

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
 Data File : BF111292.D
 Acq On : 11 Dec 2018 22:50
 Operator : JU/SJ
 Sample : J6157-10
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-5-DISSOLVED

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_F\METHODS\8270-BF120818.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	2.816	118	124	132	rVB	157620	261010	5.19%	0.678%
2	3.787	285	289	293	rBV	39631	57691	1.15%	0.150%
3	4.028	322	330	336	rBV	60603	81684	1.63%	0.212%
4	4.981	486	492	501	rVB2	179529	238194	4.74%	0.618%
5	5.404	560	564	571	rBV	925278	907813	18.06%	2.357%
6	5.916	648	651	655	rVB	78867	65299	1.30%	0.170%
7	6.416	733	736	749	rBV2	677496	938221	18.67%	2.436%
8	6.557	757	760	764	rBV	1601861	1402323	27.90%	3.641%
9	6.793	797	800	804	rBV	1609725	1321112	26.28%	3.430%
10	6.951	823	827	830	rBV	3977885	3230034	64.26%	8.386%
11	7.351	890	895	898	rBV	3335365	2958605	58.86%	7.681%
12	8.075	1014	1018	1022	rBV	2526139	2108037	41.94%	5.473%
13	9.157	1197	1202	1205	rBV	5249845	5026155	100.00%	13.049%
14	9.545	1264	1268	1272	rBV	681156	510762	10.16%	1.326%
15	9.833	1313	1317	1320	rBV	2197814	1945430	38.71%	5.051%
16	10.033	1348	1351	1359	rVB2	56945	60607	1.21%	0.157%
17	10.245	1384	1387	1390	rBV	121782	102583	2.04%	0.266%
18	10.616	1446	1450	1455	rBV	1353043	1163680	23.15%	3.021%
19	11.316	1565	1569	1572	rBV	2341618	1959364	38.98%	5.087%
20	11.704	1632	1635	1641	rVB3	61204	63734	1.27%	0.165%
