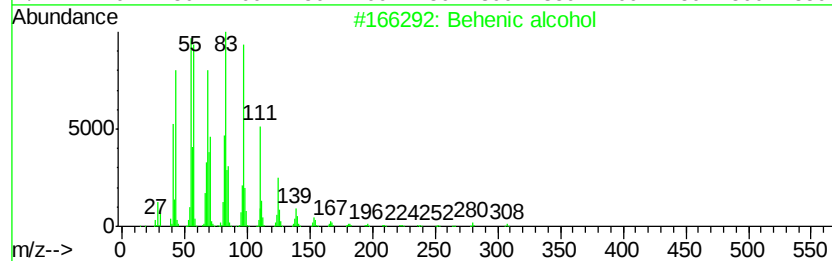
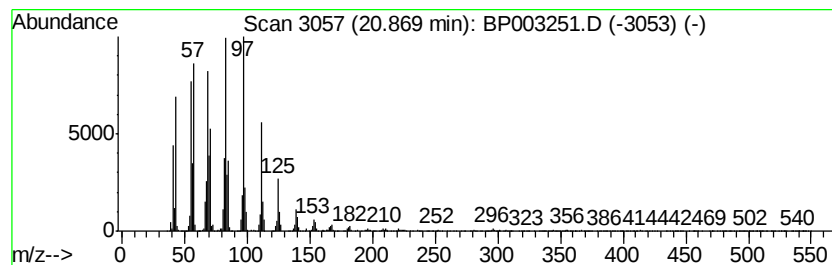
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Behenic alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	7.00 ng	861222	Chrysene-d12	21.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		1-Nonadecene	266	C19H38	018435-45-5	94
4		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



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 Sample : L3942-01
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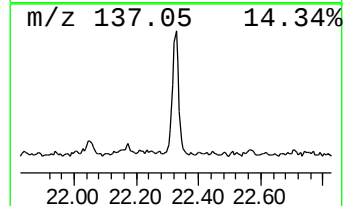
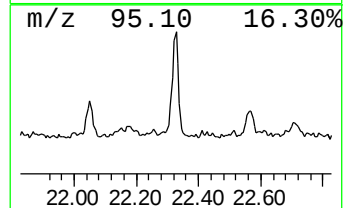
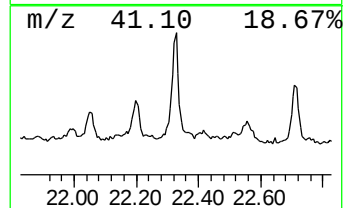
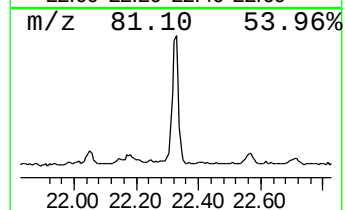
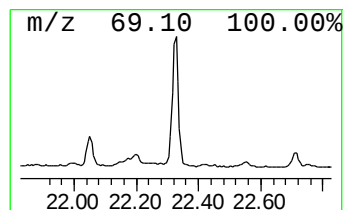
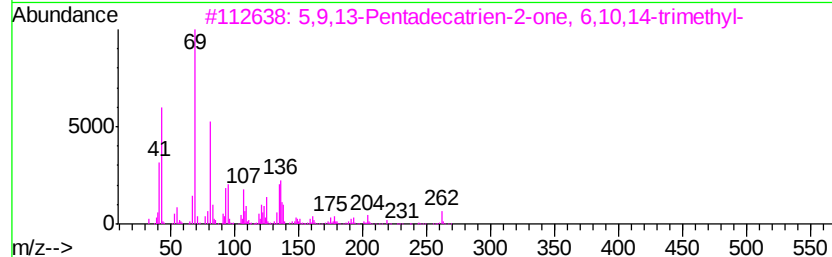
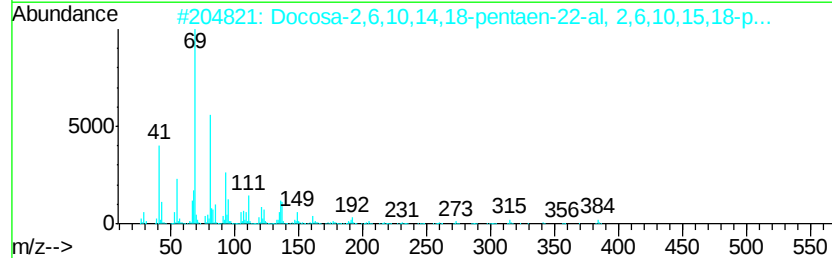
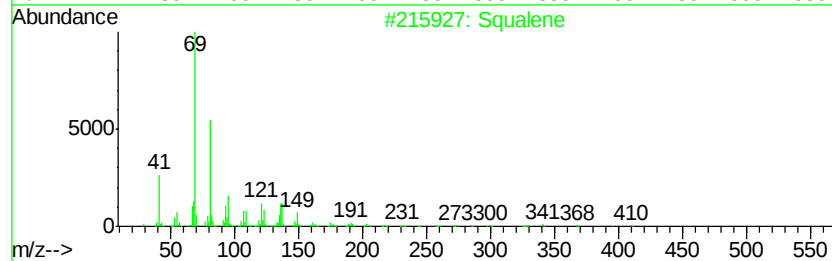
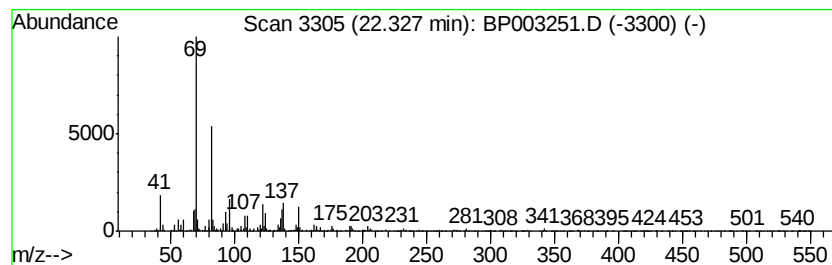
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 12 Squalene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	6.03 ng	818215	Perylene-d12	23.38
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	000111-02-4 91
2	Docosa-2,6,10,14,18-pentaen-22-a...		384 C27H44O	1000163-04-7 80
3	5,9,13-Pentadecatrien-2-one, 6,1...		262 C18H30O	000762-29-8 64
4	1,5,9-Decatriene, 2,3,5,8-tetram...		192 C14H24	230646-72-7 59
