

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
 Data File : BP001021.D
 Acq On : 11 Nov 2019 17:41
 Operator : JU
 Sample : K5760-12
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 RBR-30

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-BP110619.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	2.322	34	40	49	rVB	745262	1104020	14.90%	1.818%
2	5.734	616	620	633	rBV	479768	724596	9.78%	1.193%
3	6.305	711	717	722	rBV	3410602	4277942	57.72%	7.046%
4	7.816	966	974	981	rBV	3549189	4801978	64.79%	7.909%
5	8.010	1001	1007	1012	rBV	4035603	4839892	65.30%	7.971%
6	8.369	1063	1068	1074	rBV	1273168	1471905	19.86%	2.424%
7	8.610	1103	1109	1114	rBV	3341611	3908931	52.74%	6.438%
8	9.246	1210	1217	1221	rBV	2485512	2937301	39.63%	4.838%
9	10.398	1407	1413	1418	rBV	1697068	1890758	25.51%	3.114%
10	12.175	1709	1715	1720	rBV	5486365	6285851	84.81%	10.353%
11	12.839	1824	1828	1833	rVB	296501	317047	4.28%	0.522%
12	13.257	1893	1899	1905	rBV	1994436	2419225	32.64%	3.984%
13	14.551	2112	2119	2133	rBV	3719510	4715070	63.62%	7.766%
14	15.616	2297	2300	2302	rBV	64605	80308	1.08%	0.132%
15	15.651	2302	2306	2310	rVB	2186563	2552452	34.44%	4.204%
16	16.533	2452	2456	2464	rBV2	297806	450230	6.07%	0.742%
17	17.263	2578	2580	2587	rVB2	59406	79716	1.08%	0.131%
18	17.392	2599	2602	2606	rVB	77080	82837	1.12%	0.136%
19	17.622	2638	2641	2646	rBV	107450	140132	1.89%	0.231%
