

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081720\
 Data File : BP003007.D
 Acq On : 17 Aug 2020 17:44
 Operator : CG/JU
 Sample : L3691-09
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S711-N-SO-0-0.5-081320

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-BP073020.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	2.958	8	12	25	rVB	1581676	1698608	13.72%	1.506%
2	4.828	325	330	337	rVB2	90989	126552	1.02%	0.112%
3	5.293	402	409	429	rBV	3463350	4922935	39.77%	4.366%
4	6.863	668	676	691	rBV	3119528	5095069	41.16%	4.519%
5	7.287	743	748	756	rBV	73046	123855	1.00%	0.110%
6	7.687	808	816	826	rBV	1193985	1871106	15.11%	1.659%
7	8.828	999	1010	1024	rBV	2196209	3567361	28.82%	3.164%
8	10.463	1280	1288	1305	rBV	1460335	2424956	19.59%	2.151%
9	12.945	1702	1710	1723	rBV	5609977	8520086	68.82%	7.556%
10	13.781	1844	1852	1866	rBV	1172372	1651221	13.34%	1.464%
11	14.322	1937	1944	1951	rBV	2415325	3633796	29.35%	3.223%
12	15.816	2188	2198	2211	rBV	4117897	5891340	47.59%	5.225%
13	17.075	2406	2412	2416	rBV	2744270	3852078	31.12%	3.416%
14	17.116	2416	2419	2424	rVB	672837	878859	7.10%	0.779%
15	17.204	2430	2434	2440	rVB	102009	159416	1.29%	0.141%
16	17.475	2473	2480	2493	rBV	107849	192922	1.56%	0.171%
17	17.951	2555	2561	2564	rBV	79745	125493	1.01%	0.111%
18	17.998	2564	2569	2586	rVV	1089468	1623552	13.11%	1.440%
19	18.139	2588	2593	2597	rVV3	133820	187221	1.51%	0.166%
20	18.469	2646	2649	2657	rVB	181678	246903	1.99%	0.219%
21	19.098	2750	2756	2762	rBV	2561420	3495594	28.24%	3.100%
22	19.233	2775	2779	2785	rBV2	468409	697945	5.64%	0.619%