5	Cyclopropanecarboxylic acid, 4-i...		204 C13H16O2	1000331-01-9 50



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
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Sample : L3942-01
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Instrument :
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ClientSampleId :
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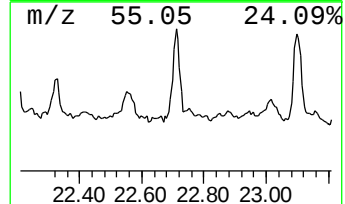
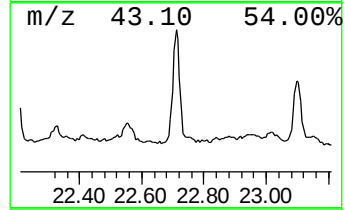
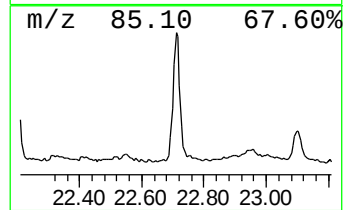
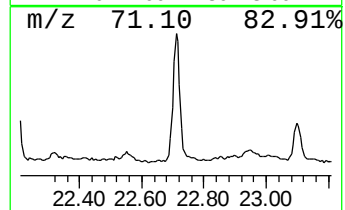
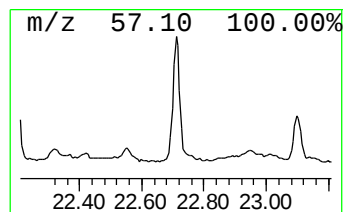
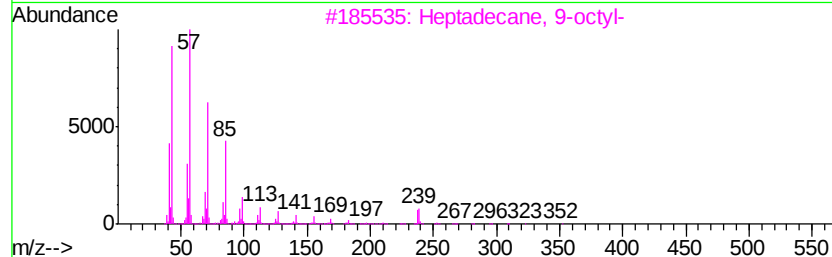
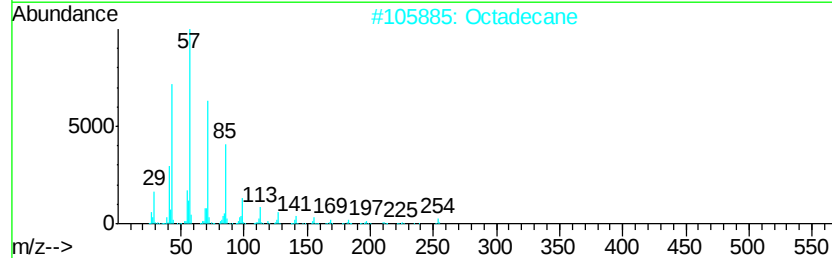
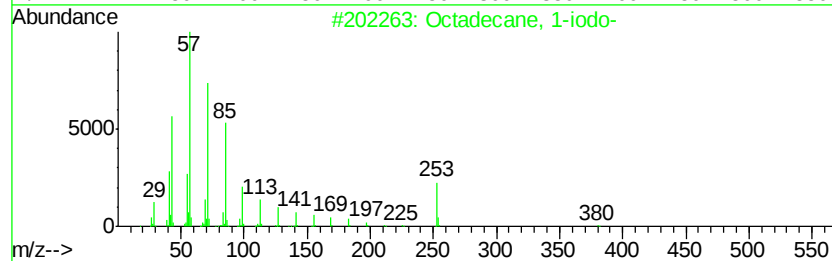
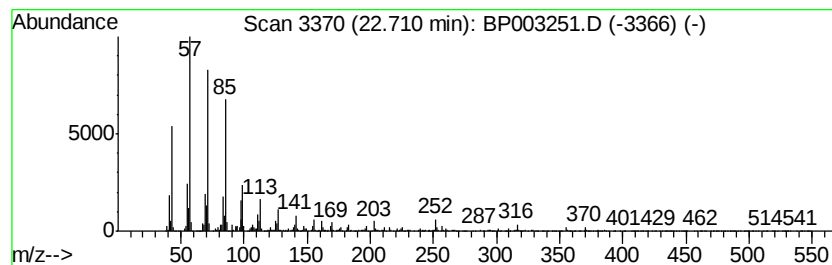
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octadecane, 1-iodo- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.71	4.40 ng	597482	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	98
2		Octadecane	254	C18H38	000593-45-3	97
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
4		Heneicosane	296	C21H44	000629-94-7	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
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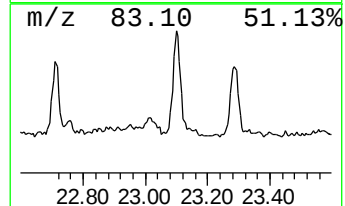
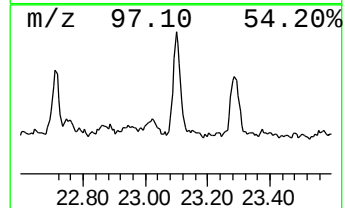
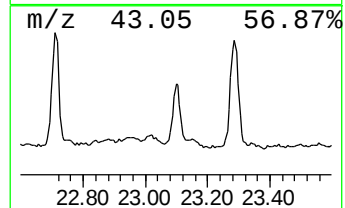