21	11.857	1655	1661	1676	rBV	1763752	2011703	40.02%	5.223%
22	12.539	1773	1777	1778	rBV2	71866	74782	1.49%	0.194%
23	12.557	1778	1780	1790	rVB4	60169	80480	1.60%	0.209%
24	12.639	1790	1794	1807	rBV	1381887	1387869	27.61%	3.603%
25	12.904	1834	1839	1842	rBV	4658156	3990566	79.40%	10.360%
26	13.121	1873	1876	1885	rBV6	31869	57931	1.15%	0.150%
27	13.386	1913	1921	1924	rVB6	27565	56812	1.13%	0.147%
28	13.810	1989	1993	2001	rBV	683386	937313	18.65%	2.433%
29	13.951	2013	2017	2021	rBV	2259125	1973986	39.27%	5.125%
30	14.133	2045	2048	2053	rBV	112862	121125	2.41%	0.314%
31	14.439	2097	2100	2108	rBV2	146803	193115	3.84%	0.501%
32	14.739	2148	2151	2156	rVB	180967	165127	3.29%	0.429%
33	15.068	2203	2207	2210	rBV	202033	227467	4.53%	0.591%
34	15.386	2256	2261	2267	rBV	1349346	1699335	33.81%	4.412%

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

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.445	2267	2271	2276	rVV	163877	231548	4.61%	0.601%
36	15.868	2338	2343	2348	rBV	147125	230666	4.59%	0.599%
37	15.927	2348	2353	2362	rVV4	115872	276031	5.49%	0.717%
38	16.351	2422	2425	2432	rVB2	79160	125284	2.49%	0.325%
39	16.592	2462	2466	2473	rVB2	109445	186824	3.72%	0.485%
40	17.504	2616	2621	2622	rBV4	48438	87417	1.74%	0.227%

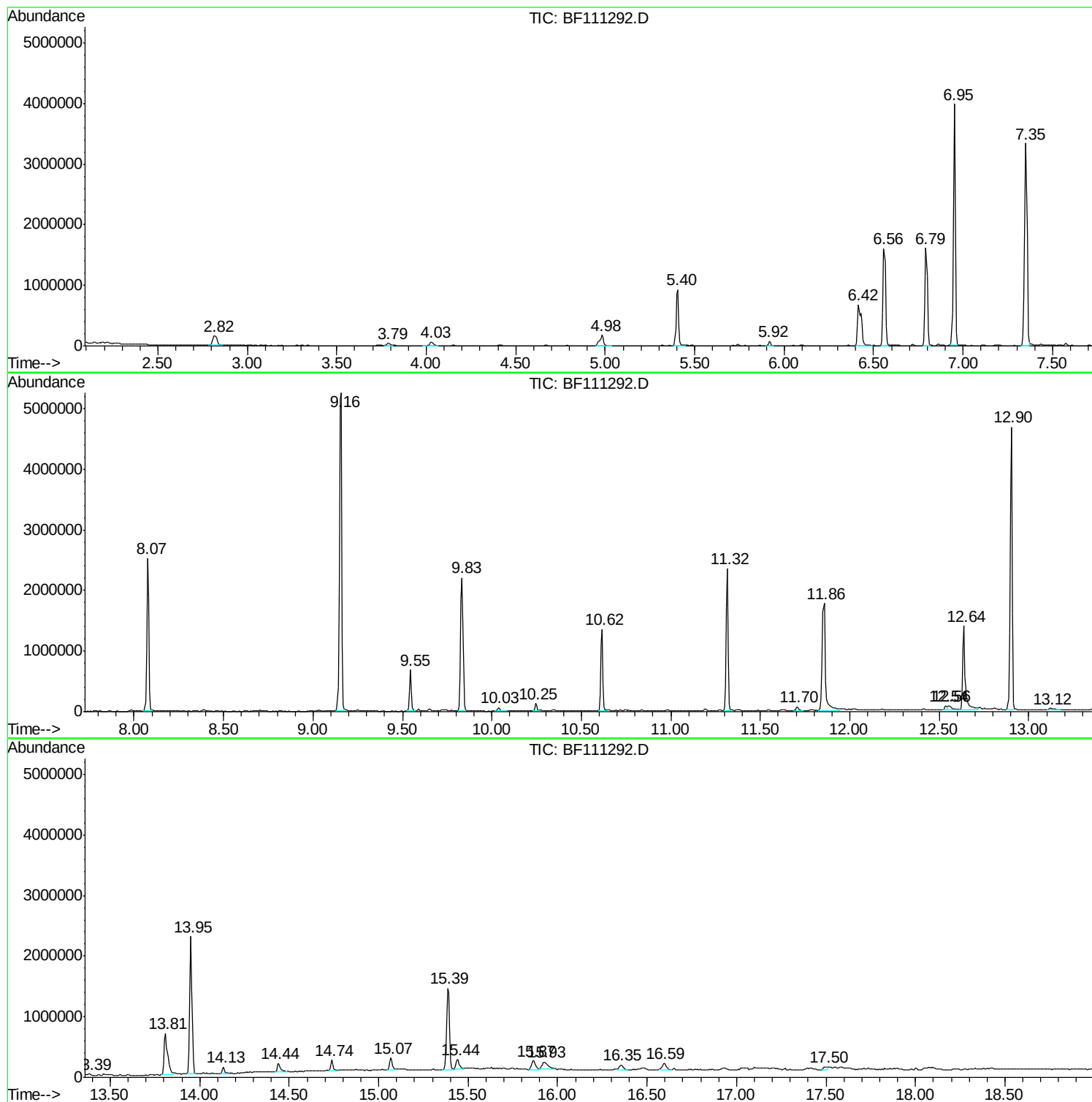
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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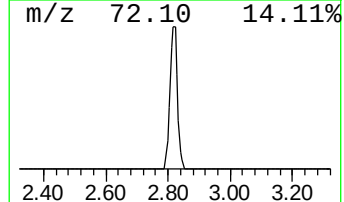
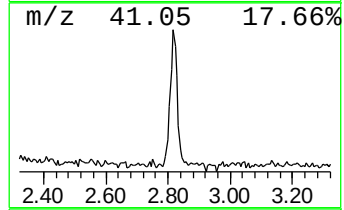