20	17.698	2650	2654	2658	rVB	103105	120137	1.62%	0.198%
21	17.933	2688	2694	2698	rBV	6702804	7411301	100.00%	12.206%
22	18.110	2720	2724	2728	rVB	281431	311870	4.21%	0.514%
23	18.551	2796	2799	2802	rBV2	132574	146242	1.97%	0.241%
24	18.616	2807	2810	2816	rVB	241688	271718	3.67%	0.448%
25	19.157	2898	2902	2911	rVB2	798320	964026	13.01%	1.588%
26	19.292	2919	2925	2928	rBV	2451966	2930638	39.54%	4.827%
27	19.322	2928	2930	2937	rVB2	229045	305203	4.12%	0.503%
28	19.974	3037	3041	3047	rVB	170343	191926	2.59%	0.316%
29	20.351	3101	3105	3115	rVB	234504	275562	3.72%	0.454%
30	20.433	3115	3119	3125	rVB	361507	413741	5.58%	0.681%
31	20.574	3139	3143	3146	rBV	95055	141615	1.91%	0.233%
32	20.610	3146	3149	3153	rVB	79080	97387	1.31%	0.160%
33	20.751	3169	3173	3182	rBV	277144	373753	5.04%	0.616%
34	21.074	3221	3228	3239	rVB	1944572	2802998	37.82%	4.617%

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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

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
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35	21.198	3244	3249	3256	rBV	210176	305508	4.12%	0.503%
36	21.710	3330	3336	3340	rBV	154106	284073	3.83%	0.468%
37	21.751	3340	3343	3354	rVB	93172	181952	2.46%	0.300%
38	22.292	3430	3435	3444	rBV3	57139	106751	1.44%	0.176%

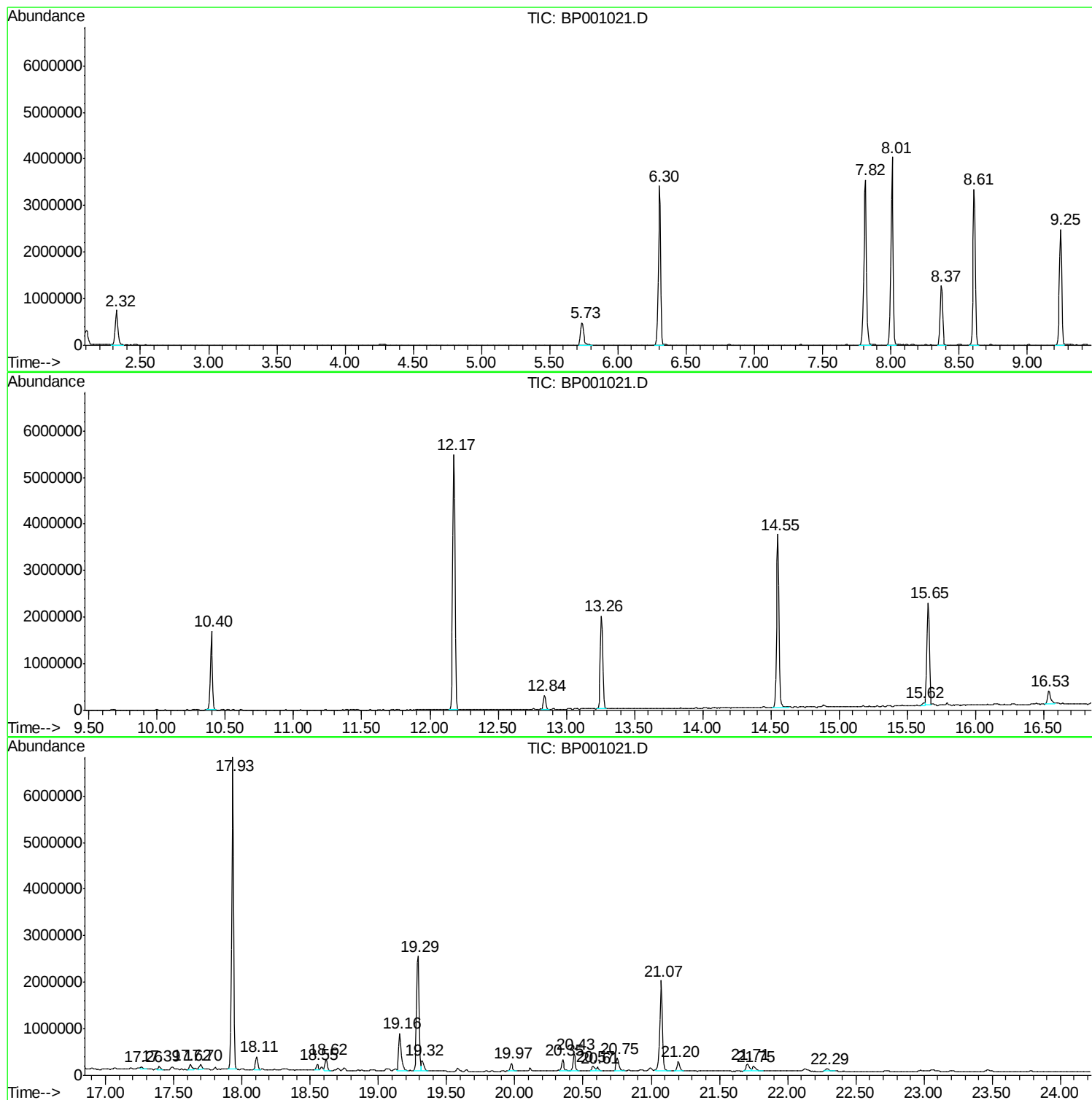
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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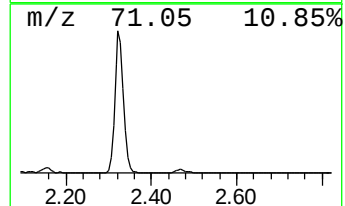
