

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
 Data File : BF111285.D
 Acq On : 11 Dec 2018 19:02
 Operator : JU/SJ
 Sample : J6157-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-2-TOTAL

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	2.822	119	125	133	rVB	263436	431728	8.08%	0.785%
2	4.034	326	331	335	rVB	59937	74566	1.40%	0.136%
3	4.357	381	386	394	rBV	1408819	1591232	29.78%	2.892%
4	4.987	486	493	499	rBV	688935	720702	13.49%	1.310%
5	5.404	560	564	579	rBV	1897300	1692741	31.68%	3.077%
6	5.922	648	652	654	rVB	75258	65373	1.22%	0.119%
7	6.422	733	737	738	rBV	1368626	1318245	24.67%	2.396%
8	6.434	738	739	746	rVB	1552565	894798	16.75%	1.626%
9	6.563	757	761	765	rBV	3572150	2980892	55.79%	5.418%
10	6.798	797	801	804	rBV	1911100	1696985	31.76%	3.084%
11	6.863	809	812	819	rBV	79151	80084	1.50%	0.146%
12	6.951	823	827	831	rBV	4183735	3628698	67.92%	6.596%
13	7.351	891	895	898	rBV	3520105	3182645	59.57%	5.785%
14	7.575	930	933	937	rVB	84513	74579	1.40%	0.136%