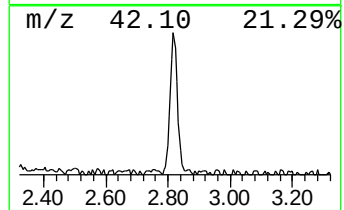
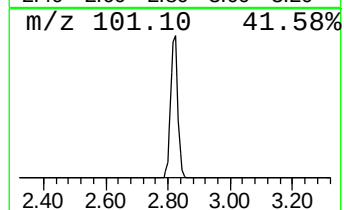
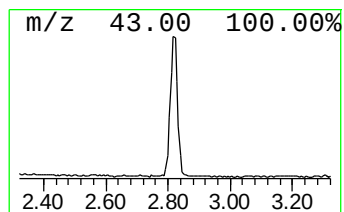
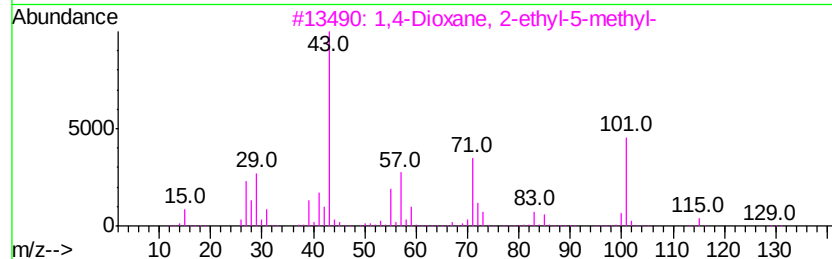
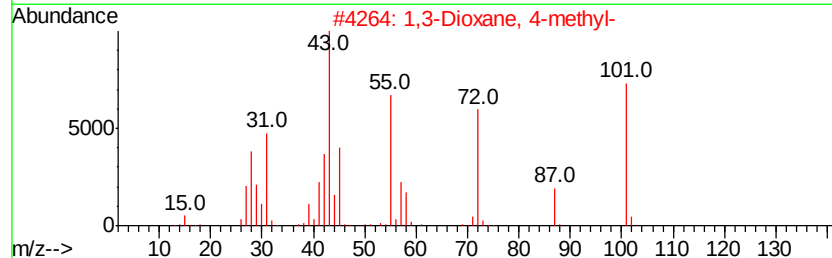
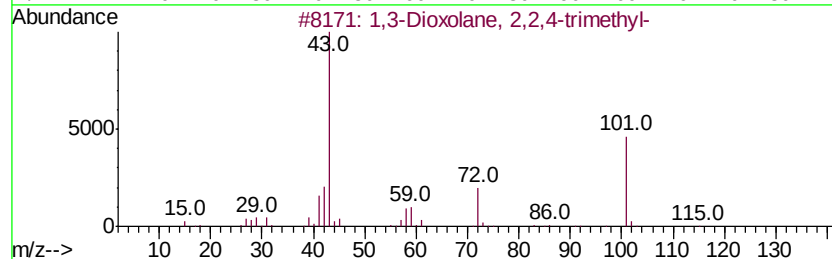
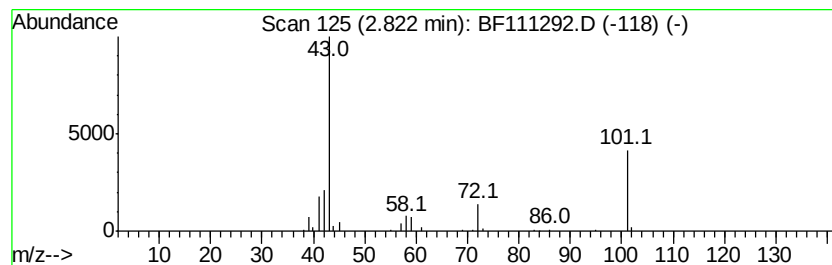
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.82	3.95 ng	261010	1,4-Dichlorobenzene-d4	6.79

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	64
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	42
3		1,4-Dioxane, 2-ethyl-5-methyl-	130	C7H14O2	053907-91-8	36
4		1,3-Dioxolane-4-carboxaldehyde, ...	130	C6H10O3	015186-48-8	33
5		Ethanethioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	10



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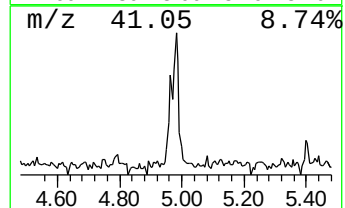
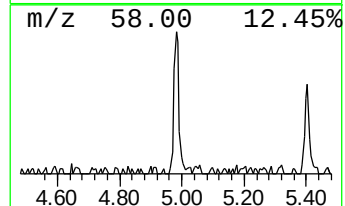
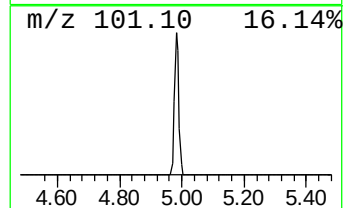
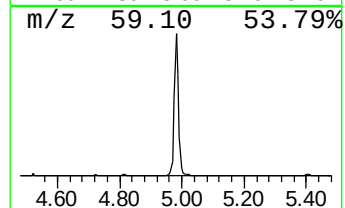
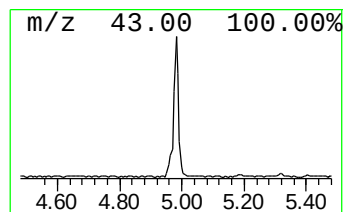
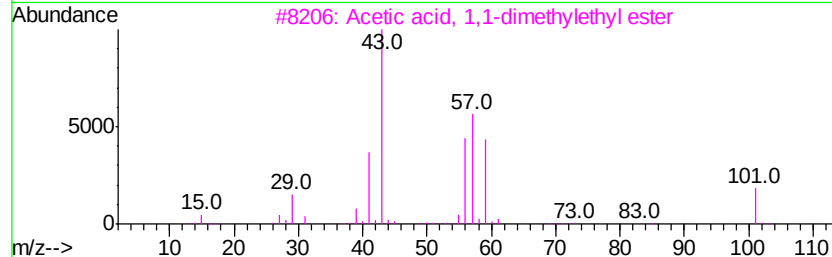
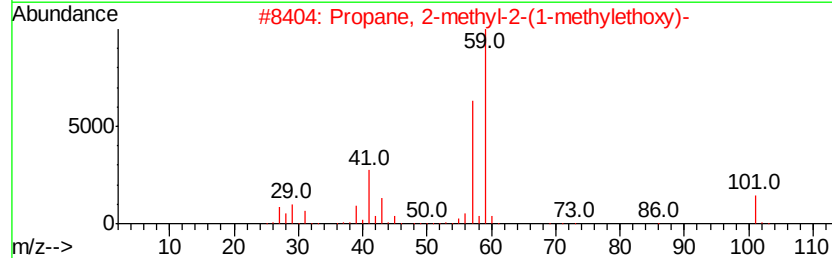
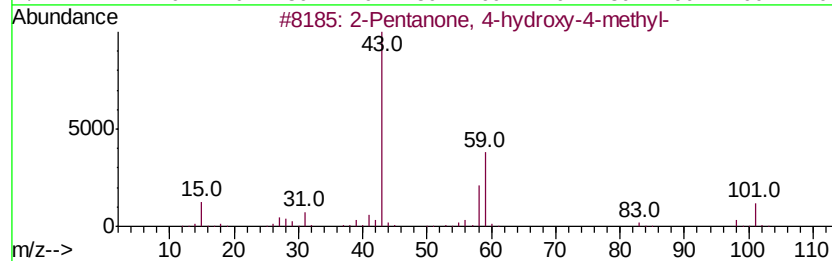
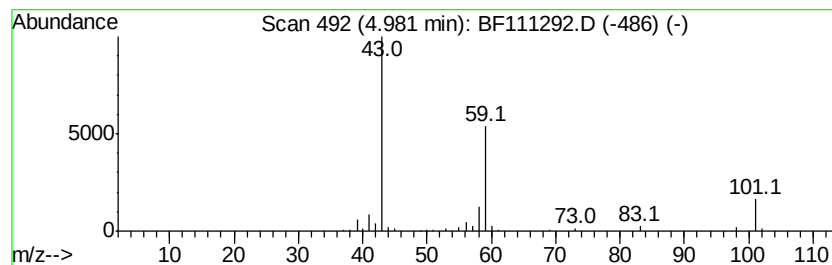
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	3.61 ng	238194	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25



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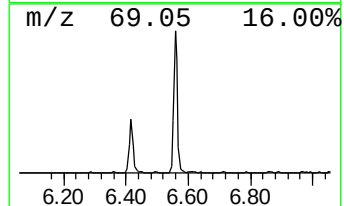
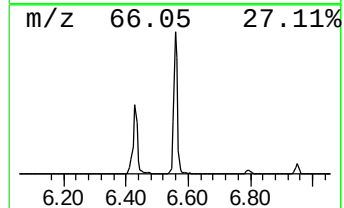
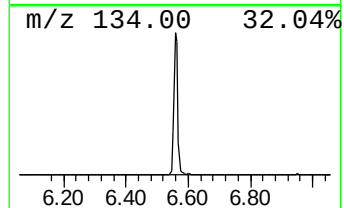
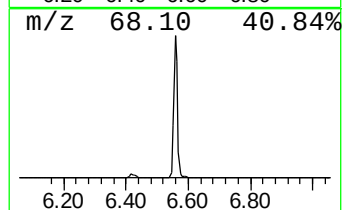