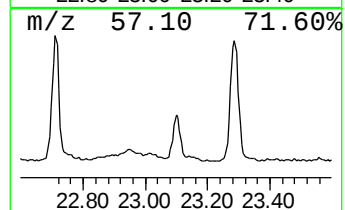
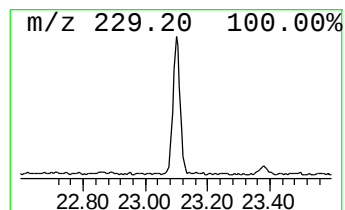
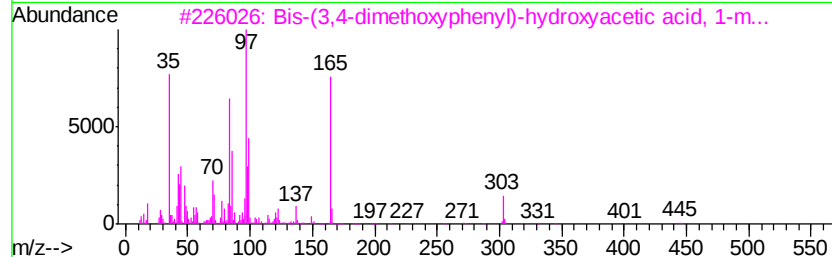
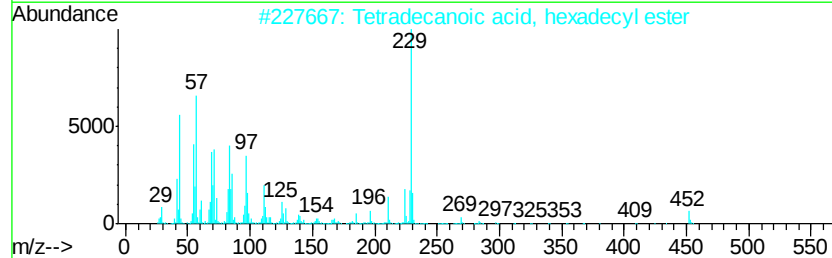
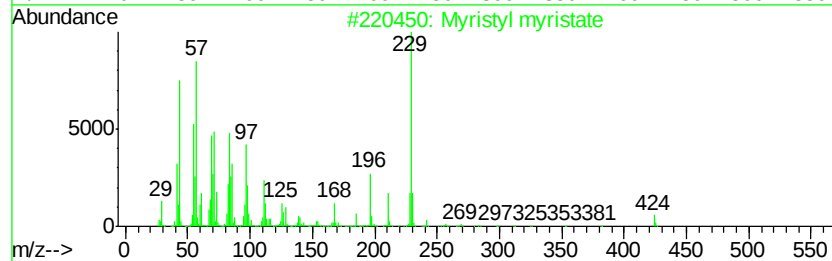
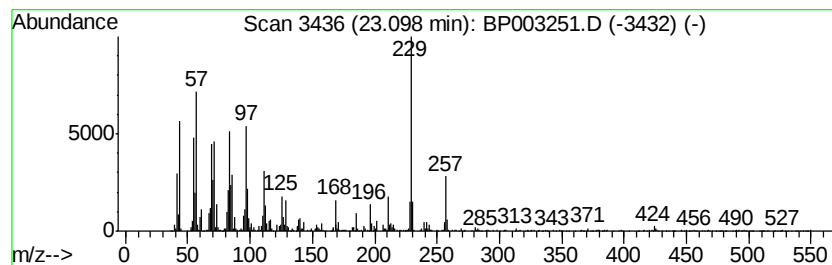
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Myristyl myristate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.10	4.02 ng	546000	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Myristyl myristate	424	C28H56O2	003234-85-3	90
2		Tetradecanoic acid, hexadecyl ester	452	C30H60O2	002599-01-1	68
3		Bis-(3,4-dimethoxyphenyl)-hydrox...	445	C24H31NO7	095805-62-2	35
4		Hexadecanoic acid, tetradecyl ester	452	C30H60O2	004536-26-9	27
5		Tetramethyl ethenetetracarboxylate	260	C10H12O8	1000341-25-0	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
Operator : CG/JU
Sample : L3942-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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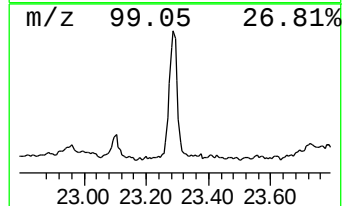
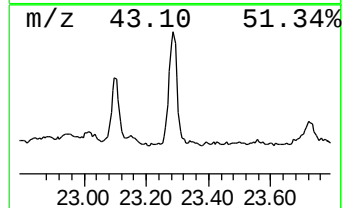
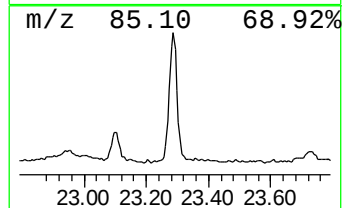
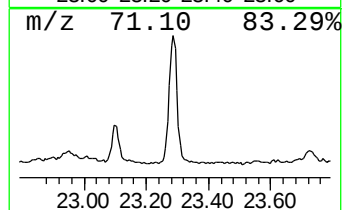
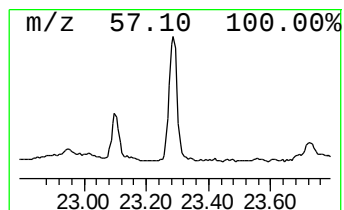
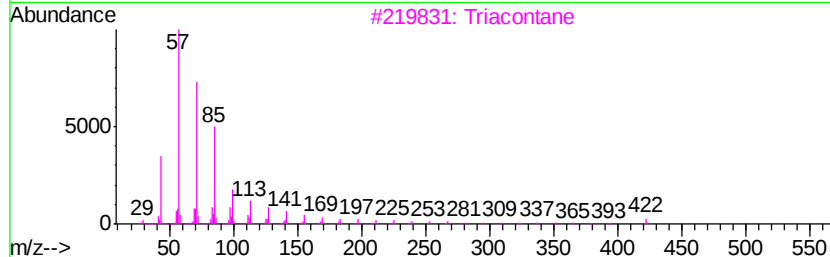
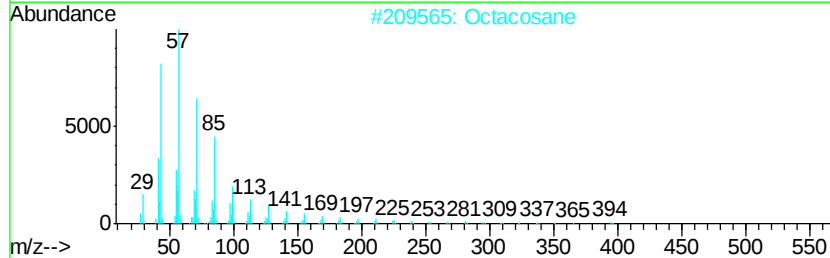
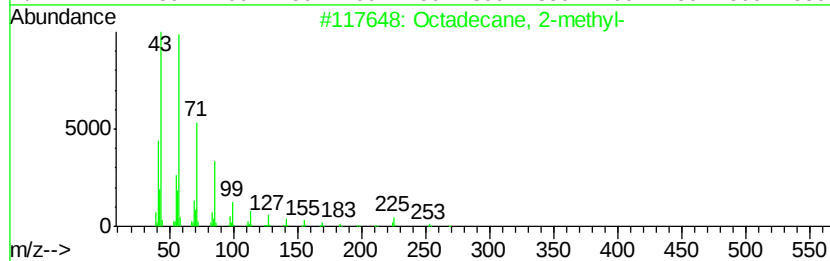