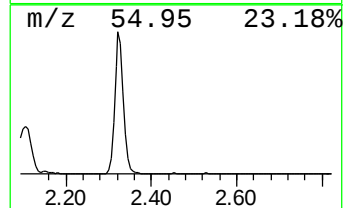
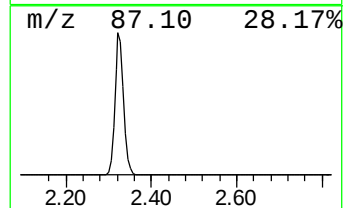
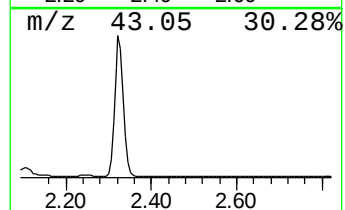
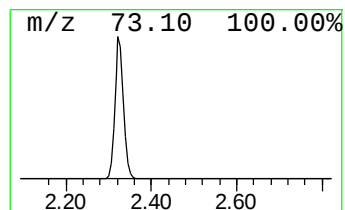
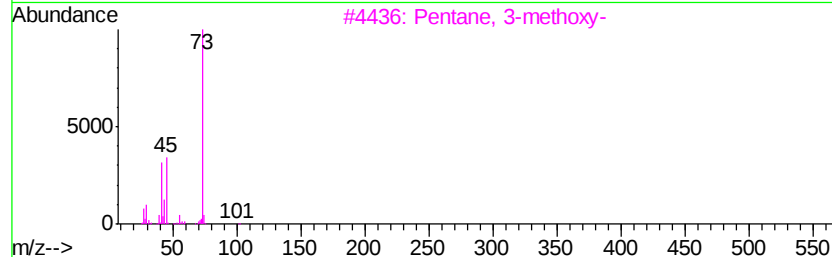
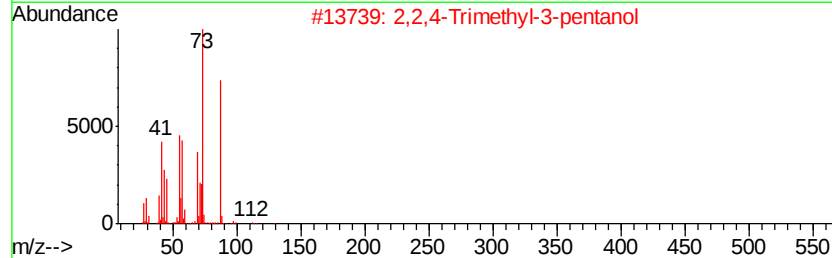
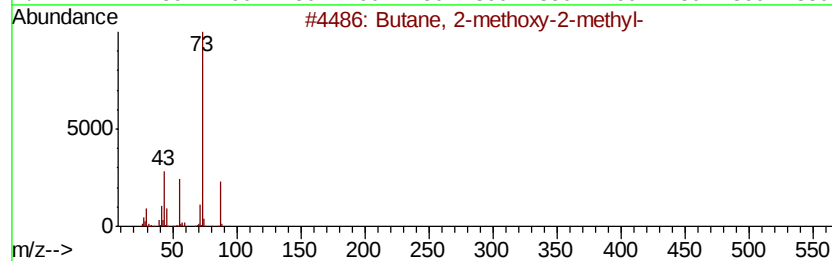
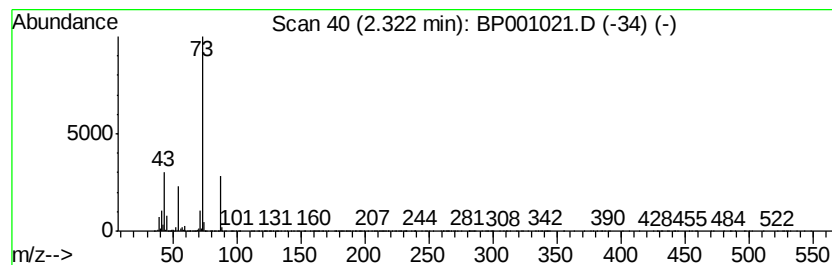
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	15.00 ng	1104020	1,4-Dichlorobenzene-d4	8.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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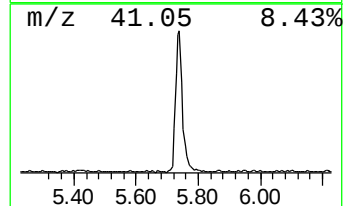
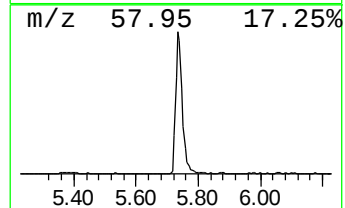
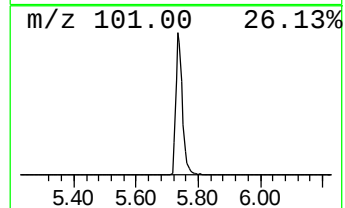
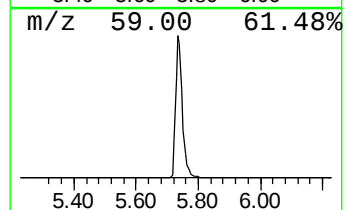
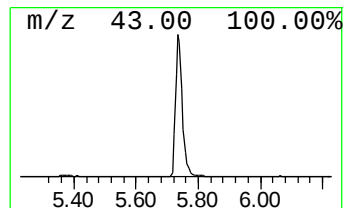
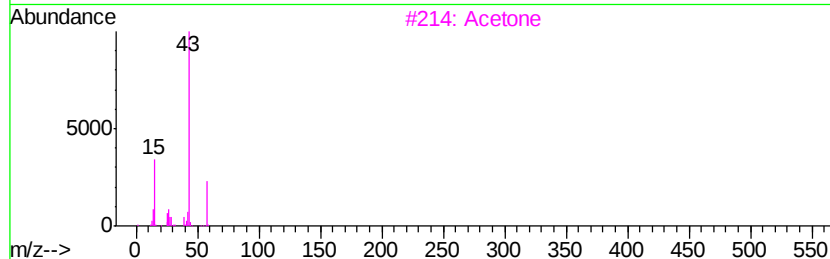
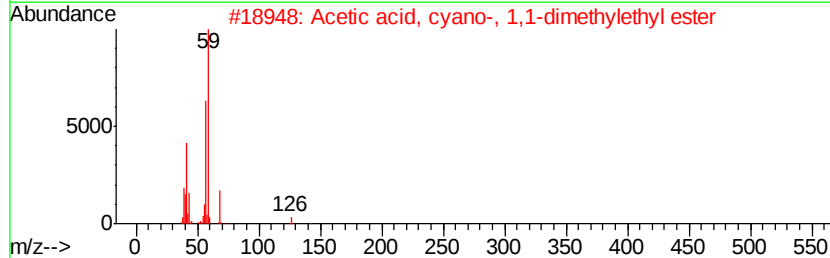
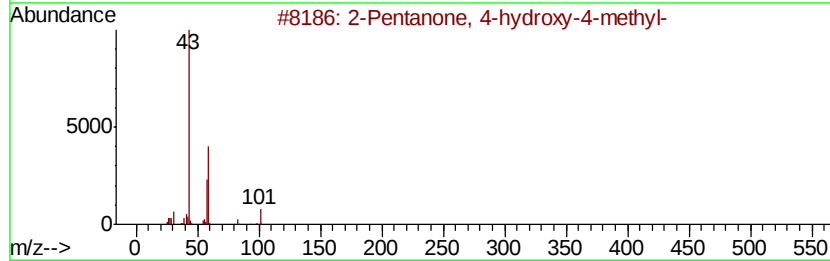
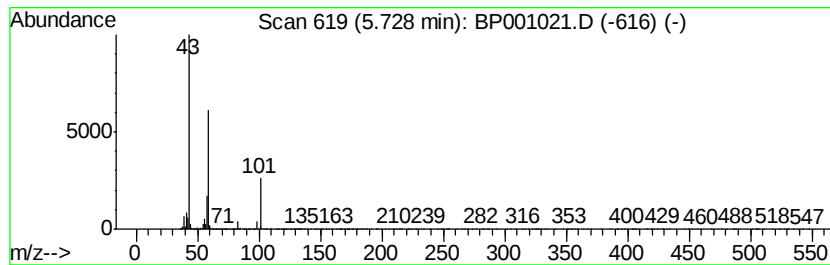
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	9.85 ng	724596	1,4-Dichlorobenzene-d4	8.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			Acetone	58	C3H6O	000067-64-1	10
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Guanidine	59	CH5N3	000113-00-8	9



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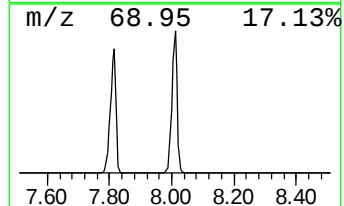
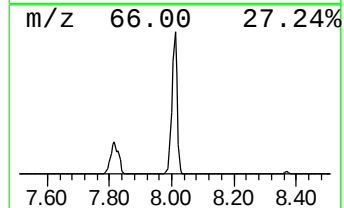
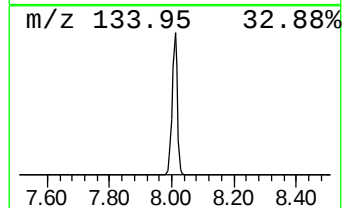
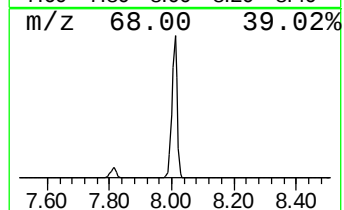