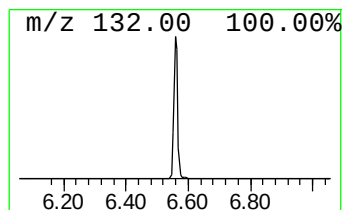
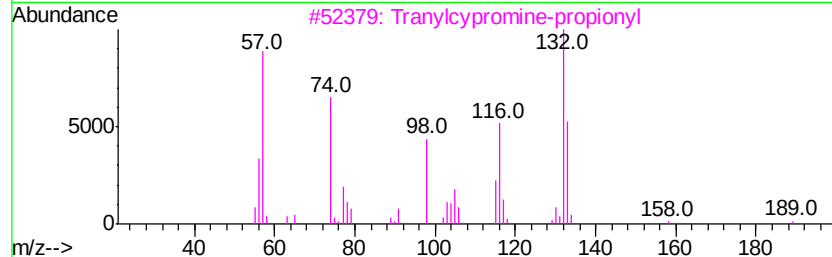
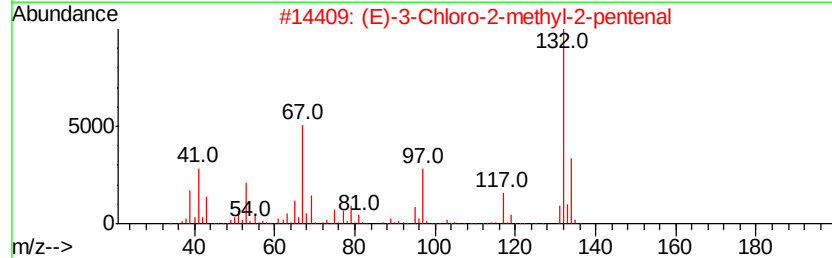
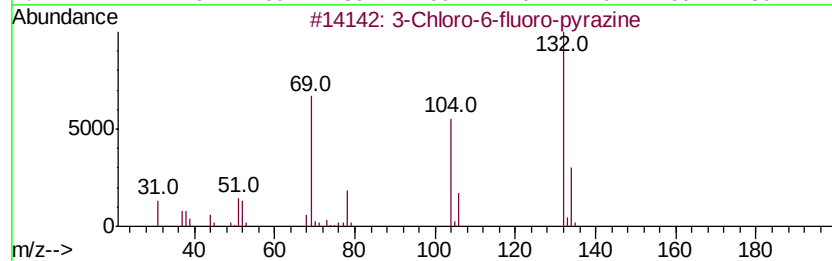
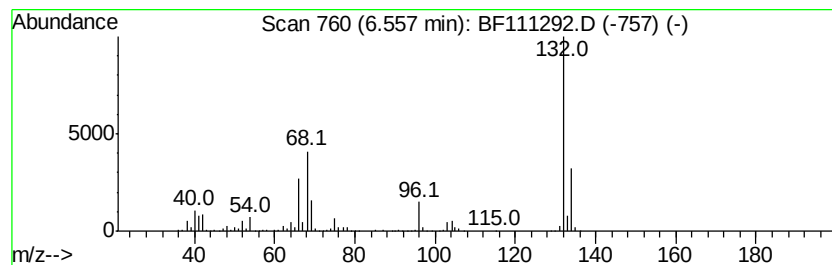
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	21.23 ng	1402320	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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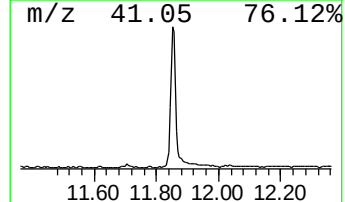
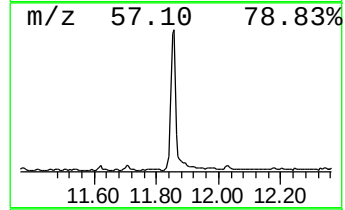
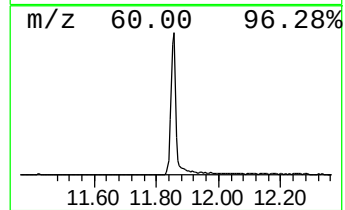
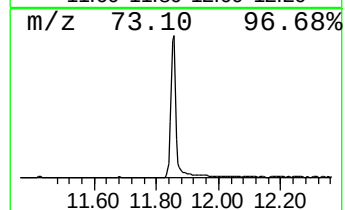
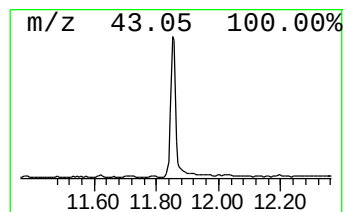
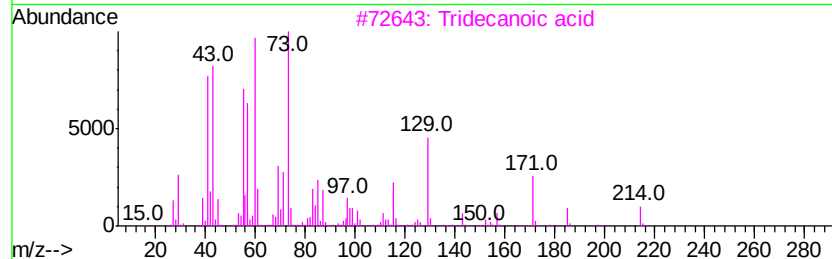
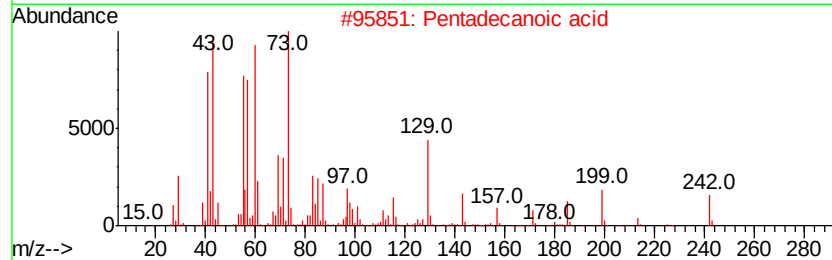
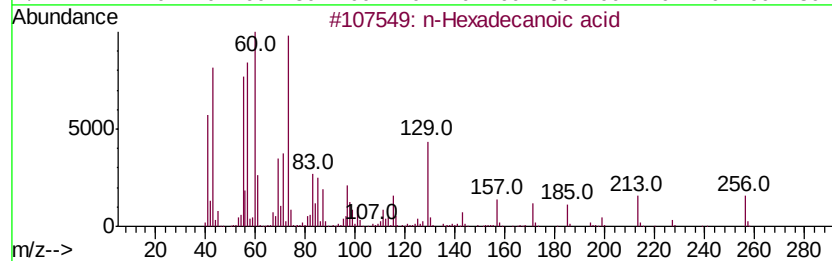
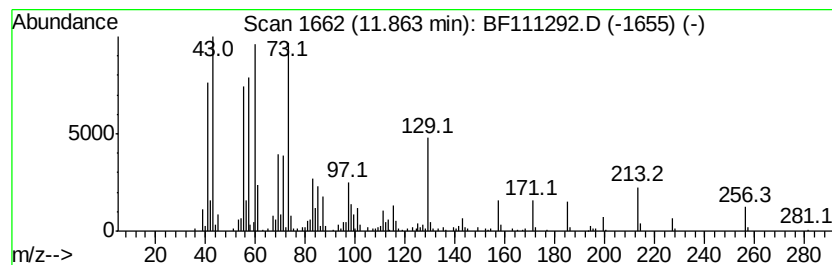
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	20.53 ng	2011700	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	38



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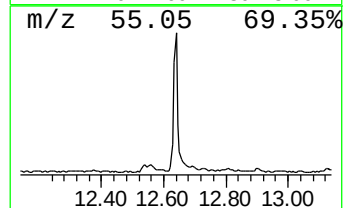
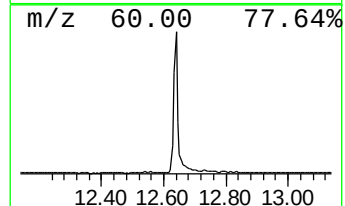
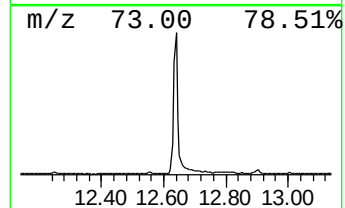
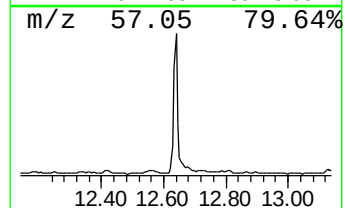
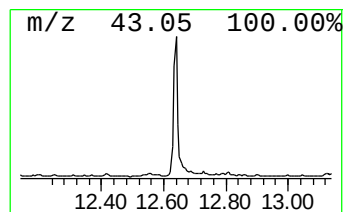
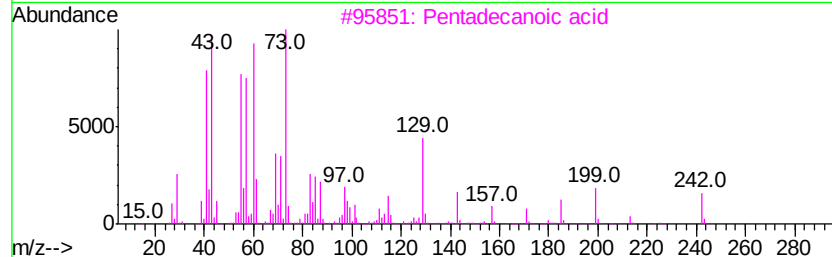
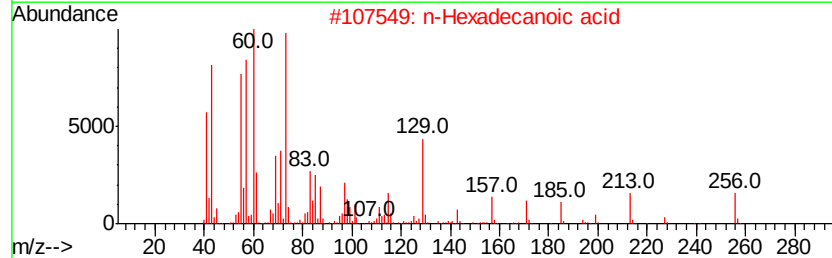
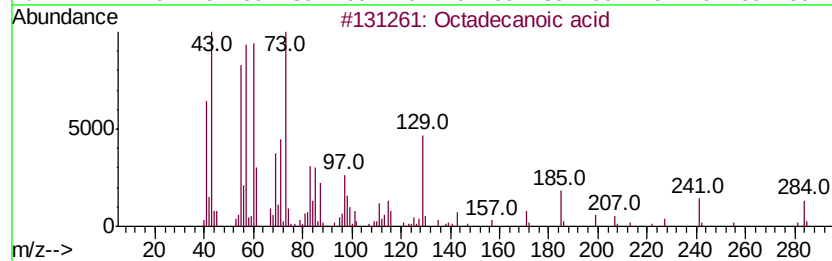
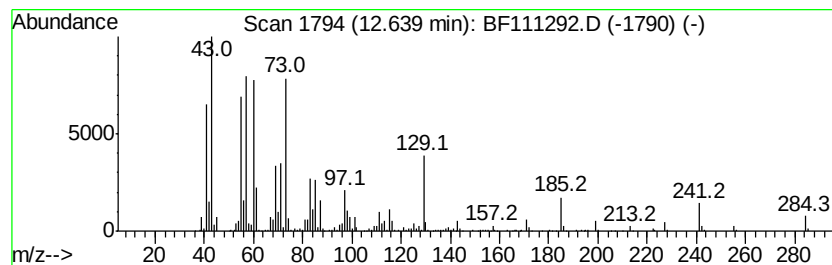
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	14.06 ng	1387870	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	72