23	19.445	2806	2815	2824	rBV	2108901	3400538	27.47%	3.016%
24	19.651	2842	2850	2860	rVB	9483782	12379536	100.00%	10.979%
25	19.898	2888	2892	2894	rBV2	86419	132428	1.07%	0.117%
26	19.933	2895	2898	2903	rVB3	257877	403043	3.26%	0.357%
27	20.033	2911	2915	2919	rBV	176438	214941	1.74%	0.191%
28	20.086	2919	2924	2927	rBV2	165097	249701	2.02%	0.221%
29	20.227	2944	2948	2951	rBV3	120829	175508	1.42%	0.156%
30	20.657	3018	3021	3028	rVB	250868	345391	2.79%	0.306%
31	20.821	3043	3049	3052	rBV2	327750	558467	4.51%	0.495%
32	20.863	3053	3056	3059	rVB	251911	271448	2.19%	0.241%
33	20.904	3059	3063	3068	rBV3	2572174	3544940	28.64%	3.144%
34	21.104	3094	3097	3101	rVB	533897	531843	4.30%	0.472%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP073020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.169	3101	3108	3112	rVV2	4774426	7995635	64.59%	7.091%
36	21.204	3112	3114	3122	rVB	1751370	1993404	16.10%	1.768%
37	21.321	3131	3134	3136	rBV	211371	228753	1.85%	0.203%
38	21.474	3156	3160	3164	rBV2	284716	425014	3.43%	0.377%
39	21.792	3207	3214	3220	rBV4	743639	1541052	12.45%	1.367%
40	22.480	3327	3331	3340	rVB4	470670	770385	6.22%	0.683%
41	22.739	3369	3375	3385	rBV	1799644	5794150	46.80%	5.139%
42	23.221	3452	3457	3465	rVB	1046731	1933449	15.62%	1.715%
43	23.315	3467	3473	3483	rBV	1207564	2432487	19.65%	2.157%
44	23.415	3484	3490	3496	rBV2	2773951	5210259	42.09%	4.621%
45	24.021	3588	3593	3600	rVB	510304	950571	7.68%	0.843%
46	24.098	3601	3606	3621	rVV	581120	1370377	11.07%	1.215%
47	25.698	3870	3878	3892	rVB2	1209755	3586849	28.97%	3.181%
48	26.245	3966	3971	3982	rVB3	414522	1064845	8.60%	0.944%