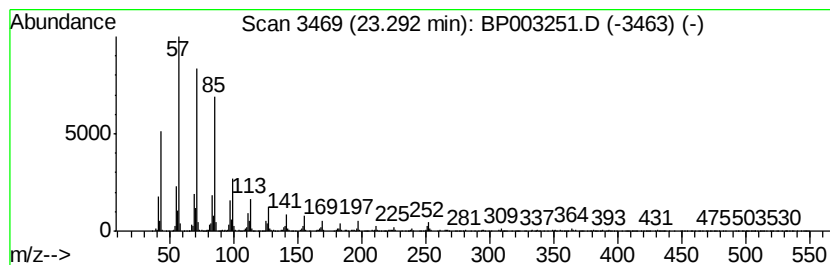
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Octadecane, 2-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	4.68 ng	634934	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Eicosane	282	C20H42	000112-95-8	91
5		Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
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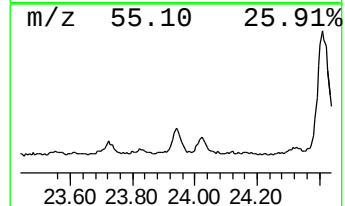
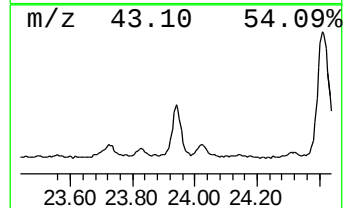
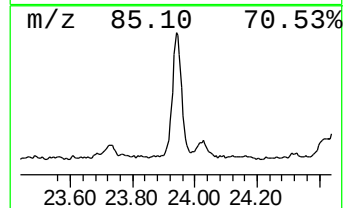
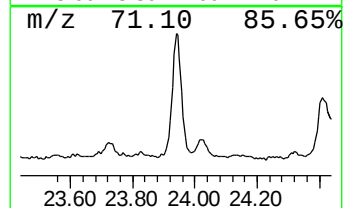
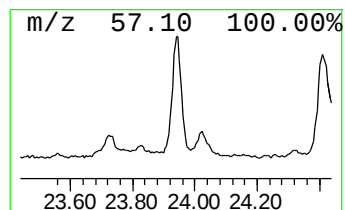
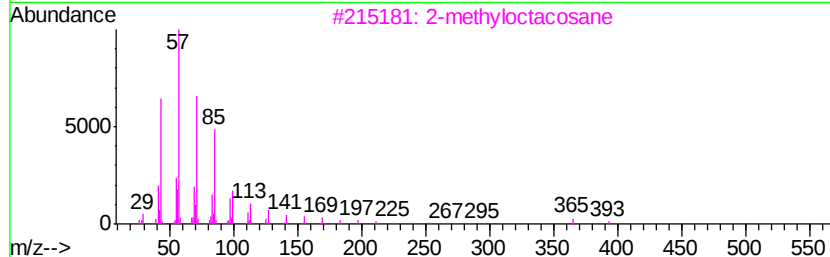
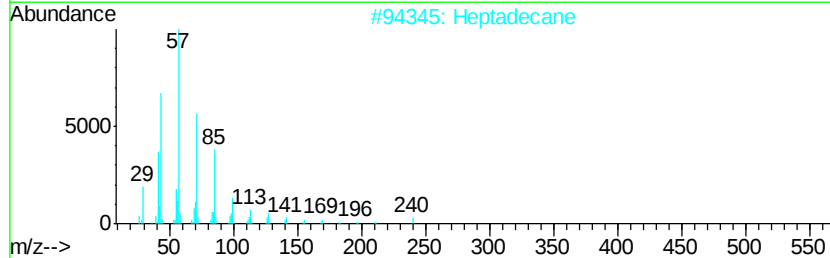
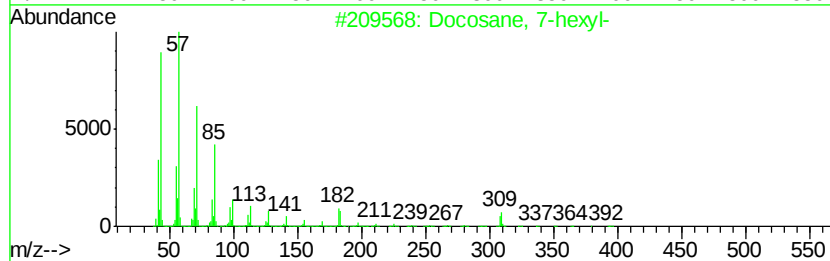
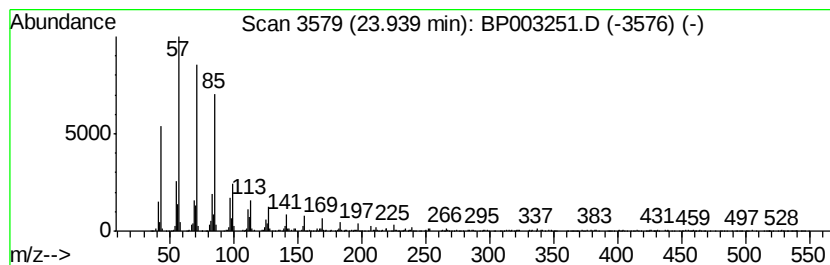
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Docosane, 7-hexyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.94	3.90 ng	529358	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	87
4		triacontane, 1-bromo-	500	C30H61Br	004209-22-7	87
5		Hentriacontane	437	C31H64	000630-04-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
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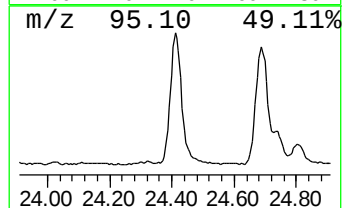
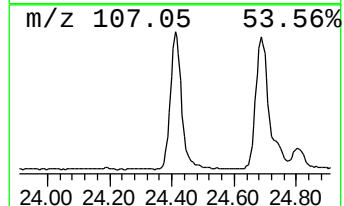
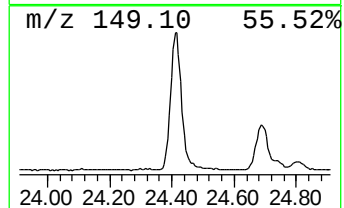
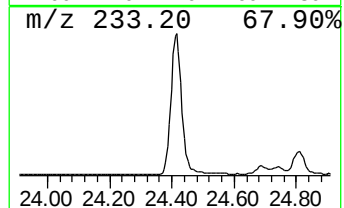