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Operator : JU/SJ
Sample : J6157-10
Misc :
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ClientSampleId :
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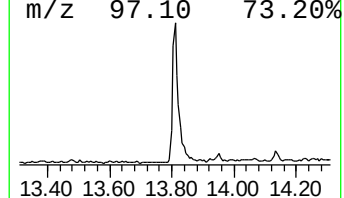
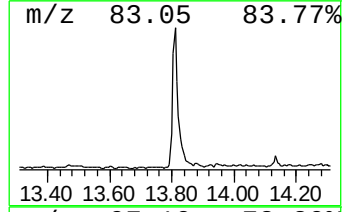
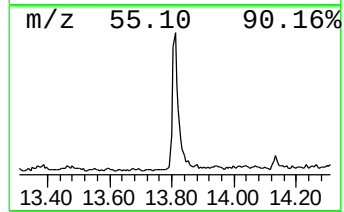
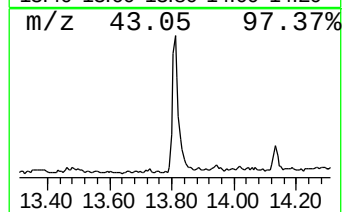
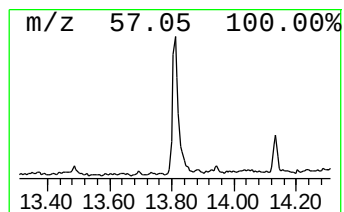
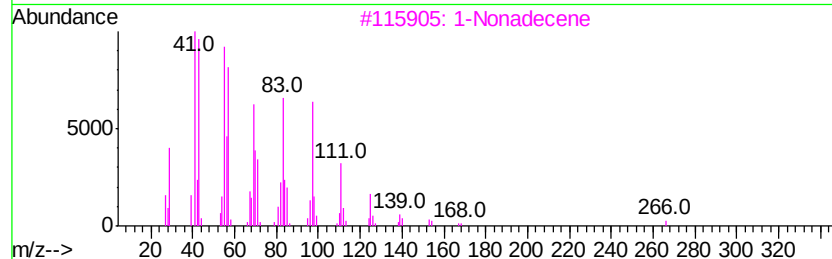
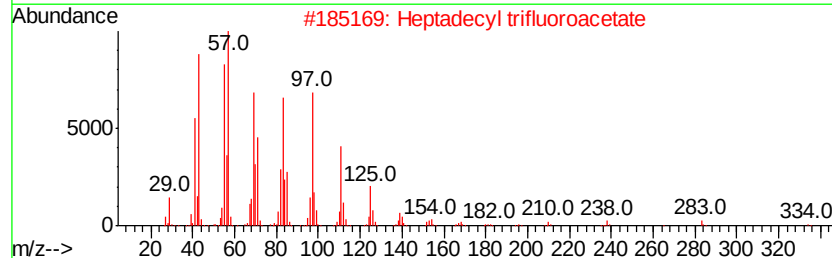
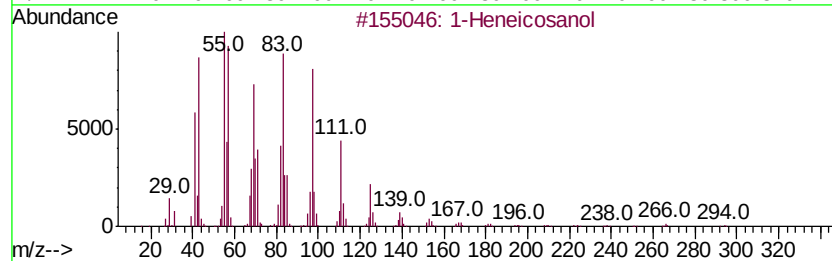
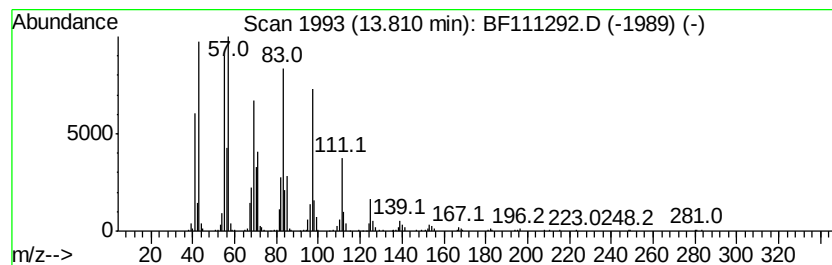
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	9.50 ng	937313	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		1-Docosene	308	C22H44	001599-67-3	91
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



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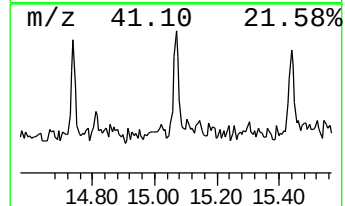
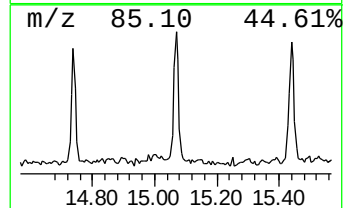
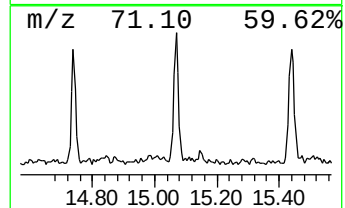
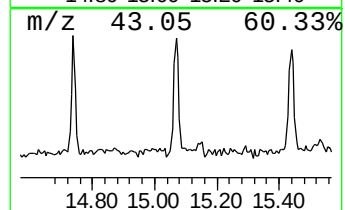
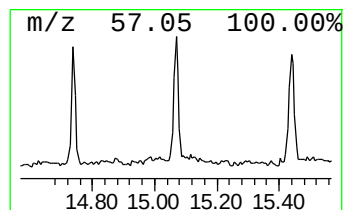
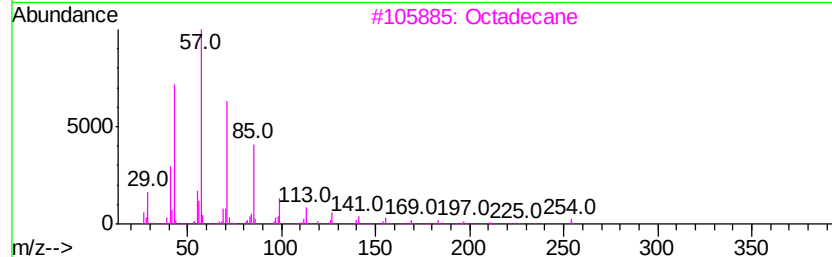
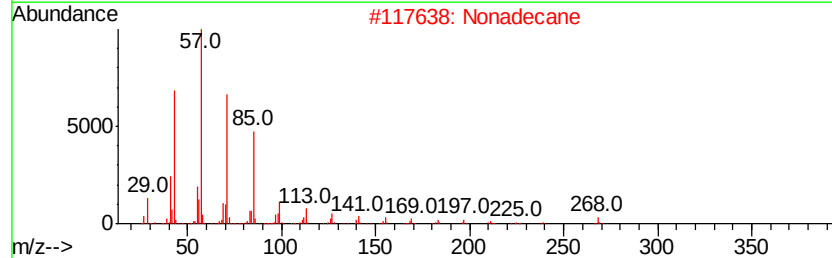
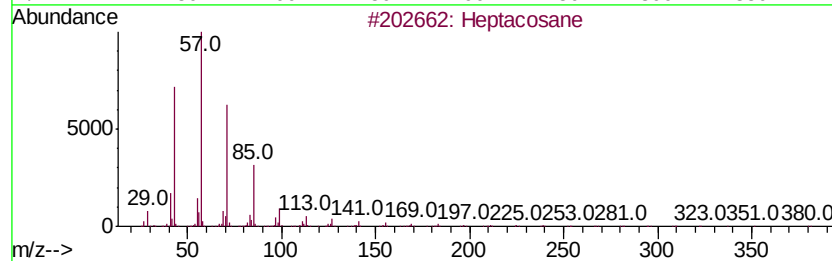
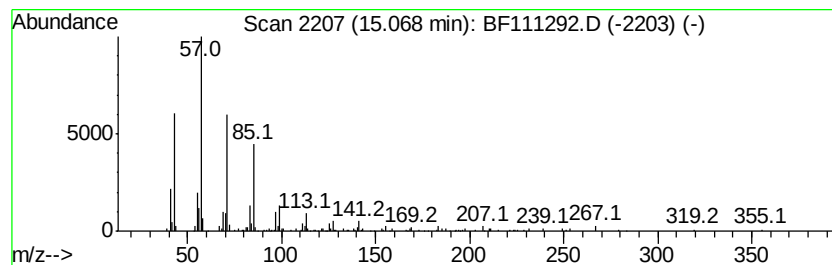
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.68 ng	227467	Perylene-d12	15.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	87
2	Nonadecane		268	C19H40	000629-92-5	86
3	Octadecane		254	C18H38	000593-45-3	86
4	Eicosane		282	C20H42	000112-95-8	86