49	26.398	3990	3997	4010	rVB	622385	1866339	15.08%	1.655%
50	26.574	4020	4027	4039	rBV	468509	1362098	11.00%	1.208%
51	26.968	4089	4094	4103	rVB3	386587	1038446	8.39%	0.921%

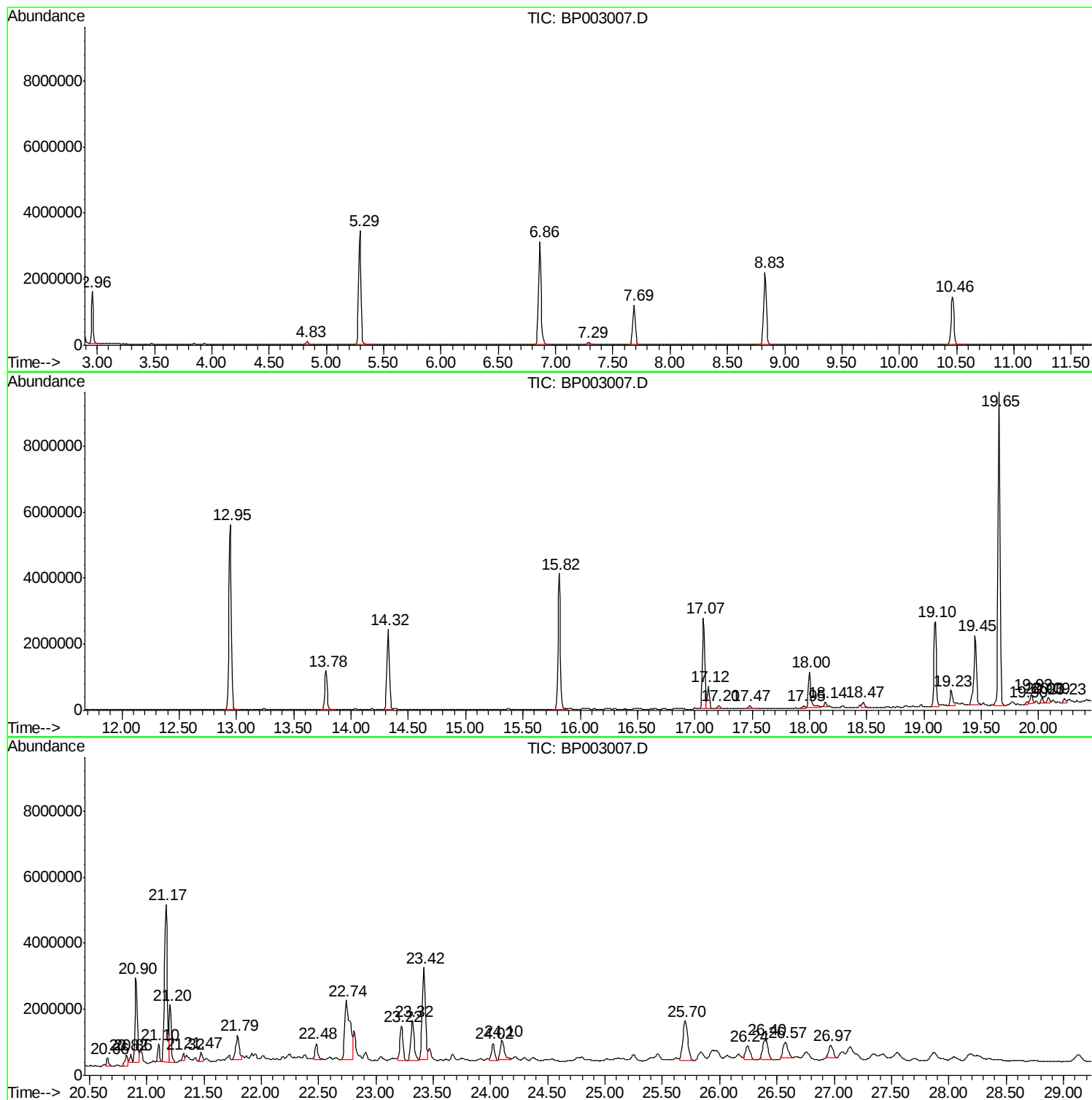
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP073020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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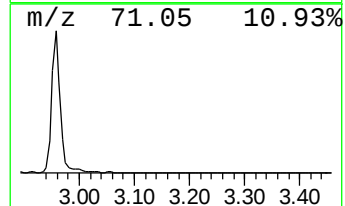
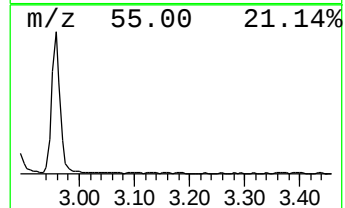
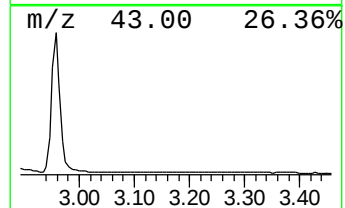
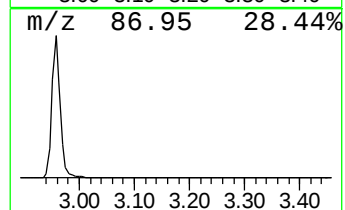
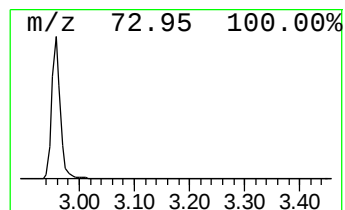
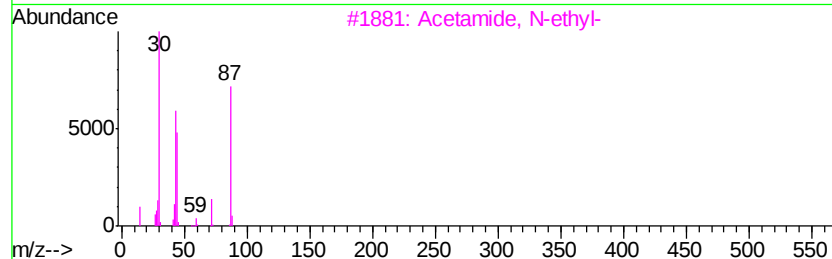
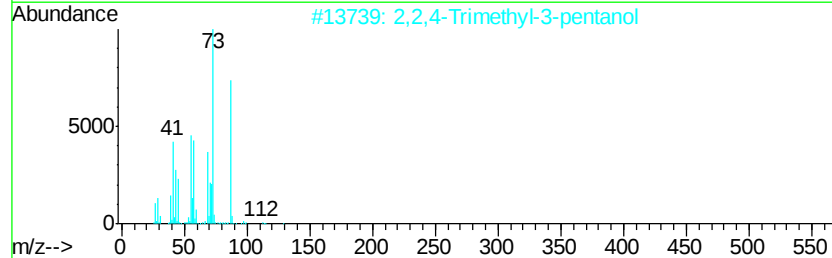
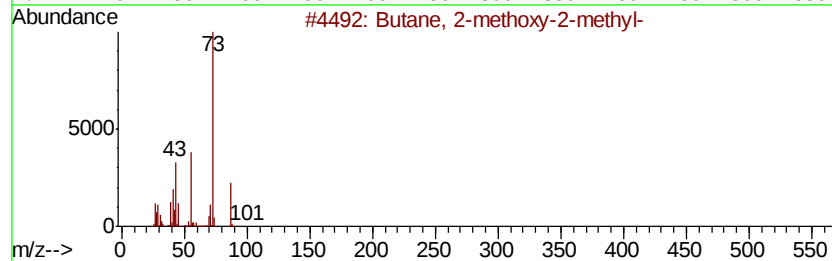
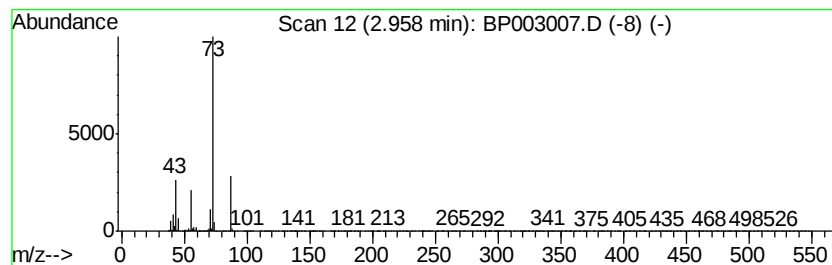
Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP073020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.96	18.16 ng	1698610	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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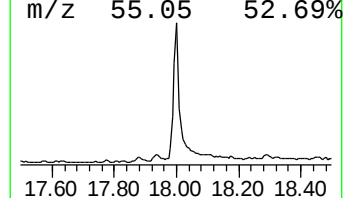
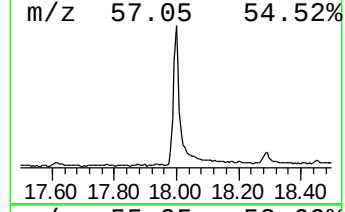
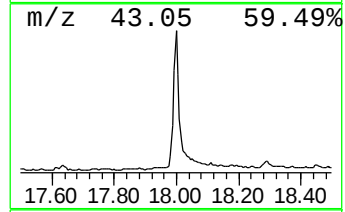
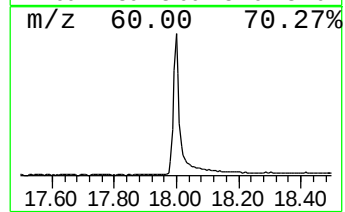
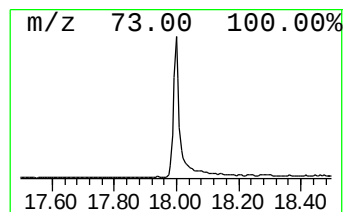
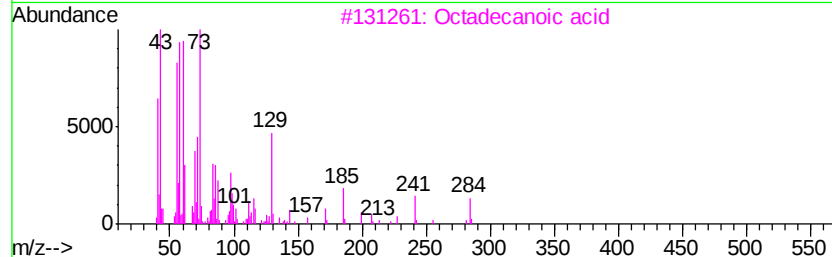
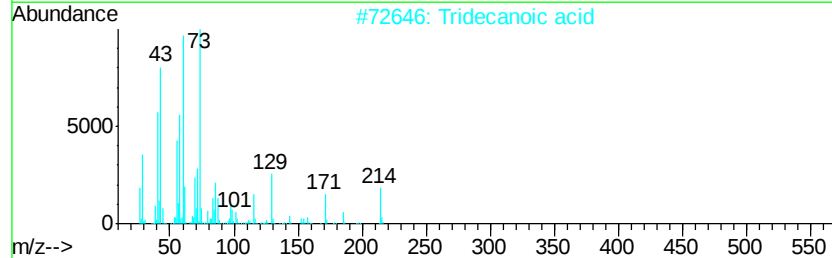
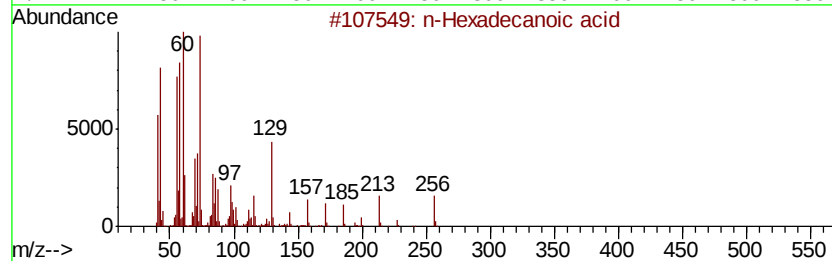
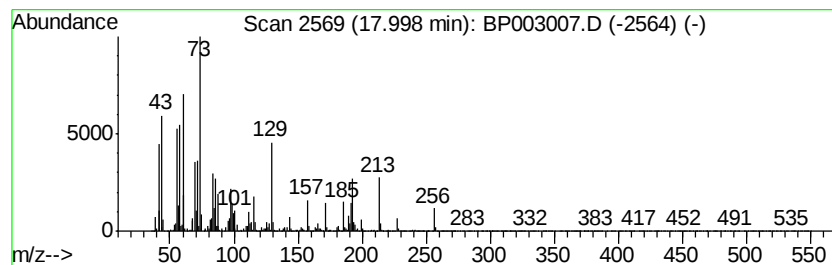
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.00	8.43 ng	1623550	Phenanthrene-d10		17.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49



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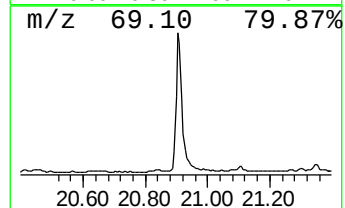