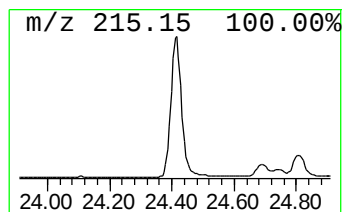
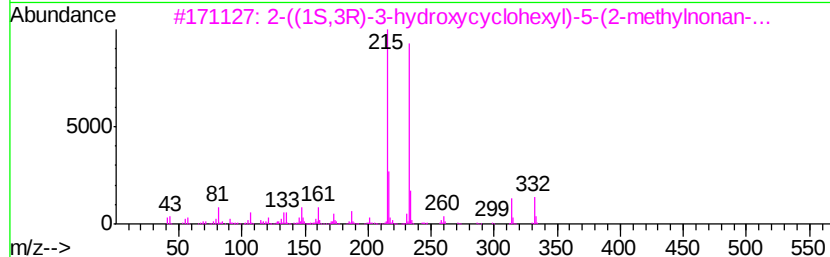
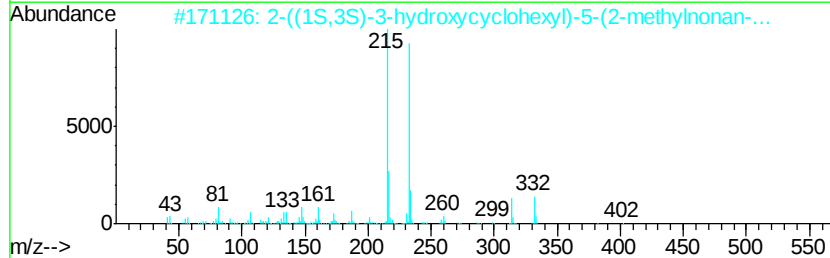
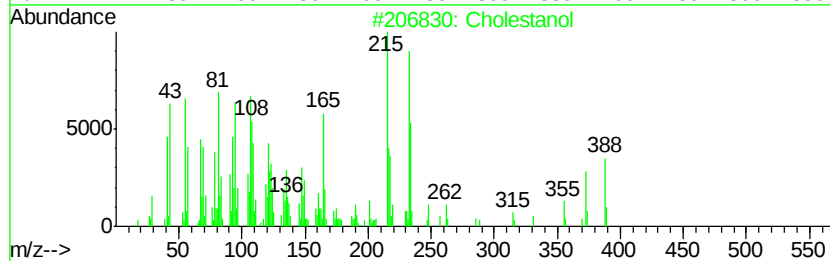
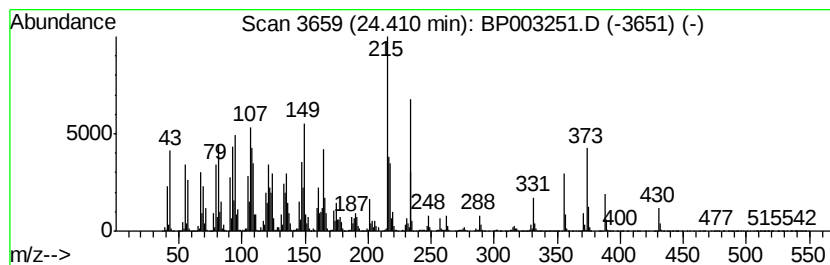
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Cholesterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
24.41	58.41 ng	7925010	Perylene-d12	23.38		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cholesterol	388	C27H48O	000080-97-7	96
2		2-((1S,3S)-3-hydroxycyclohexyl)-...	332	C22H36O2	1000372-26-3	46
3		2-((1S,3R)-3-hydroxycyclohexyl)-...	332	C22H36O2	1000372-26-4	46
4		5-(2-Methyloctan-2-yl)-3-(1R,3R)-...	332	C22H36O2	070434-92-3	38
5		trans-3-[2-Hydroxy-4-(2-methyl-2...	332	C22H36O2	1000370-41-7	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
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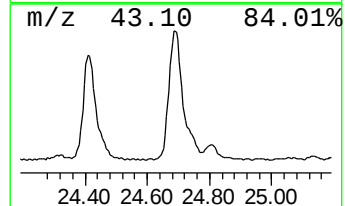
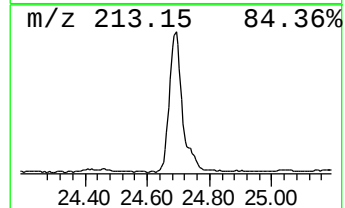
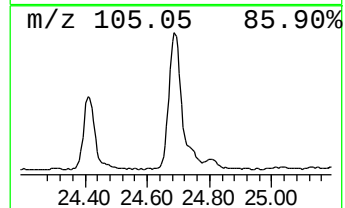
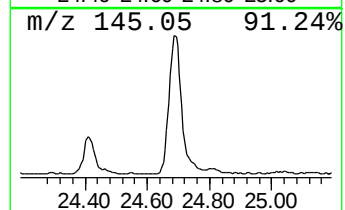
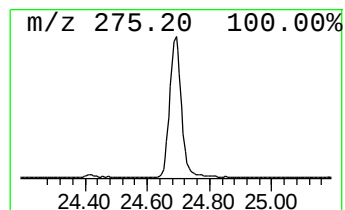
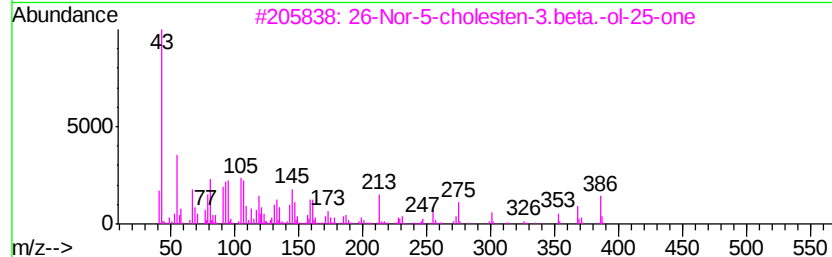
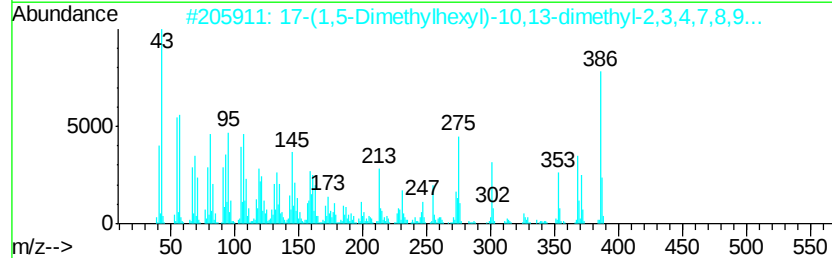
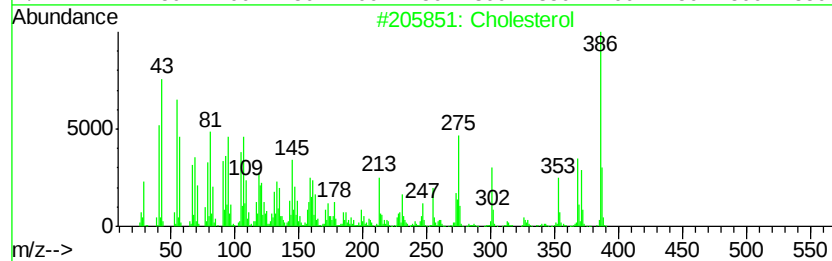
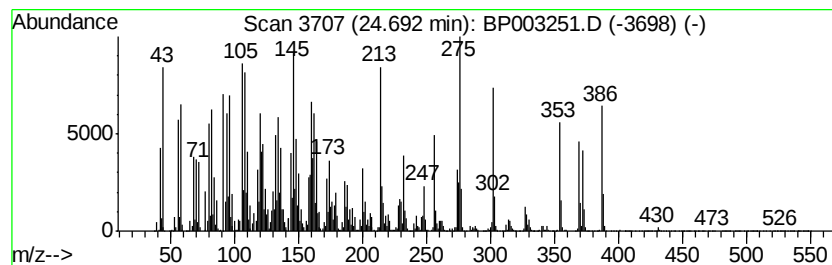