15	8.081	1015	1019	1022	rBV	2613626	2364839	44.26%	4.298%
16	8.392	1069	1072	1077	rBV	56244	64855	1.21%	0.118%
17	9.157	1197	1202	1205	rBV	6461563	5342778	100.00%	9.711%
18	9.551	1264	1269	1272	rBV	1611281	1458398	27.30%	2.651%
19	9.833	1313	1317	1321	rVB2	3004538	2515314	47.08%	4.572%
20	10.039	1348	1352	1355	rBV	87409	87117	1.63%	0.158%
21	10.251	1384	1388	1390	rBV	191890	149523	2.80%	0.272%
22	10.616	1446	1450	1454	rBV	2796751	2469420	46.22%	4.488%
23	11.316	1565	1569	1573	rBV	3155025	2584895	48.38%	4.698%
24	11.710	1632	1636	1639	rVB2	143262	128580	2.41%	0.234%
25	11.857	1655	1661	1676	rBV	2897949	3236295	60.57%	5.882%
26	12.539	1773	1777	1779	rBV2	123367	134821	2.52%	0.245%
27	12.557	1779	1780	1786	rVB3	93687	95518	1.79%	0.174%
28	12.639	1789	1794	1807	rBV	1998845	2085252	39.03%	3.790%
29	12.904	1835	1839	1842	rBV	5282937	4651079	87.05%	8.454%
30	13.374	1914	1919	1924	rBV8	64615	149483	2.80%	0.272%
31	13.810	1989	1993	1999	rBV2	687656	976920	18.28%	1.776%