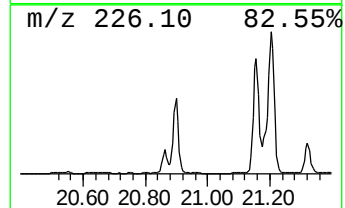
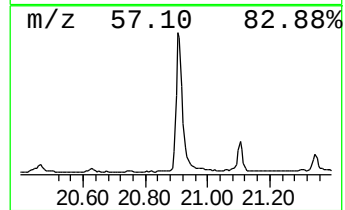
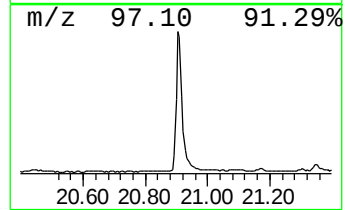
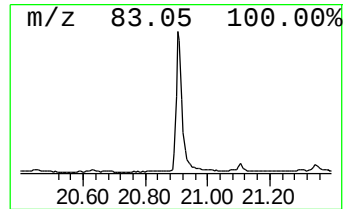
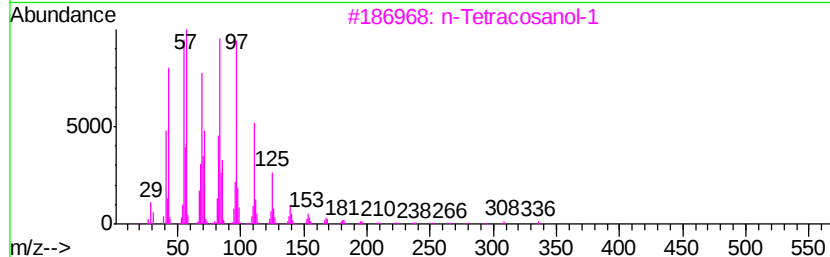
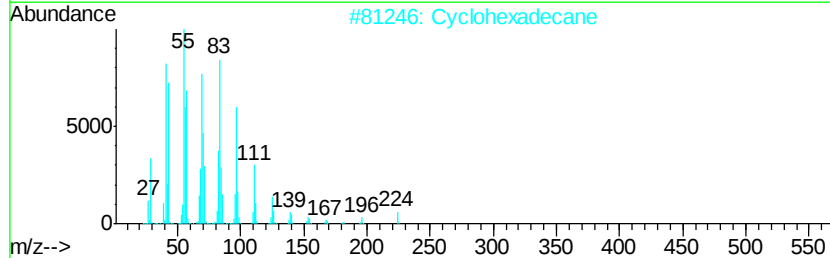
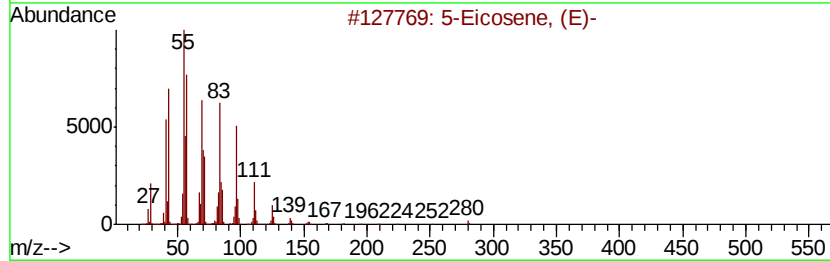
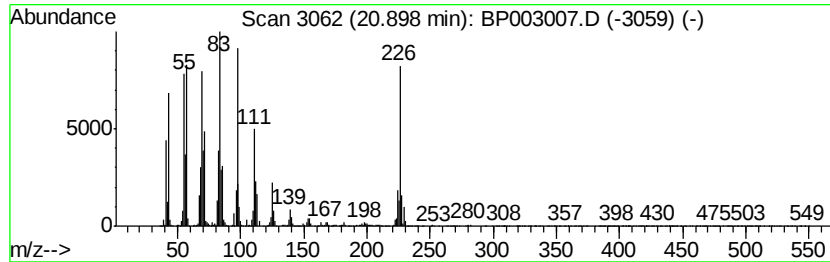
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.90	8.87 ng	3544940	Chrysene-d12	21.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Cyclohexadecane	224	C16H32	000295-65-8	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93



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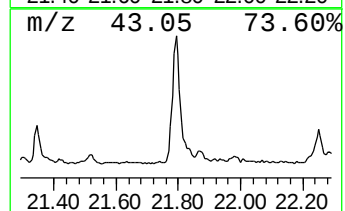
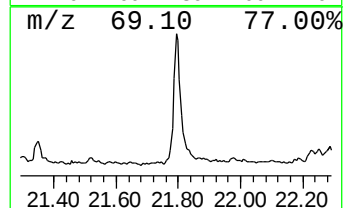
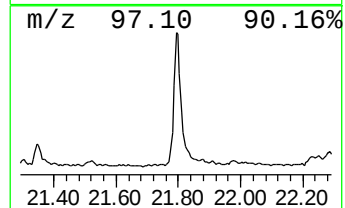
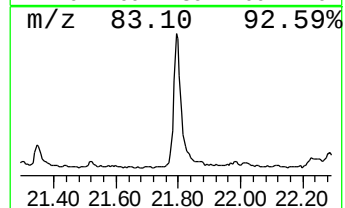
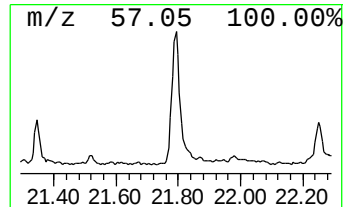
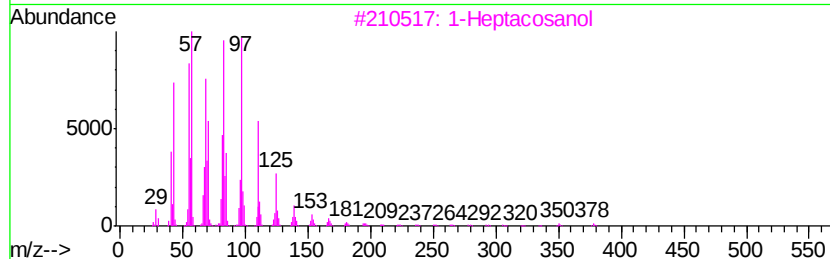
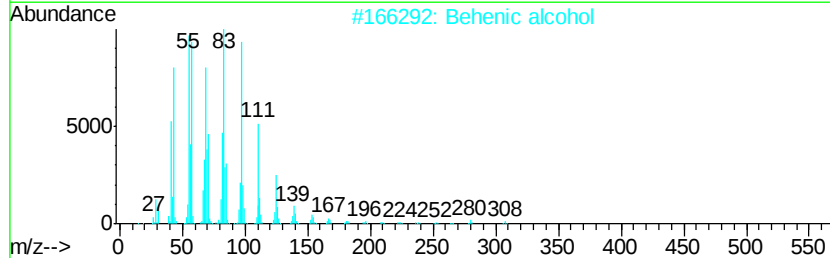
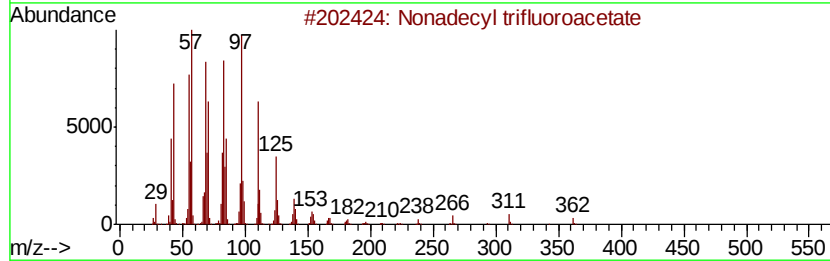
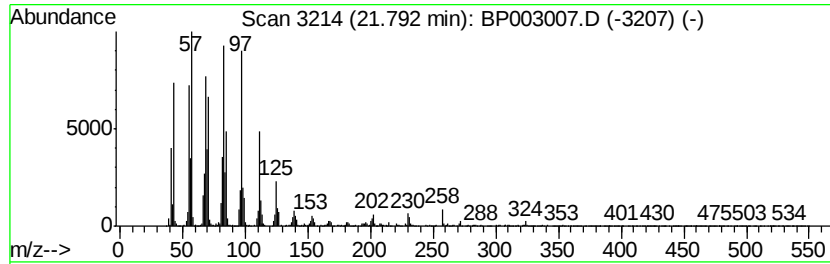
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonadecyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
21.79	3.85 ng	1541050	Chrysene-d12		21.17
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	94
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90



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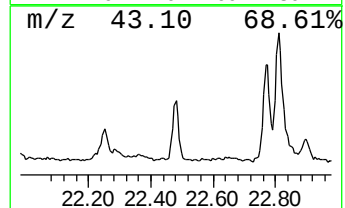
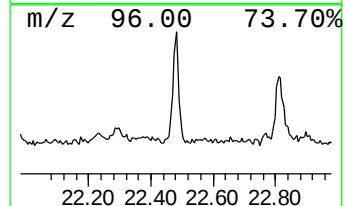
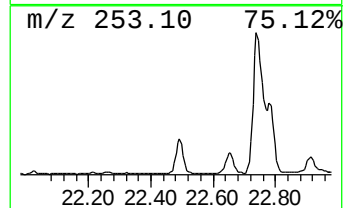
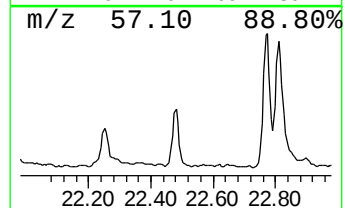
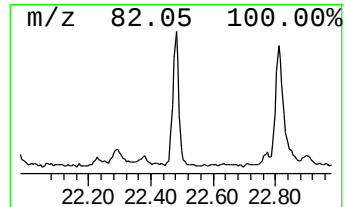