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Cholesterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.69	76.33 ng	10357200	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholesterol	386	C27H46O	000057-88-5	99
2		17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	99
3		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
4		Cholest-5-en-3-ol, (3.alpha.)-	386	C27H46O	000474-77-1	64
5		Cholest-8-en-3-ol, (3.beta.)-	386	C27H46O	007199-91-9	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
Data File : BP003251.D
Acq On : 10 Sep 2020 16:54
Operator : CG/JU
Sample : L3942-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
N35868

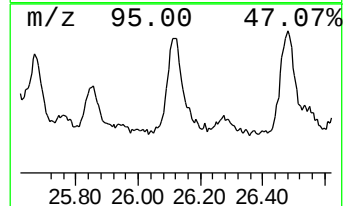
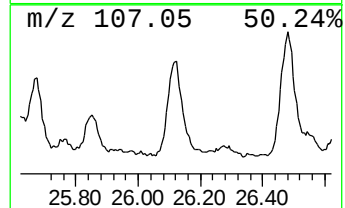
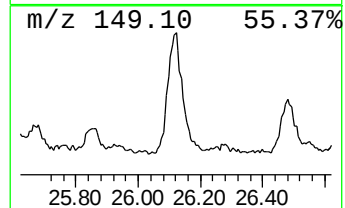
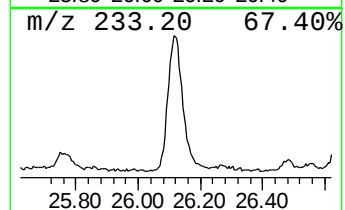
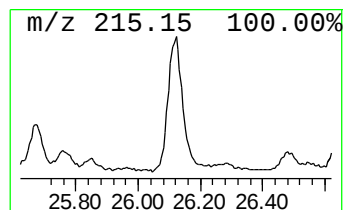
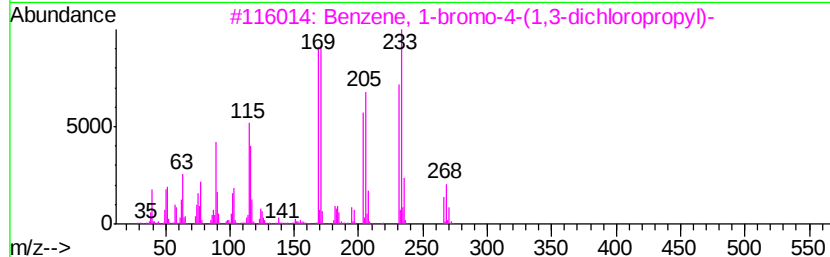
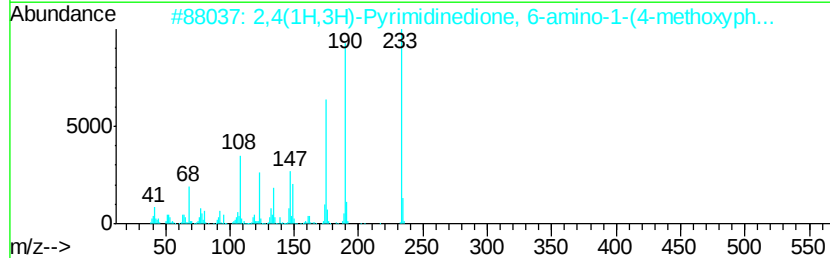
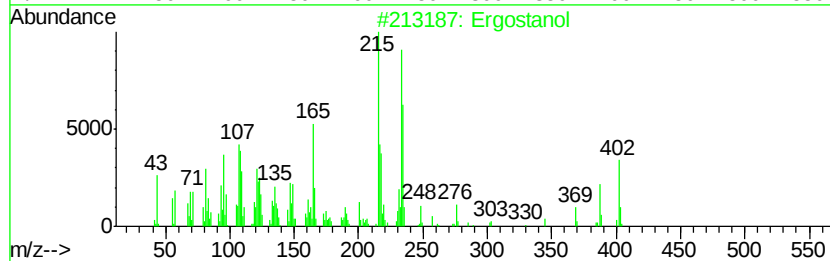
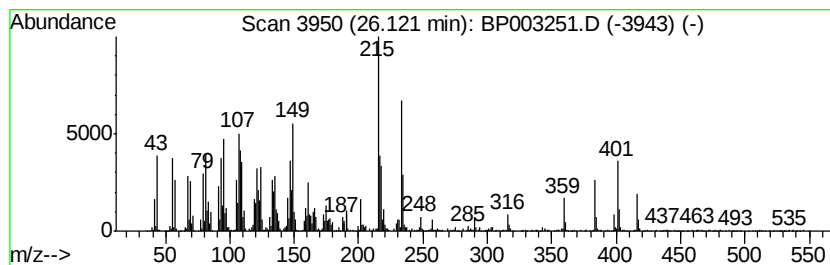
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown26.12 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.12	12.77 ng	1732970	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ergostanol	402	C28H50O	006538-02-9	27
2		2,4(1H,3H)-Pyrimidinedione, 6-am...	233	C11H11N3O3	1000337-88-3	25
3		Benzene, 1-bromo-4-(1,3-dichloro...	266	C9H9BrCl2	1000327-43-1	25