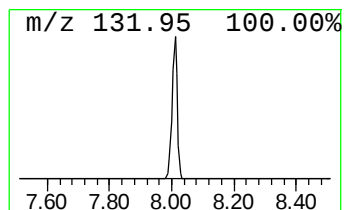
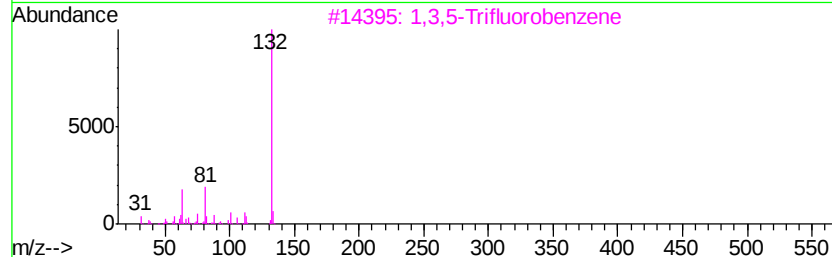
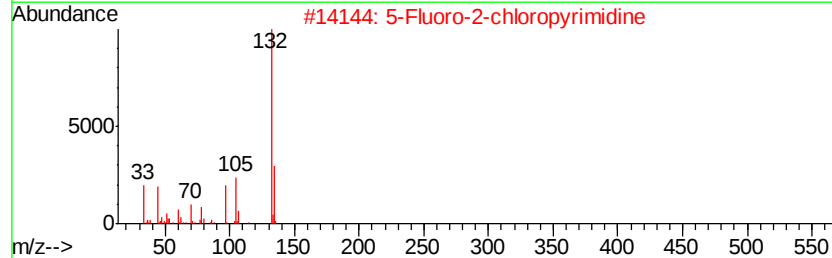
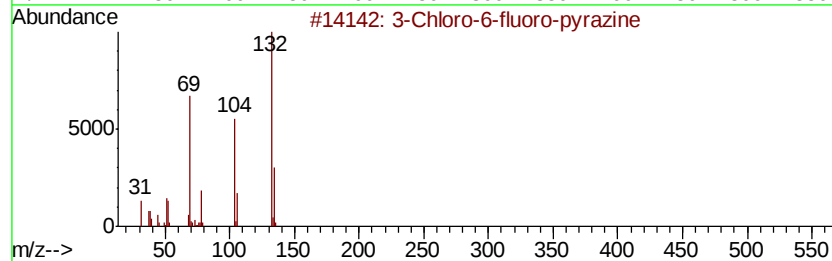
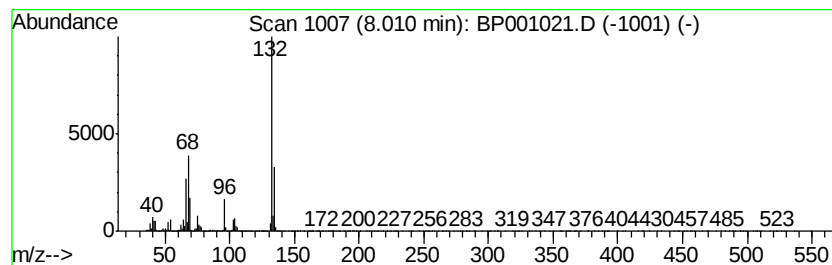
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown8.01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.01	65.76 ng	4839890	1,4-Dichlorobenzene-d4	8.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
3	1,3,5-Trifluorobenzene			132	C6H3F3	000372-38-3	10
4	N-(-3,4-Methylenedioxyphenylisop...			267	C17H17NO2	1000378-96-6	10
5	1,2,4-Trifluorobenzene			132	C6H3F3	000367-23-7	9



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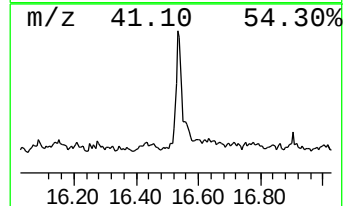
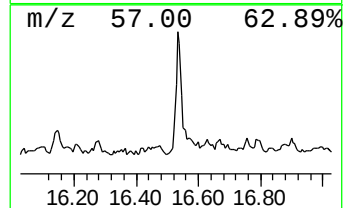
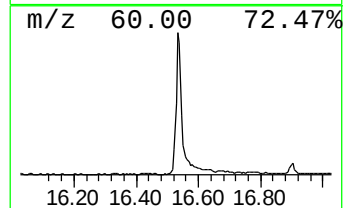
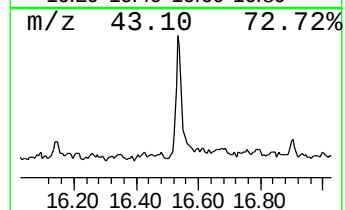
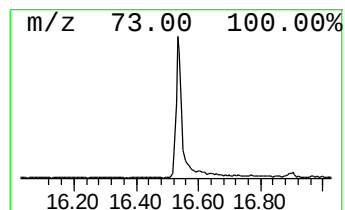
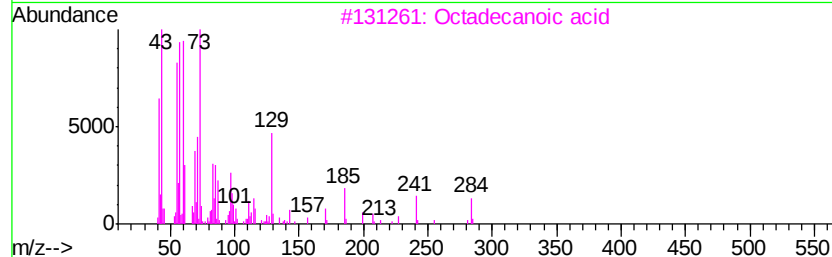
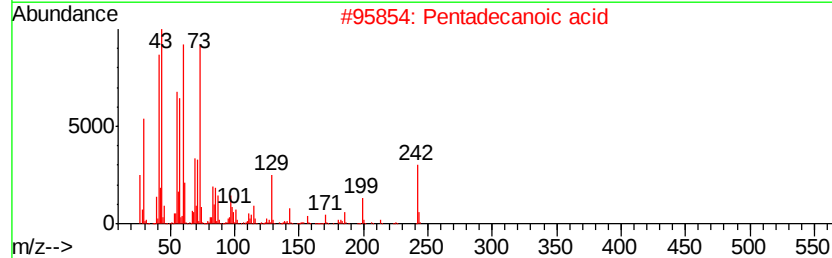
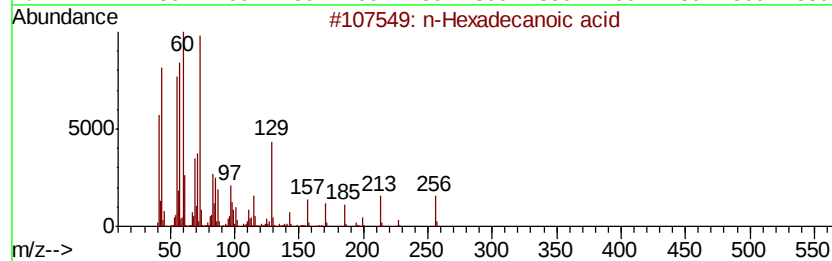
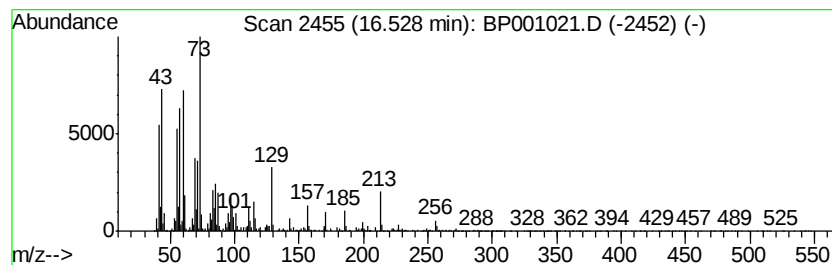
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	3.53 ng	450230	Phenanthrene-d10	15.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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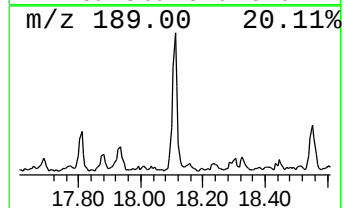
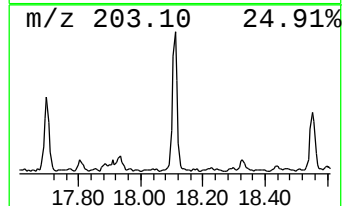
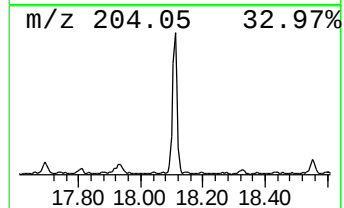
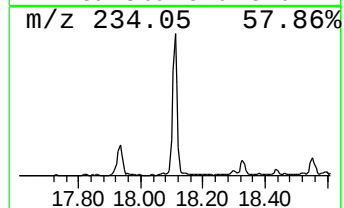