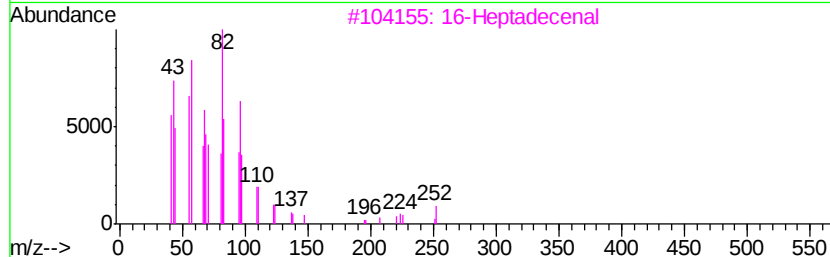
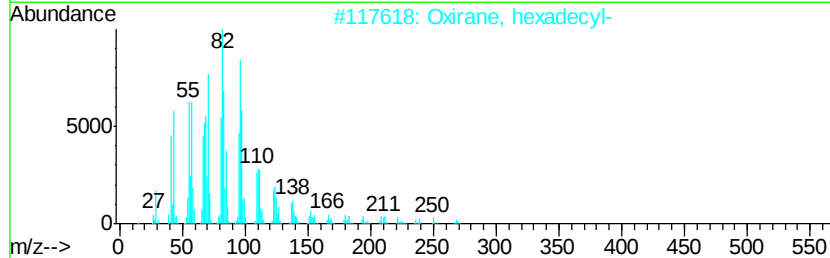
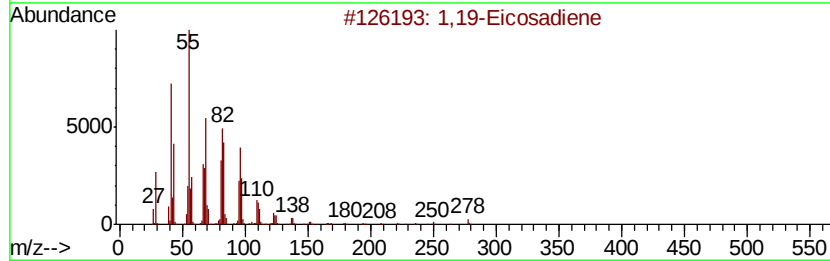
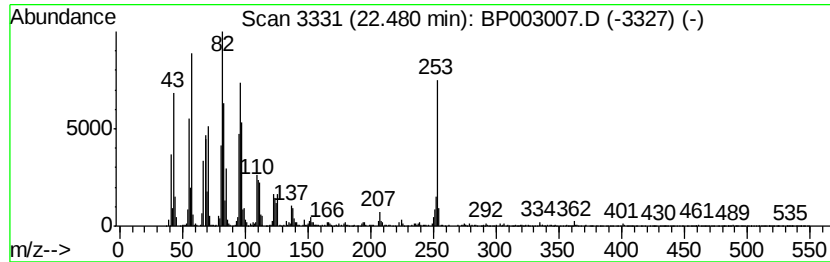
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,19-Eicosadiene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.48	2.96 ng	770385	Perylene-d12	23.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	96
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	89
3	16-Heptadecenal	252	C17H32O	1000144-57-9	83
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	76
5	Octadecanal	268	C18H36O	000638-66-4	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081720\
Data File : BP003007.D
Acq On : 17 Aug 2020 17:44
Operator : CG/JU
Sample : L3691-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S711-N-SO-0-0.5-081320

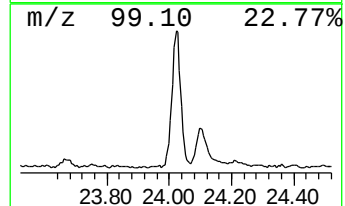
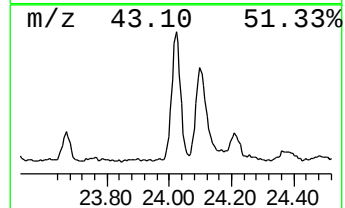
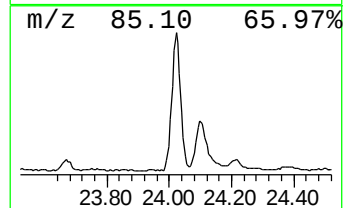
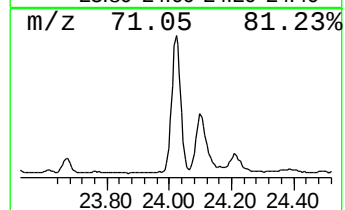
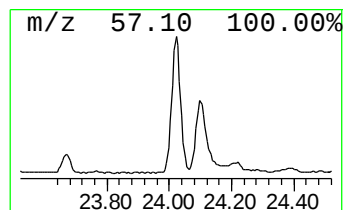
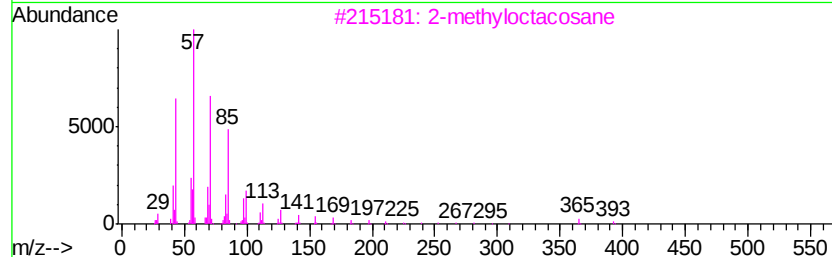
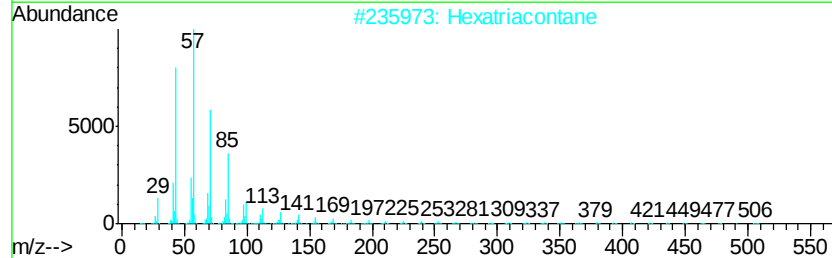
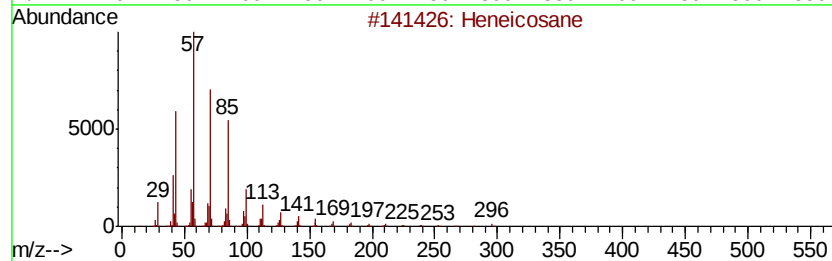
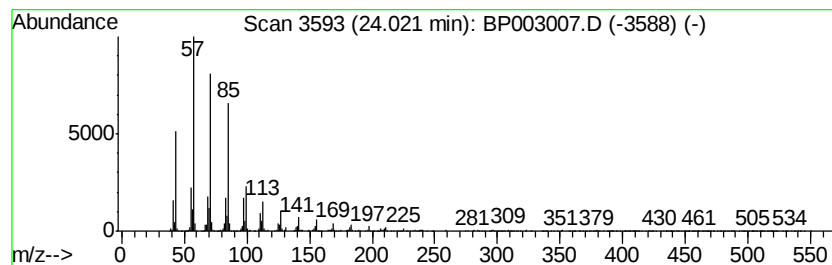
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.02	3.65 ng	950571	Perylene-d12	23.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	97
2	Hexatriacontane		507	C36H74	000630-06-8	93
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Tetracosane		338	C24H50	000646-31-1	91
5	Pentacosane		352	C25H52	000629-99-2	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081720\
Data File : BP003007.D
Acq On : 17 Aug 2020 17:44