5	Docosane		310	C22H46	000629-97-0	86



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Sample : J6157-10
Misc :
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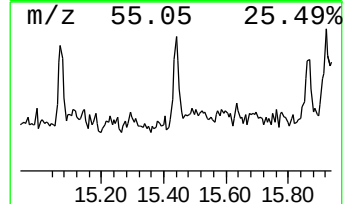
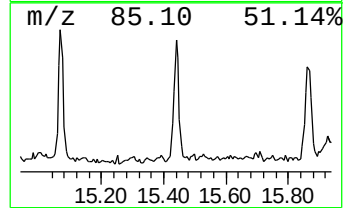
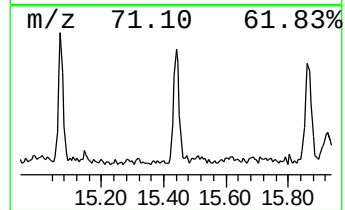
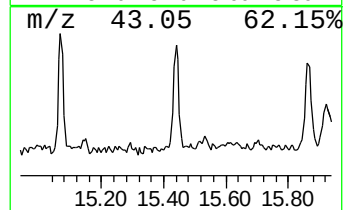
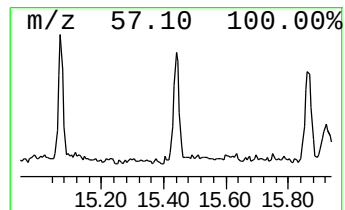
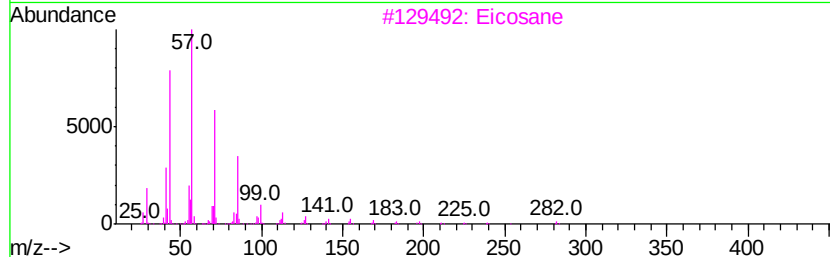
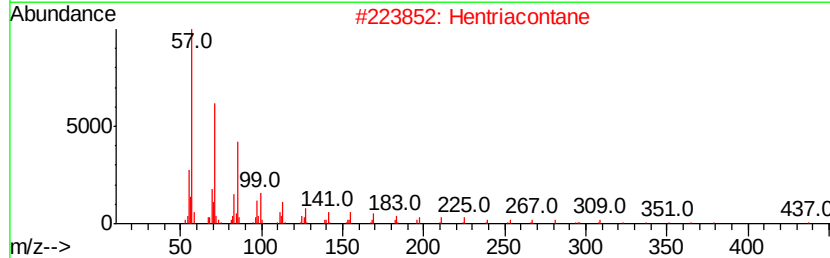
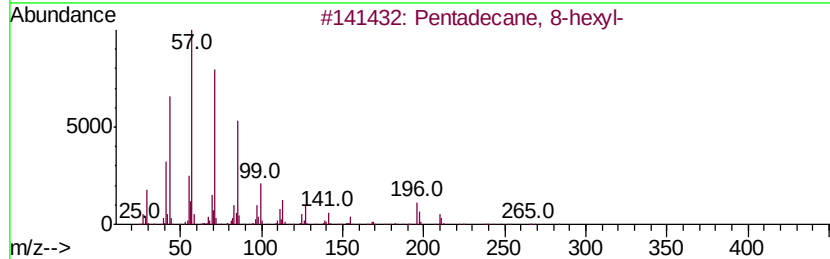
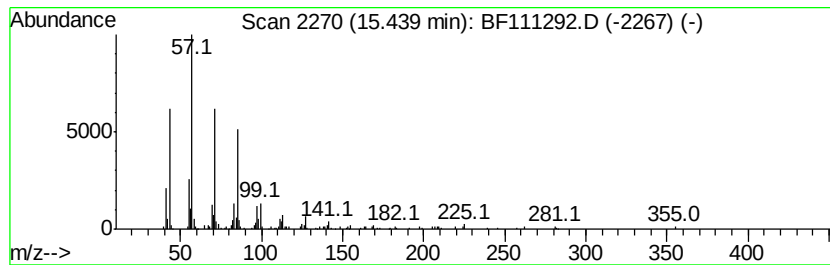
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	2.73 ng	231548	Perylene-d12	15.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pentadecane, 8-hexyl-	296 C21H44	013475-75-7 87
2		Hentriacontane	437 C31H64	000630-04-6 87
3		Eicosane	282 C20H42	000112-95-8 87
4		Pentacosane	352 C25H52	000629-99-2 86
5		Eicosane, 2-methyl-	296 C21H44	001560-84-5 86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
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Acq On : 11 Dec 2018 22:50
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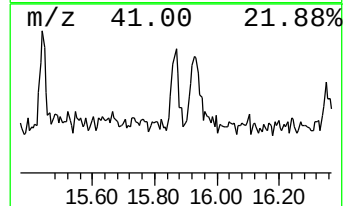
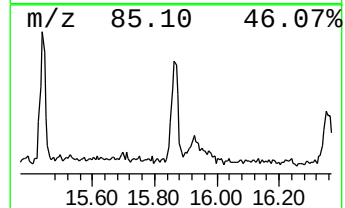
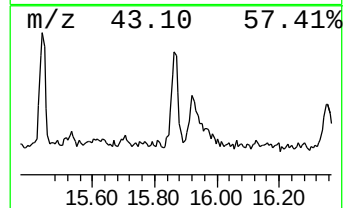
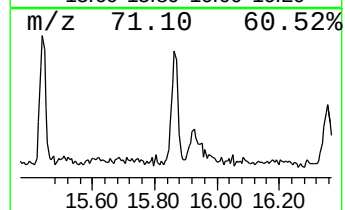
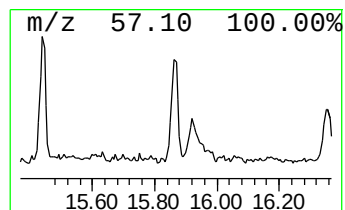
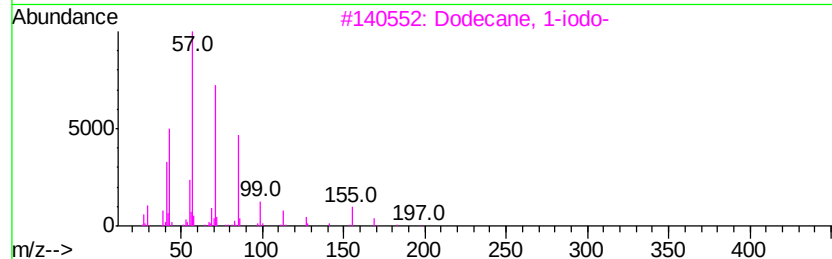
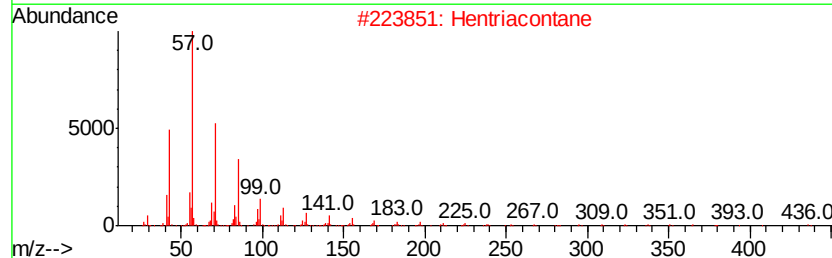
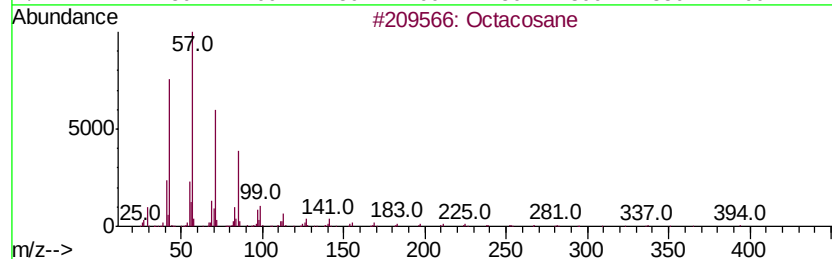
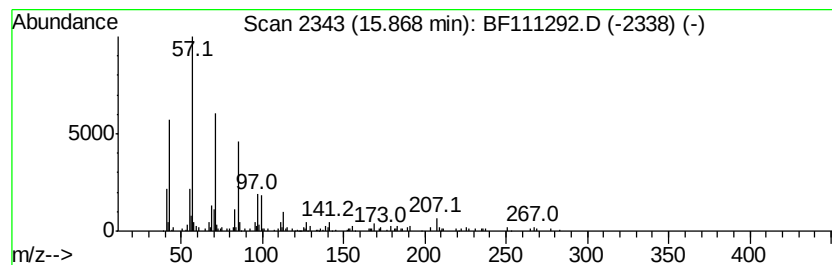