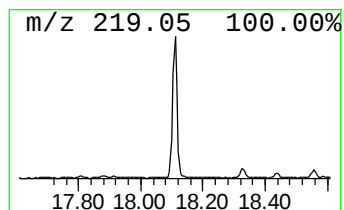
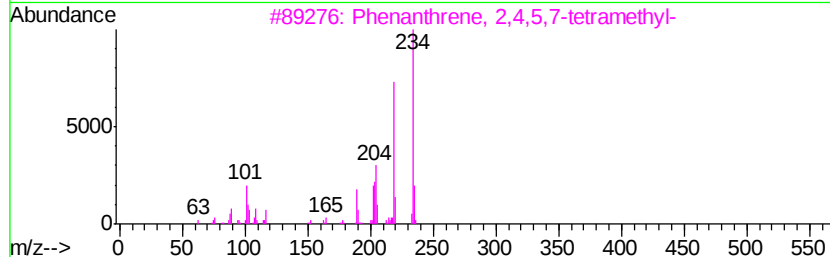
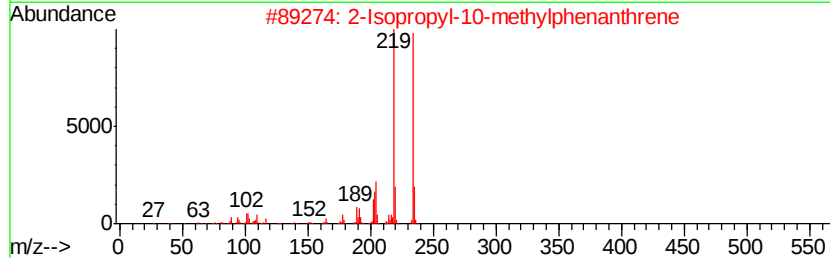
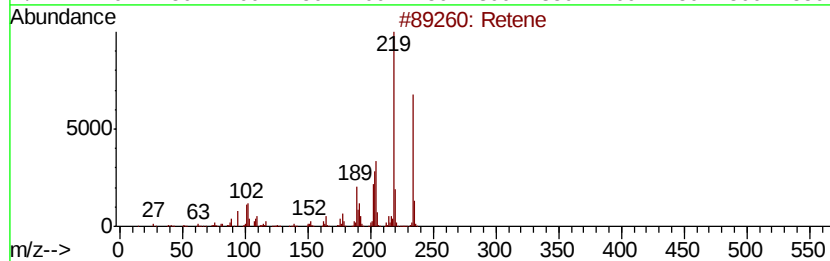
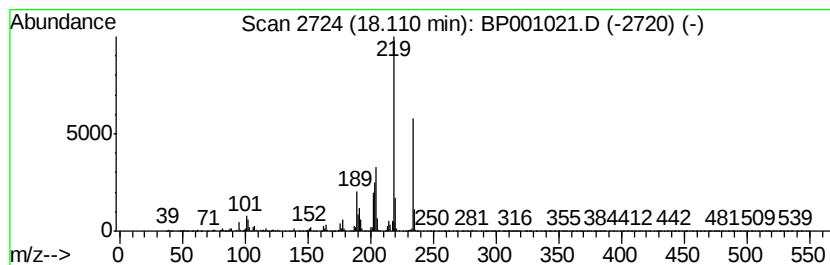
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Retene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.11	2.13 ng	311870	Chrysene-d12	19.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Retene	234	C18H18	000483-65-8	98
2		2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	95
3		Phenanthrene, 2,4,5,7-tetramethyl-	234	C18H18	007396-38-5	68
4		Phenanthrene, 3,4,5,6-tetramethyl-	234	C18H18	007343-06-8	64
5		Anthracene, 2-(1,1-dimethylethyl)-	234	C18H18	018801-00-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001021.D
Acq On : 11 Nov 2019 17:41
Operator : JU
Sample : K5760-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RBR-30

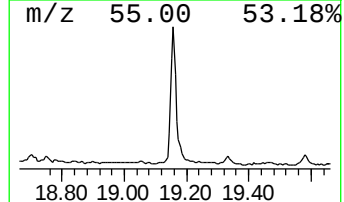
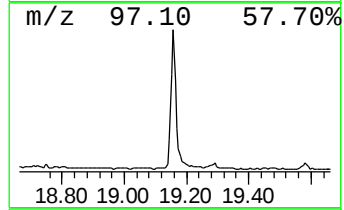
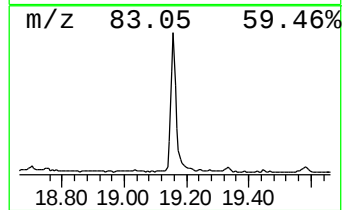
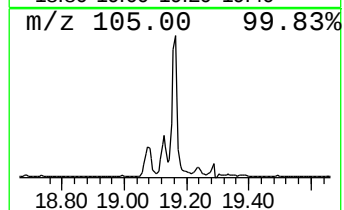
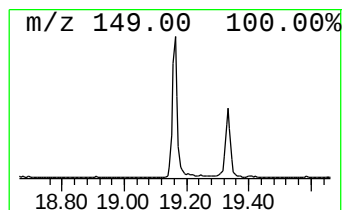
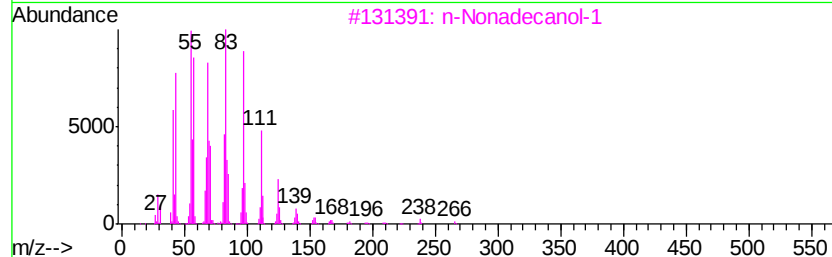
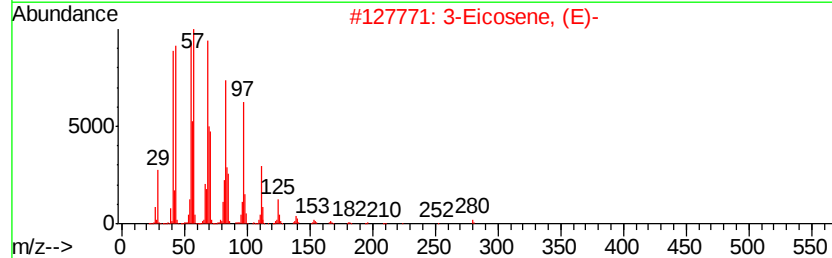
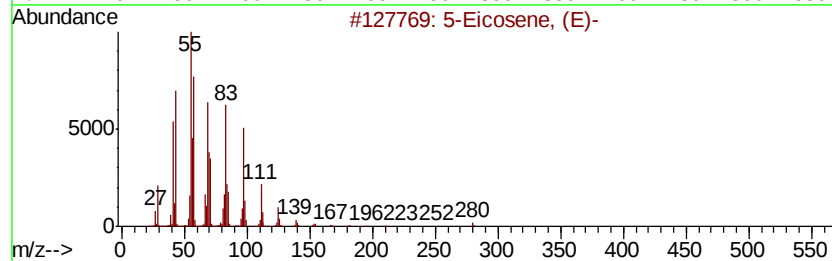
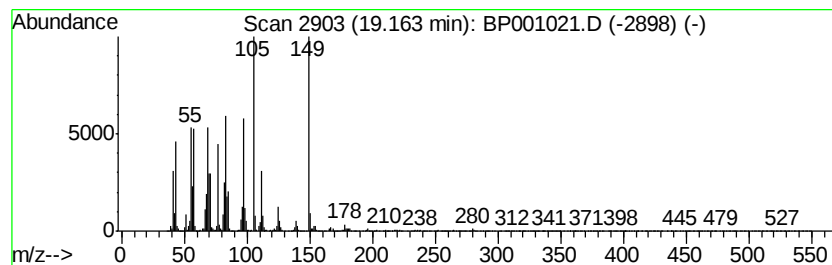
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	6.58 ng	964026	Chrysene-d12	19.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	94