Operator : CG/JU
Sample : L3691-09
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ALS Vial : 14 Sample Multiplier: 1

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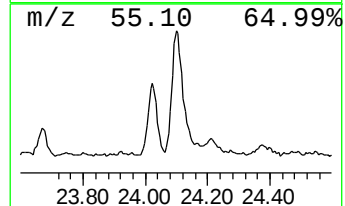
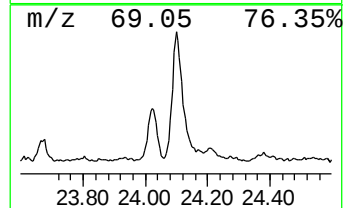
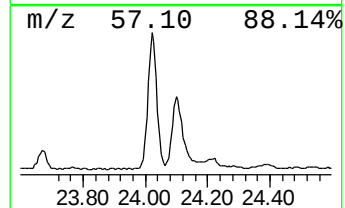
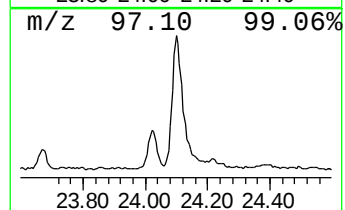
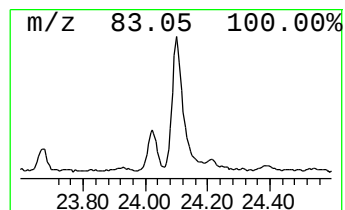
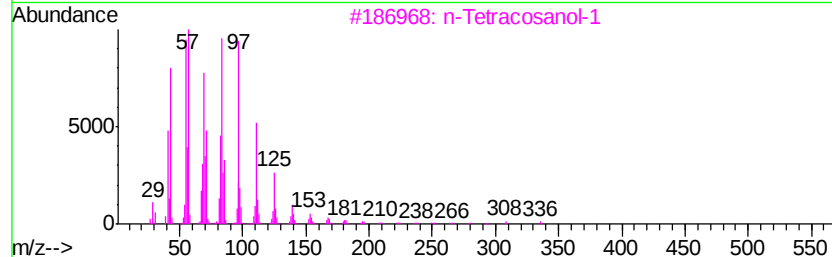
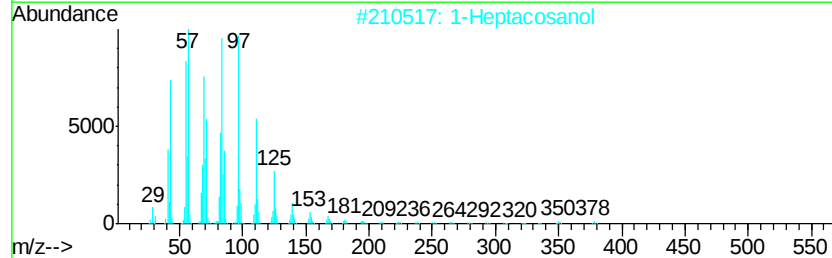
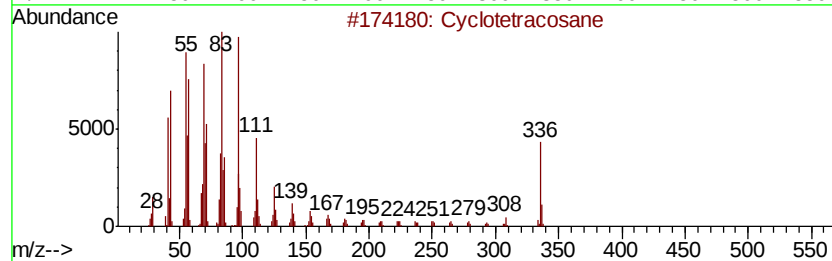
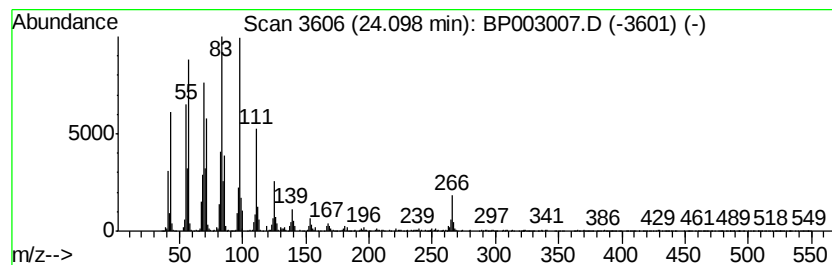
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.10	5.26 ng	1370380	Perylene-d12	23.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	95
2		1-Heptacosanol	396	C27H56O	002004-39-9	95
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Behenic alcohol	326	C22H46O	000661-19-8	93
5		Heptacosyl acetate	438	C29H58O2	1000351-78-2	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081720\
Data File : BP003007.D
Acq On : 17 Aug 2020 17:44
Operator : CG/JU
Sample : L3691-09
Misc :
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Instrument :
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ClientSampleId :
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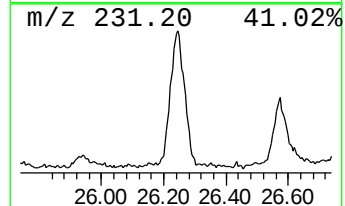
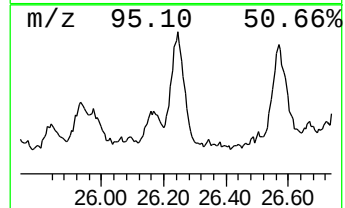
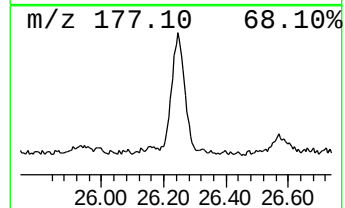
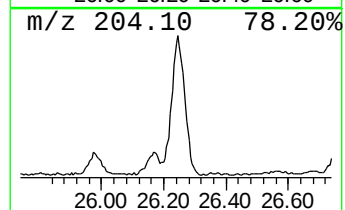
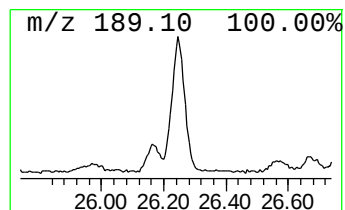
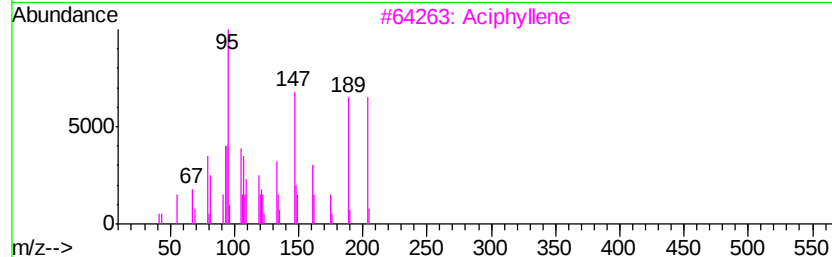
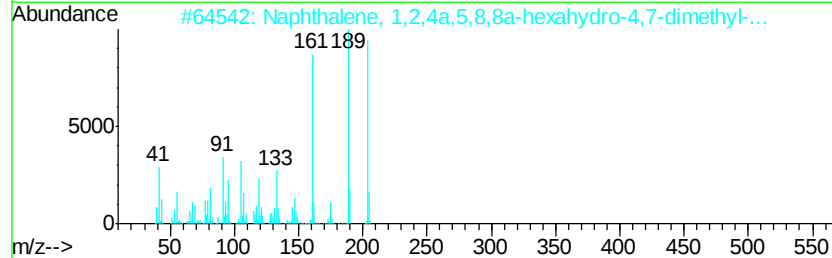
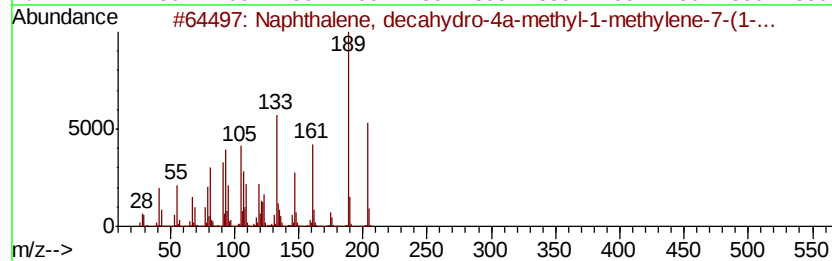
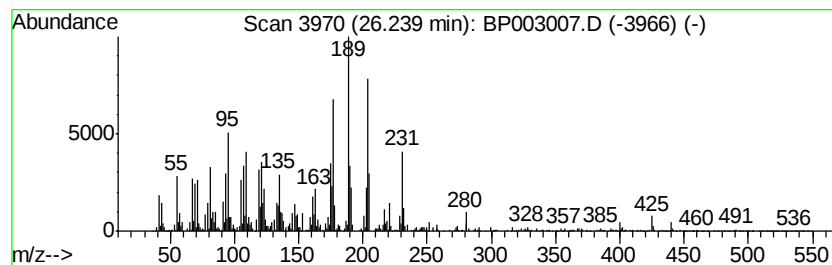