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	2.71 ng	230666	Perylene-d12	15.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Hentriacontane	437	C31H64	000630-04-6	86
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
4			Heneicosane	296	C21H44	000629-94-7	78
5			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111292.D
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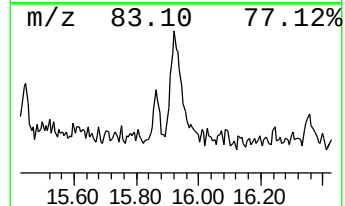
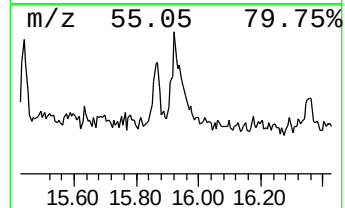
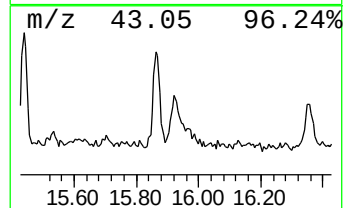
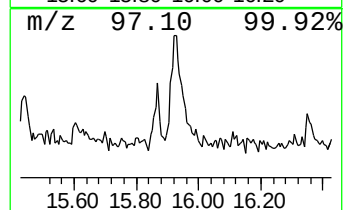
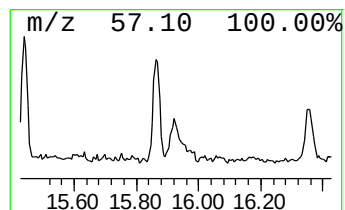
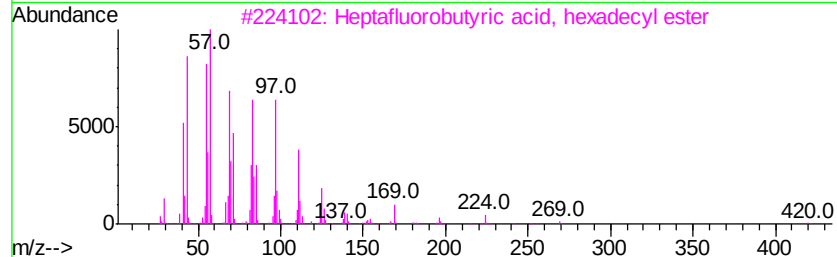
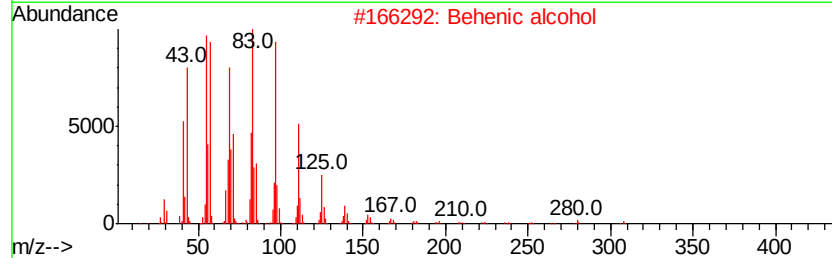
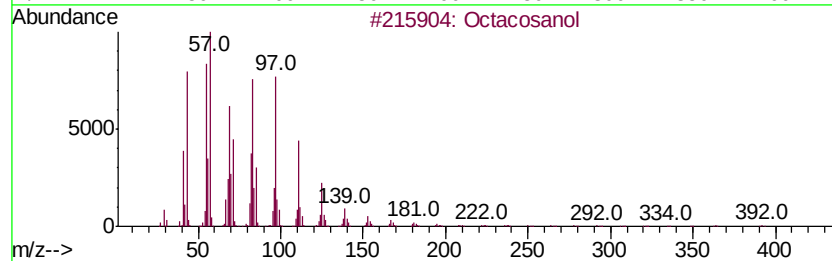
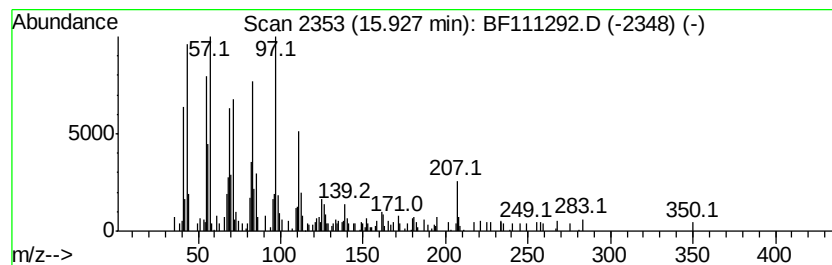
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.25 ng	276031	Perylene-d12	15.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	90
2			Behenic alcohol	326	C22H46O	000661-19-8	83
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	81
4			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	81
5			Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	81



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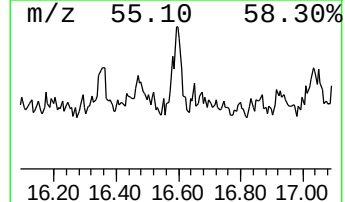
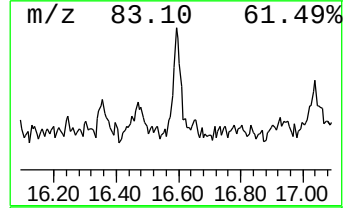
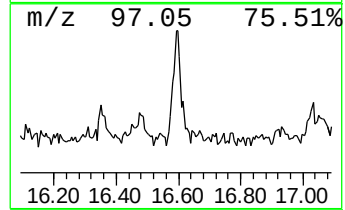
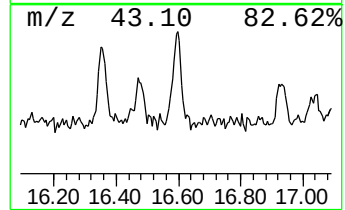
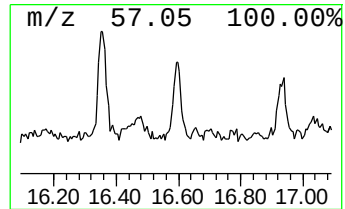
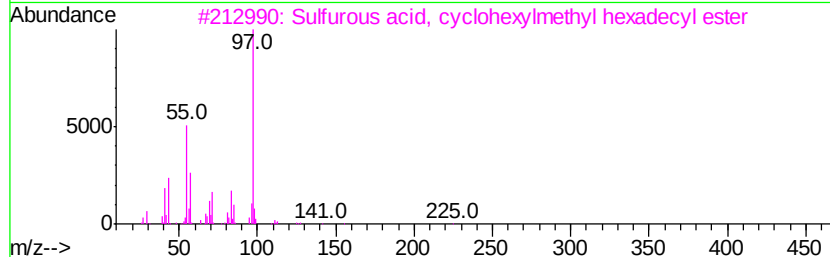
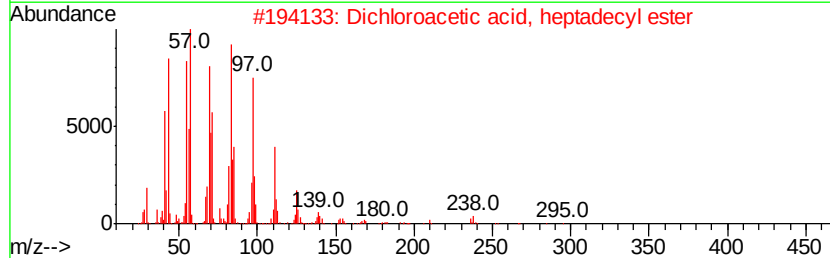