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Cyclopentadecane	210	C15H30	000295-48-7	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
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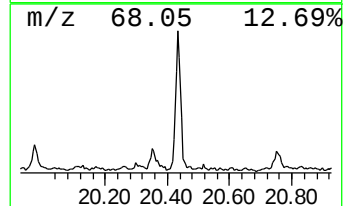
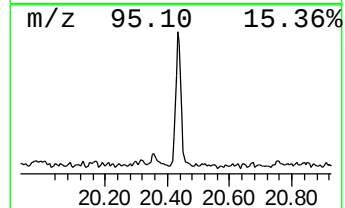
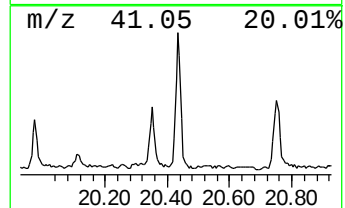
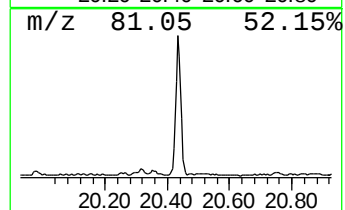
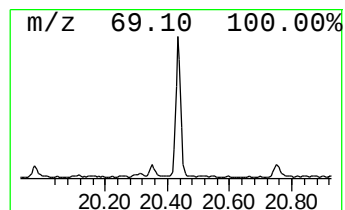
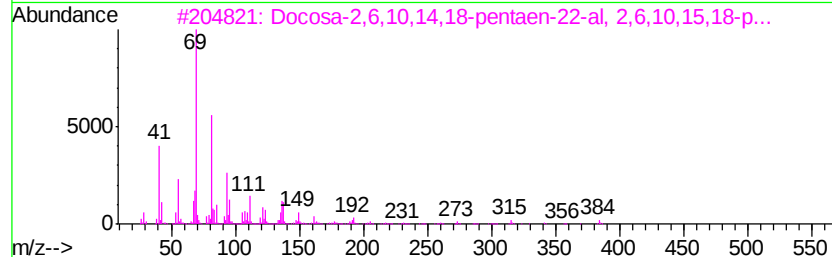
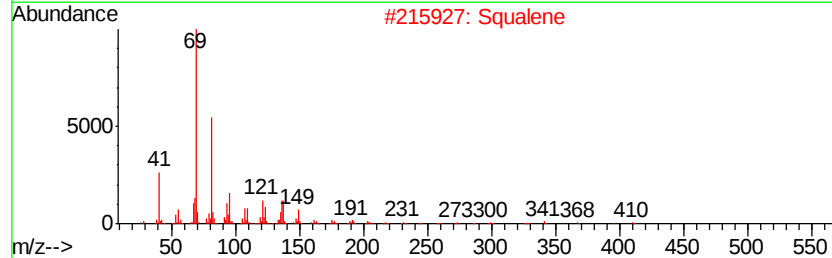
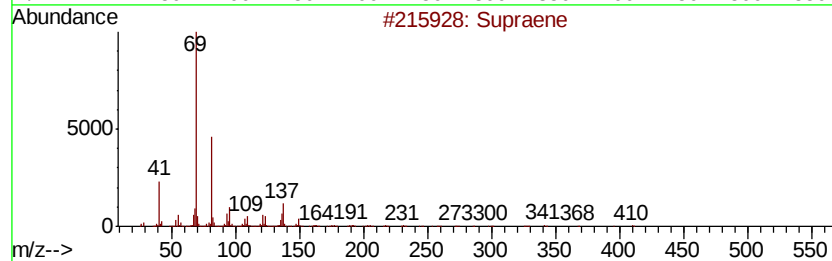
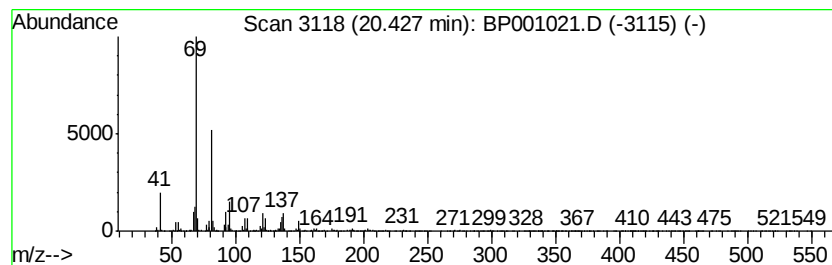
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	2.95 ng	413741	Perylene-d12	21.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Supraene		410 C30H50	007683-64-9 98
2	Squalene		410 C30H50	000111-02-4 95
3	Docosa-2,6,10,14,18-pentaen-22-a...		384 C27H44O	1000163-04-7 83
4	2,6,10,14-Hexadecatetraenoic aci...		332 C22H36O2	024035-35-6 83
5	2,6,10,14-Hexadecatetraenoic aci...		318 C21H34O2	042207-88-5 78



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001021.D
Acq On : 11 Nov 2019 17:41
Operator : JU
Sample : K5760-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

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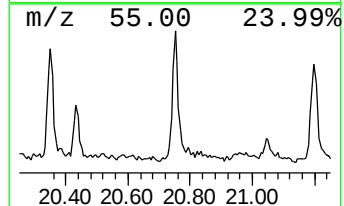
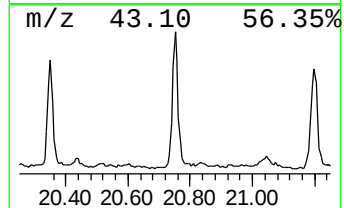
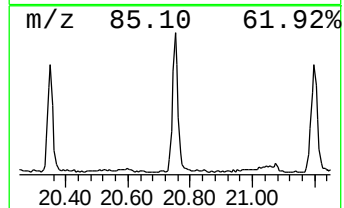
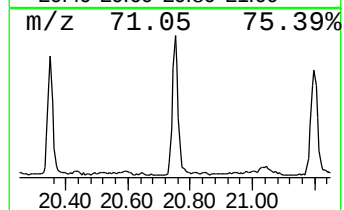
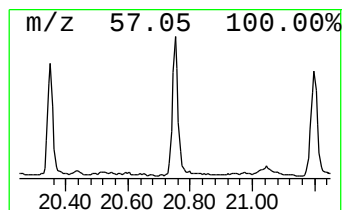
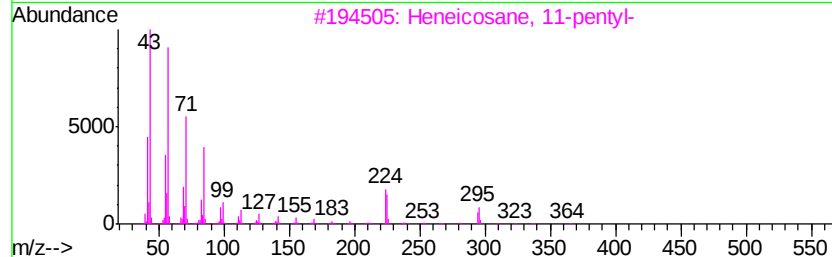