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown26.24 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.24	4.09 ng	1064850	Perylene-d12	23.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	49
2		Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	43
3		Aciphvllene	204	C15H24	087745-31-1	43
4		Naphthalene, 2,3,4,4a,5,6-hexahy...	204	C15H24	000473-14-3	38
5		2,3-Dimethoxy-5-aminocinnamonitrile	204	C11H12N2O2	1000214-46-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081720\
Data File : BP003007.D
Acq On : 17 Aug 2020 17:44
Operator : CG/JU
Sample : L3691-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

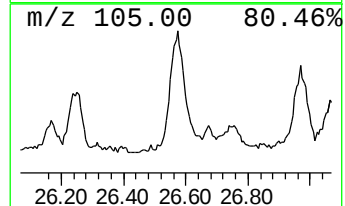
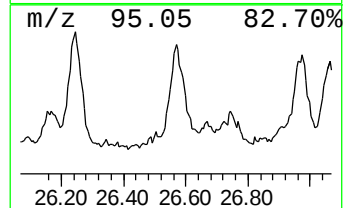
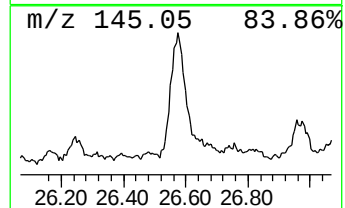
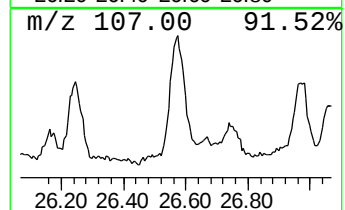
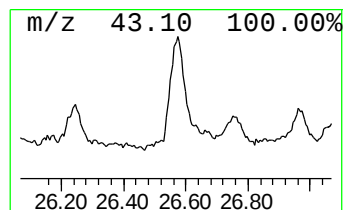
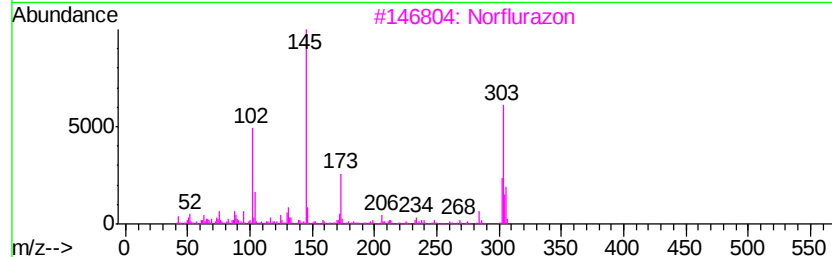
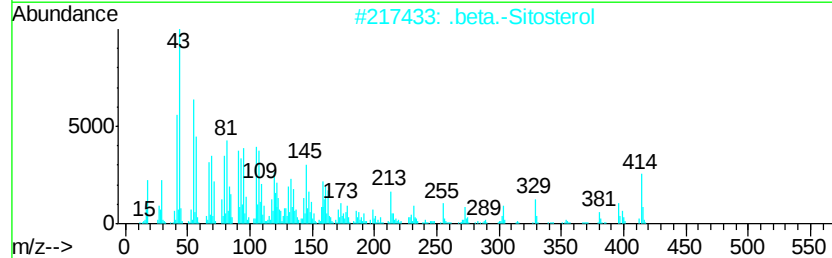
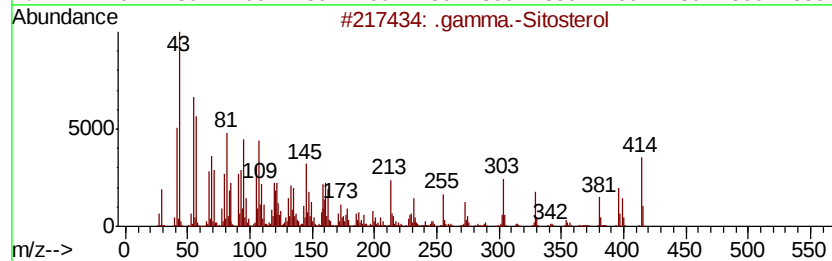
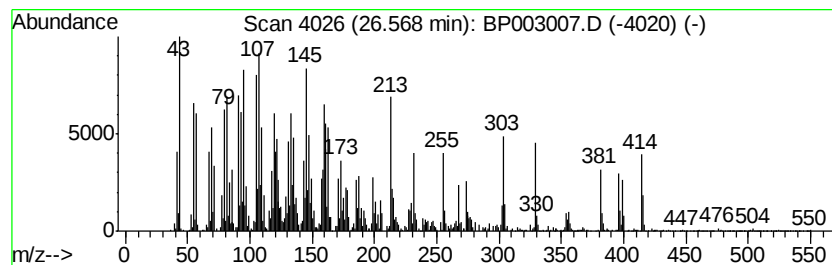
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Sitosterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.57	5.23 ng	1362100	Perylene-d12	23.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3	Norflurazon	303	C12H9ClF3N3O	027314-13-2	20
4	N-(3-Chloro-4-fluoro-phenyl)-2-(...	329	C14H10Cl2FNOS	1000295-12-7	18
5	Furan-2-carboxylic acid, (4-benz...	303	C19H13NO3	1000316-79-6	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP081720\
Data File : BP003007.D
Acq On : 17 Aug 2020 17:44
Operator : CG/JU
Sample : L3691-09
Misc :