4		Pyridin-3-ol, 2-(4-nitrophenyl)-	216	C11H8N2O3	030820-89-4	18
5		Isophthalic acid, allyl hexyl ester	290	C17H22O4	1000345-64-7	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP091020\
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Acq On : 10 Sep 2020 16:54
Operator : CG/JU
Sample : L3942-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
N35868

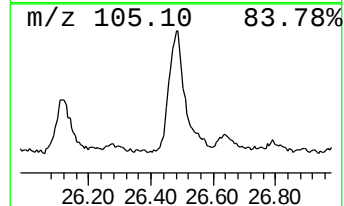
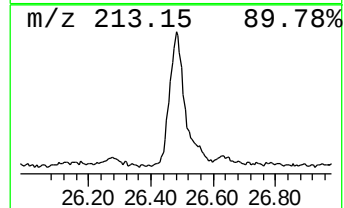
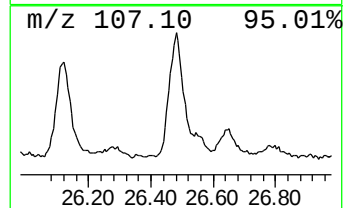
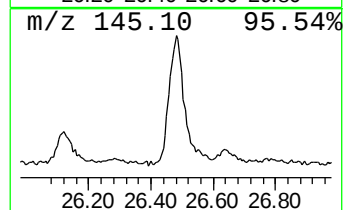
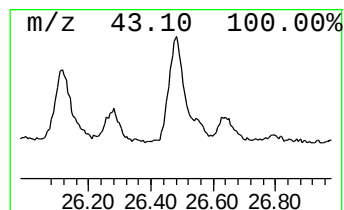
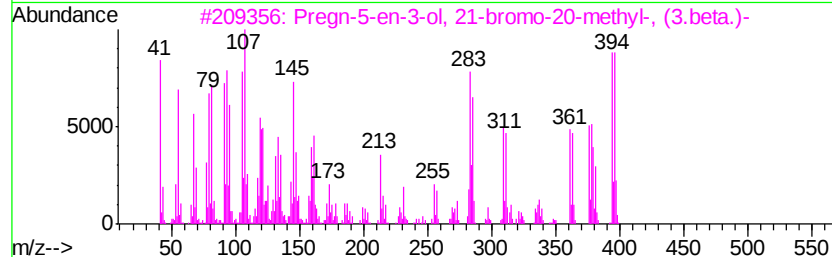
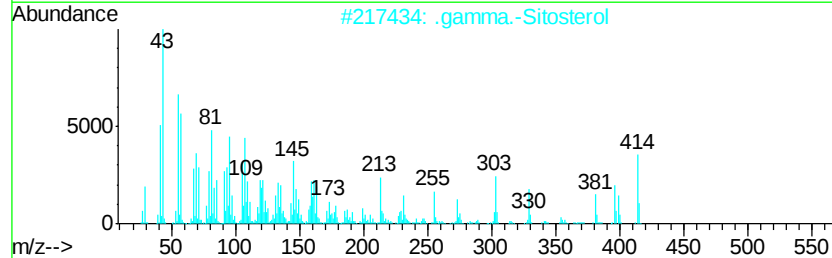
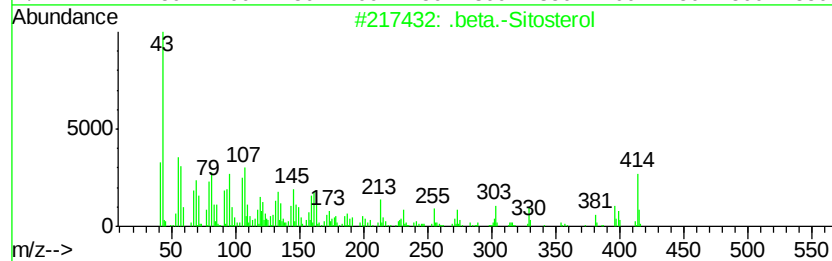
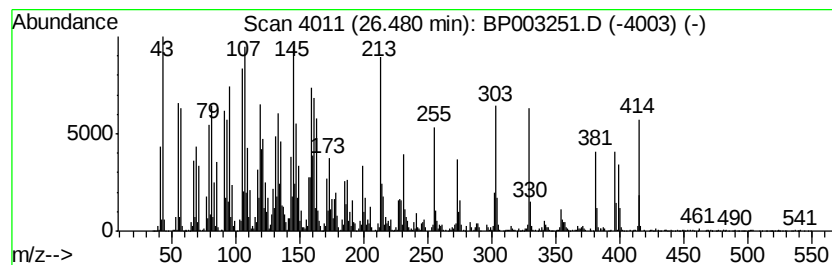
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 .beta.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.48	18.74 ng	2543090	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
3		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	90
4		Stigmast-7-en-3-ol, (3.beta.,5.a...	414	C29H50O	000521-03-9	45
5		Stigmastan-3,5-diene	396	C29H48	1000214-16-4	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP091020\
 Data File : BP003251.D
 Acq On : 10 Sep 2020 16:54
 Operator : CG/JU
 Sample : L3942-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 N35868