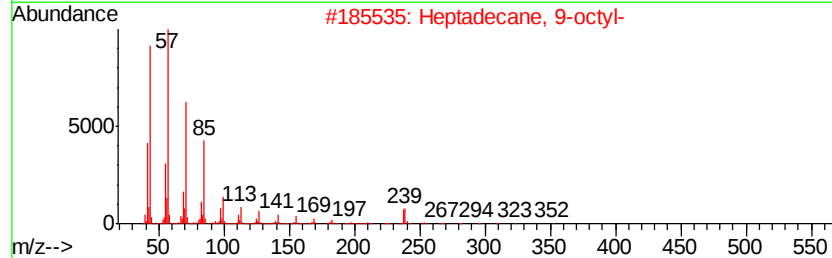
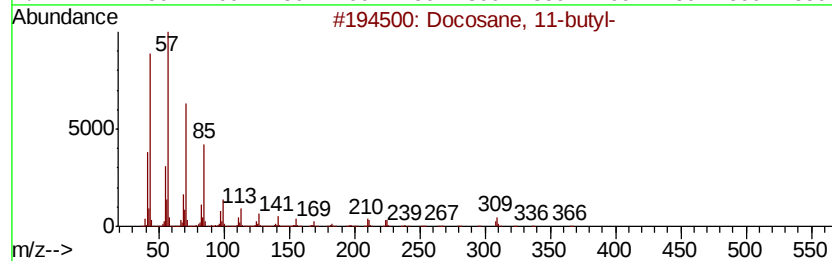
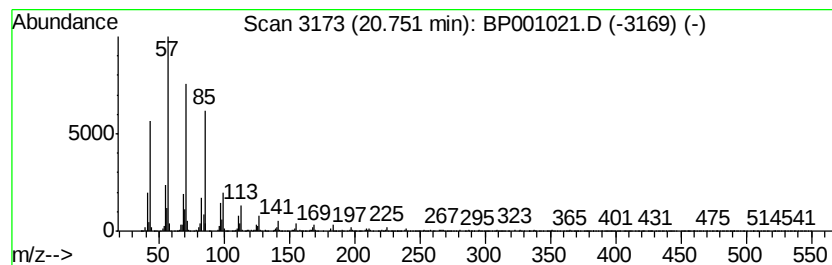
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane, 11-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	2.67 ng	373753	Perylene-d12	21.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	94
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001021.D
Acq On : 11 Nov 2019 17:41
Operator : JU
Sample : K5760-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

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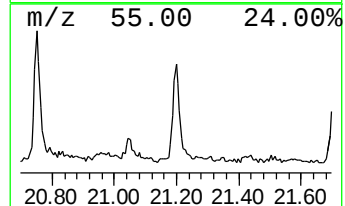
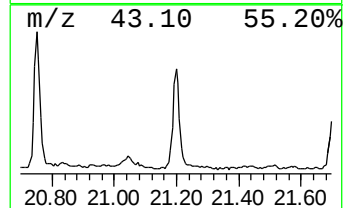
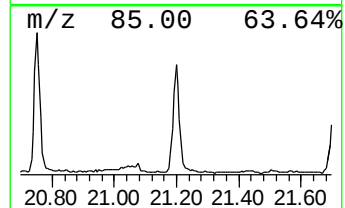
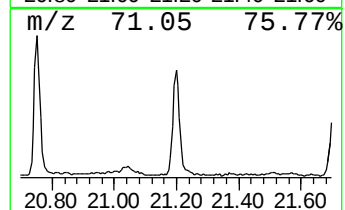
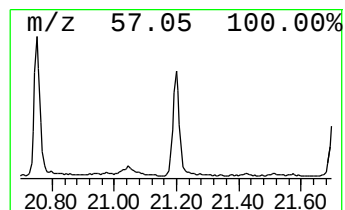
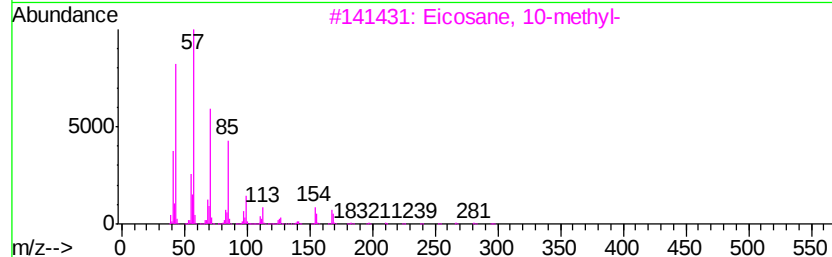
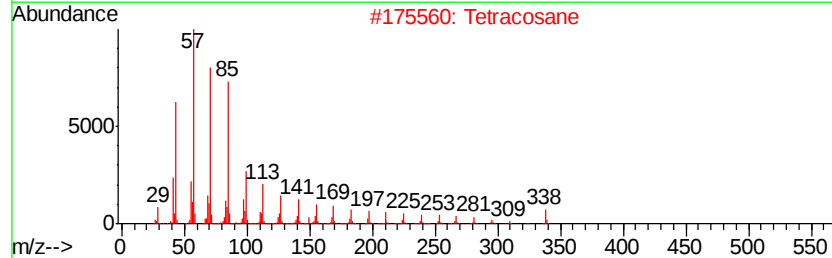
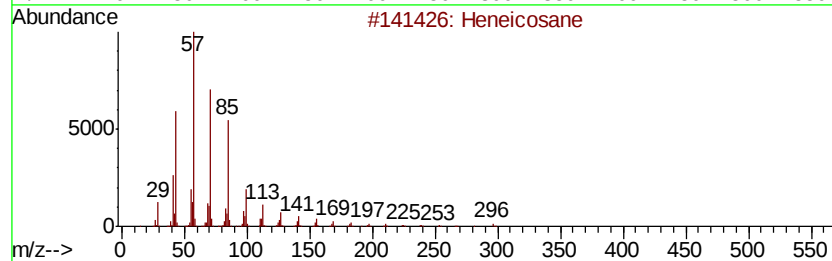
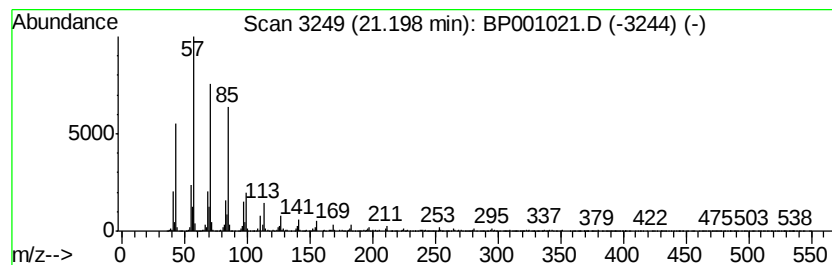
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.20	2.18 ng	305508	Perylene-d12	21.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Tetracosane	338	C24H50	000646-31-1	95
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
4			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111119\
Data File : BP001021.D
Acq On : 11 Nov 2019 17:41
Operator : JU
Sample : K5760-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

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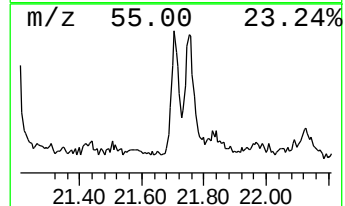