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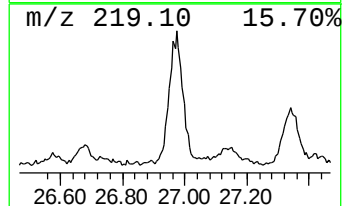
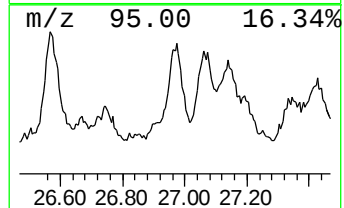
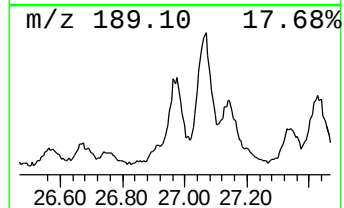
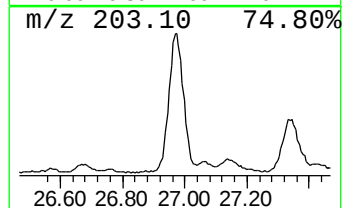
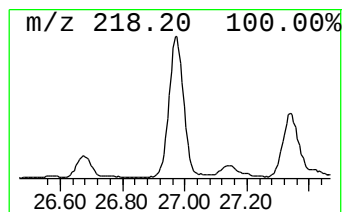
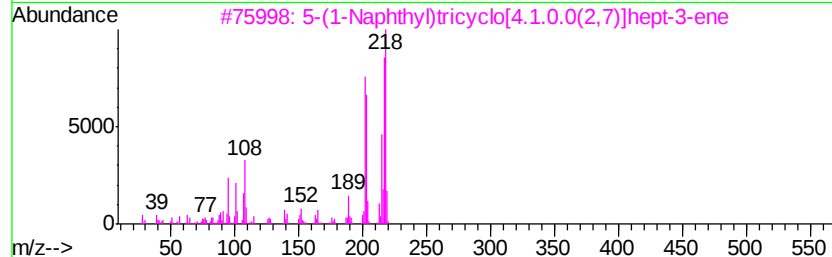
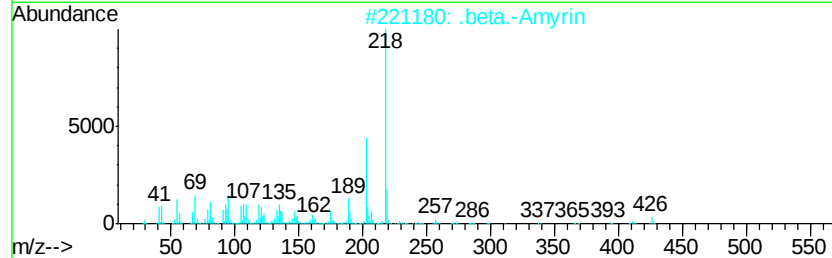
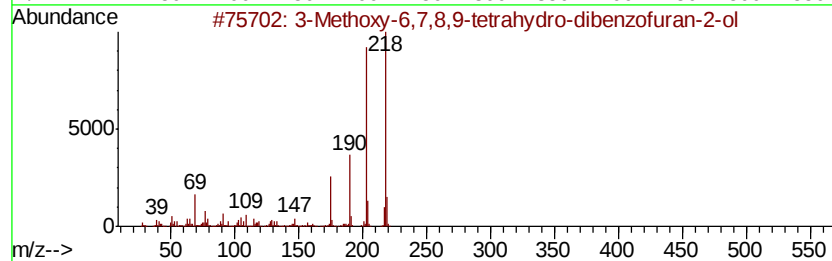
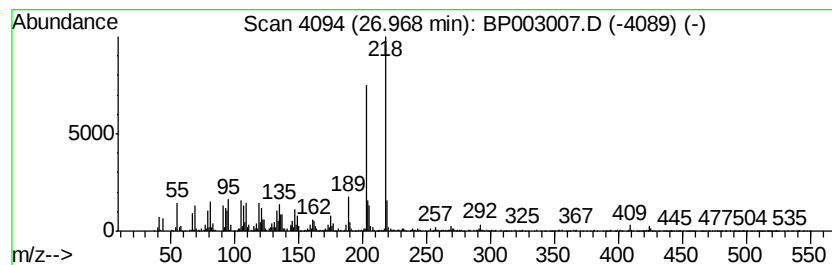
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 3-Methoxy-6,7,8,9-tetrahydr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
26.97	3.99 ng	1038450	Perylene-d12	23.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	80
2		.beta.-Amyrin	426	C30H50O	000559-70-6	58
3		5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	58
4		.alpha.-Amyrin, trimethylsilyl e...	498	C33H58OSi	1000374-76-6	49
5		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP081720\
Data File : BP003007.D
Acq On : 17 Aug 2020 17:44
Operator : CG/JU
Sample : L3691-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
Butane, 2-methoxy...	2.96	18.2	ng	1698610	1	7.69	1871110	20.0
n-Hexadecanoic acid	18.00	8.4	ng	1623550	4	17.07	3852080	20.0
5-Eicosene, (E)-	20.90	8.9	ng	3544940	5	21.17	7995640	20.0
Nonadecyl trifluo...	21.79	3.9	ng	1541050	5	21.17	7995640	20.0
1,19-Eicosadiene	22.48	3.0	ng	770385	6	23.42	5210260	20.0
Heneicosane	24.02	3.6	ng	950571	6	23.42	5210260	20.0
Cyclotetracosane	24.10	5.3	ng	1370380	6	23.42	5210260	20.0
unknown26.24	26.24	4.1	ng	1064850	6	23.42	5210260	20.0
.gamma.-Sitosterol	26.57	5.2	ng	1362100	6	23.42	5210260	20.0
3-Methoxy-6,7,8,9...	26.97	4.0	ng	1038450	6	23.42	5210260	20.0