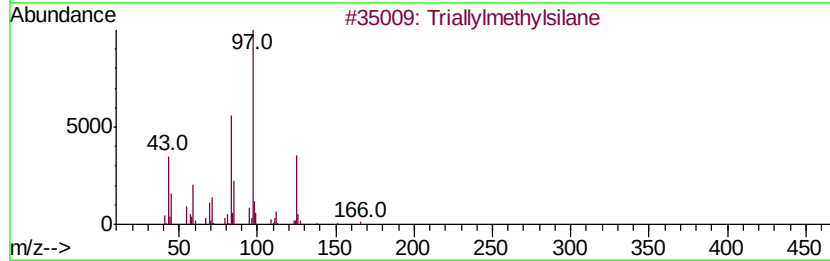
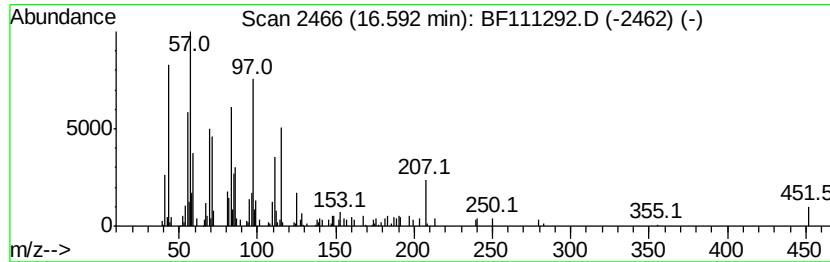
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.59 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.59	2.20 ng	186824	Perylene-d12		15.39	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triallylmethylsilane	166	C10H18Si	001112-91-0	43
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	43
3		Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	38
4		4-Isopropylidicyclohexylmethane	222	C16H30	054965-61-6	27
5		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
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Instrument :
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ClientSampleId :
COMPOSITE-5-DISSOLVED

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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
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2-Pentanone, 4-hy...	4.98	3.6	ng	238194	1	6.79	1321110	20.0
unknown6.56	6.56	21.2	ng	1402320	1	6.79	1321110	20.0
n-Hexadecanoic acid	11.86	20.5	ng	2011700	4	11.32	1959360	20.0
Octadecanoic acid	12.64	14.1	ng	1387870	5	13.95	1973990	20.0
1-Heneicosanol	13.81	9.5	ng	937313	5	13.95	1973990	20.0
Heptacosane	15.07	2.7	ng	227467	6	15.39	1699340	20.0
Pentadecane, 8-he...	15.44	2.7	ng	231548	6	15.39	1699340	20.0
Octacosane	15.87	2.7	ng	230666	6	15.39	1699340	20.0
Octacosanol	15.93	3.3	ng	276031	6	15.39	1699340	20.0
unknown16.59	16.59	2.2	ng	186824	6	15.39	1699340	20.0