32	13.957	2013	2018	2021	rBV	2479347	2534967	47.45%	4.608%
33	14.133	2046	2048	2052	rBV2	88978	79954	1.50%	0.145%
34	14.445	2098	2101	2107	rVB	198020	211909	3.97%	0.385%

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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	14.751	2150	2153	2158	rVB	316305	371071	6.95%	0.674%
36	15.080	2205	2209	2212	rVB	443079	487778	9.13%	0.887%
37	15.398	2258	2263	2268	rBV	1489172	1910662	35.76%	3.473%
38	15.451	2268	2272	2278	rVB	524665	651510	12.19%	1.184%
39	15.880	2340	2345	2350	rBV	510092	767911	14.37%	1.396%
40	16.368	2423	2428	2433	rBV	394719	646072	12.09%	1.174%
41	16.945	2521	2526	2535	rVB	216976	427120	7.99%	0.776%

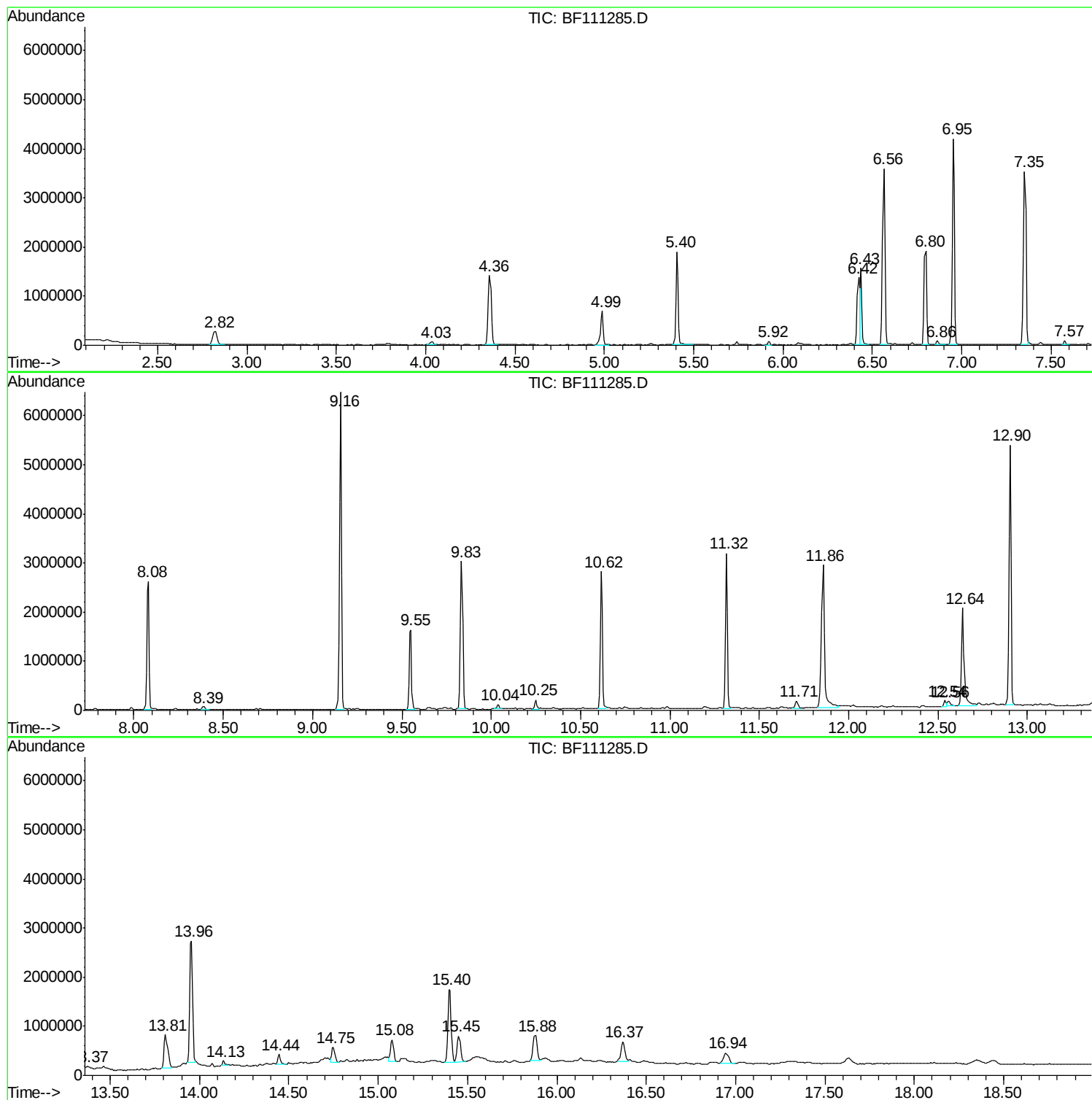
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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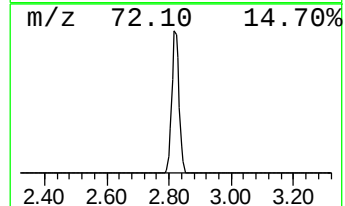
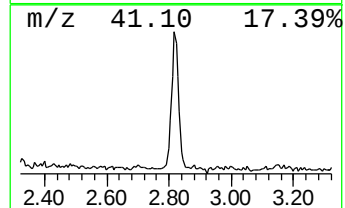
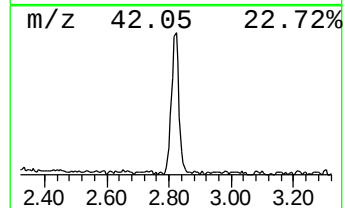