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP082420.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Crotonic acid	4.52	11.2 ng		484778	1	7.65	869552	20.0
Butanoic acid, 3-...	4.65	7.8 ng		340156	1	7.65	869552	20.0
Cyclohexanol, 5-m...	10.22	5.4 ng		360035	2	10.43	1331840	20.0
Ethanol, 2-phenoxy-	10.79	6.7 ng		443626	2	10.43	1331840	20.0
Benzeneacetic acid	11.02	6.8 ng		454501	2	10.43	1331840	20.0
unknown12.15	12.15	26.6 ng		1771030	2	10.43	1331840	20.0
Propanoic acid, 2...	12.65	6.8 ng		641490	3	14.29	1897420	20.0
1H-Indole, 2,3-di...	14.10	6.5 ng		615746	3	14.29	1897420	20.0
Caffeine	17.36	8.8 ng		928603	4	17.05	2108870	20.0
n-Hexadecanoic acid	17.97	7.7 ng		809688	4	17.05	2108870	20.0
Behenic alcohol	20.87	7.0 ng		861222	5	21.15	2460750	20.0
Squalene	22.33	6.0 ng		818215	6	23.38	2713790	20.0
Octadecane, 1-iodo-	22.71	4.4 ng		597482	6	23.38	2713790	20.0
Myristyl myristate	23.10	4.0 ng		546000	6	23.38	2713790	20.0
Octadecane, 2-met...	23.29	4.7 ng		634934	6	23.38	2713790	20.0
Docosane, 7-hexyl-	23.94	3.9 ng		529358	6	23.38	2713790	20.0
Cholesterol	24.41	58.4 ng		7925010	6	23.38	2713790	20.0
Cholesterol	24.69	76.3 ng		10357200	6	23.38	2713790	20.0
unknown26.12	26.12	12.8 ng		1732970	6	23.38	2713790	20.0
.beta.-Sitosterol	26.48	18.7 ng		2543090	6	23.38	2713790	20.0