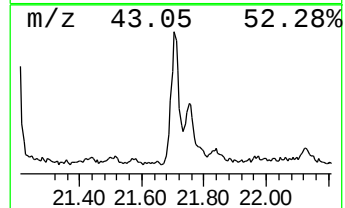
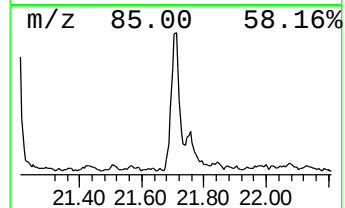
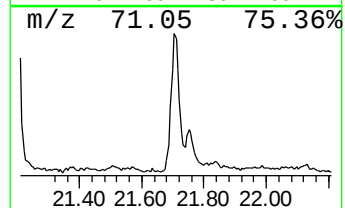
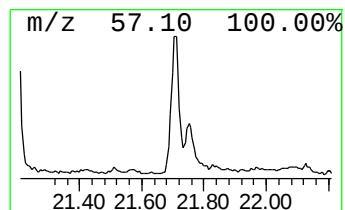
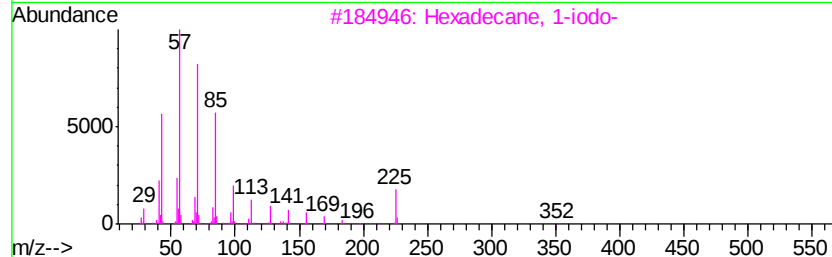
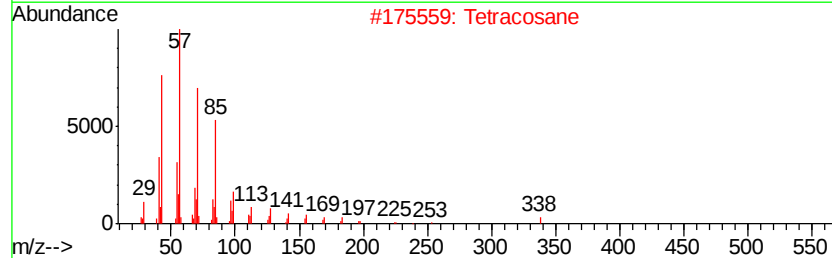
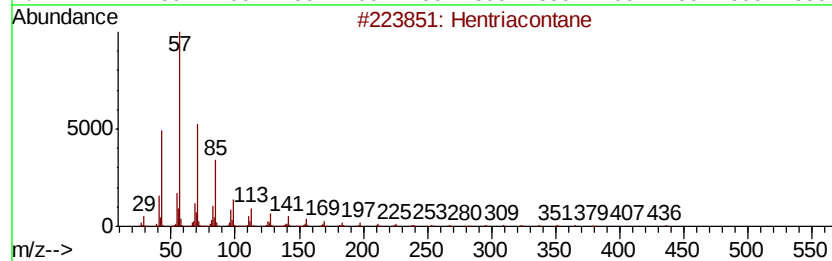
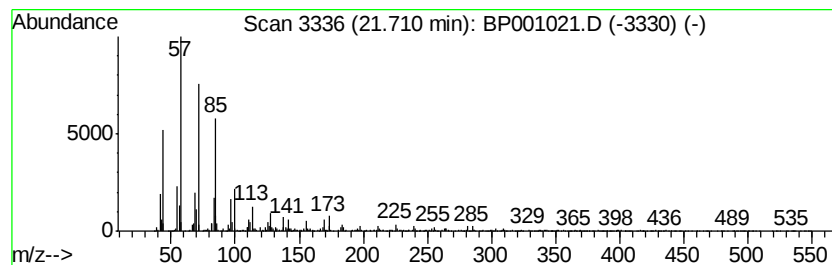
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.71	2.03 ng	284073	Perylene-d12	21.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	97
2		Tetracosane	338	C24H50	000646-31-1	94
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
4		Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP111119\
Data File : BP001021.D
Acq On : 11 Nov 2019 17:41
Operator : JU
Sample : K5760-12
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
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
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2-Pentanone, 4-hy...	5.73	9.8	ng	724596	1	8.37	1471910	20.0
unknown8.01	8.01	65.8	ng	4839890	1	8.37	1471910	20.0
n-Hexadecanoic acid	16.53	3.5	ng	450230	4	15.65	2552450	20.0
Retene	18.11	2.1	ng	311870	5	19.29	2930640	20.0
5-Eicosene, (E)-	19.16	6.6	ng	964026	5	19.29	2930640	20.0
Supraene	20.43	3.0	ng	413741	6	21.07	2803000	20.0
Docosane, 11-butyl-	20.75	2.7	ng	373753	6	21.07	2803000	20.0
Heneicosane	21.20	2.2	ng	305508	6	21.07	2803000	20.0
Hentriacontane	21.71	2.0	ng	284073	6	21.07	2803000	20.0