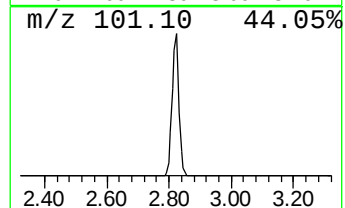
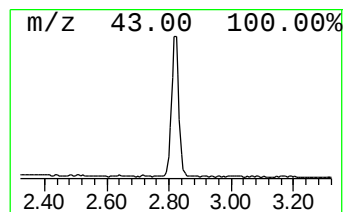
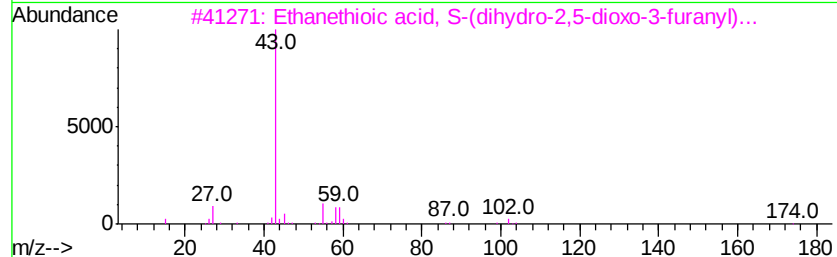
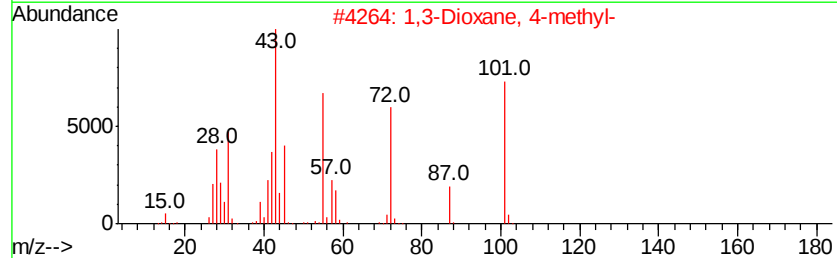
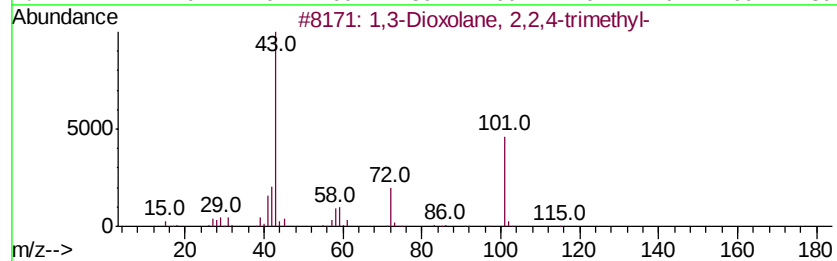
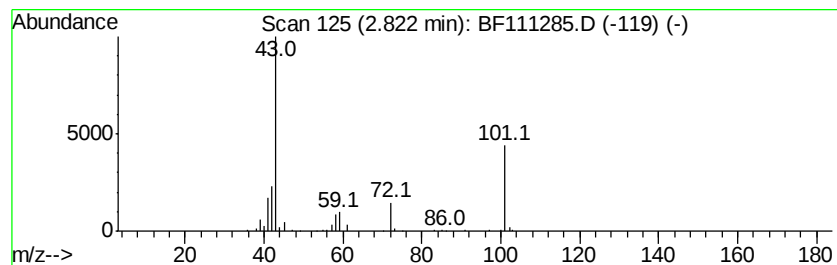
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.82	5.09 ng	431728	1,4-Dichlorobenzene-d4	6.80

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	33
3		Ethanethioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	10
4		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
5		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9



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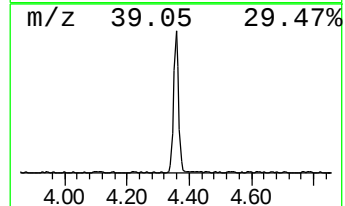
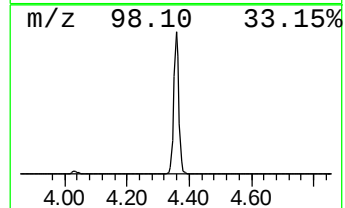
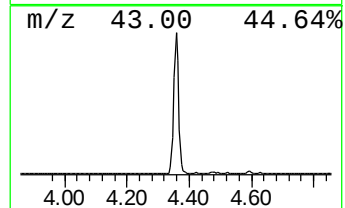
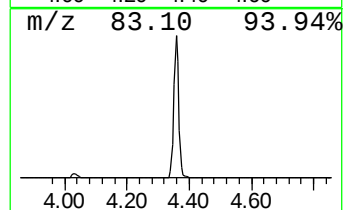
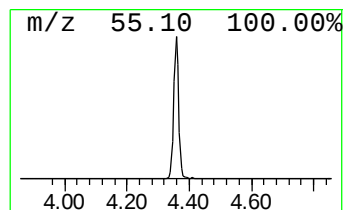
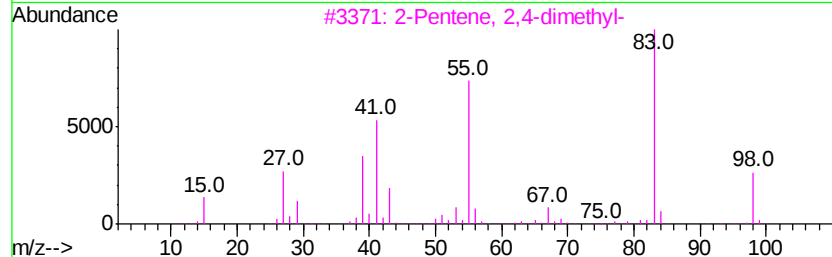
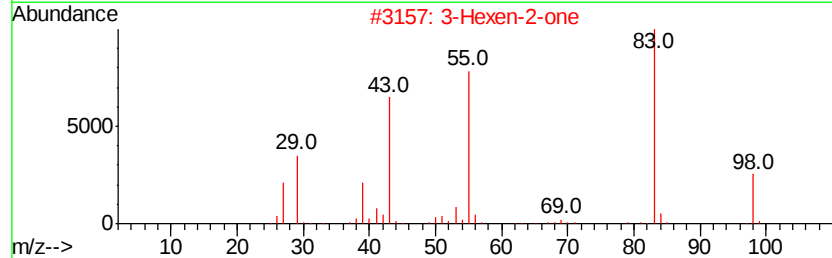
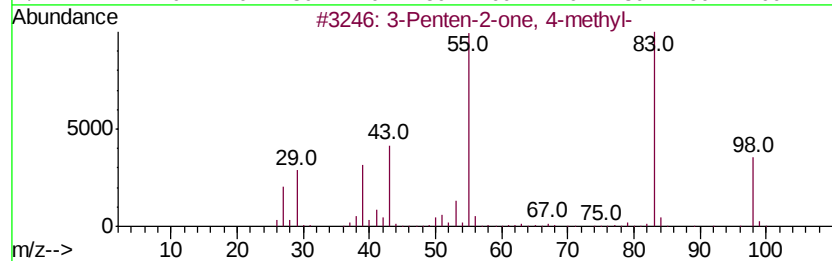
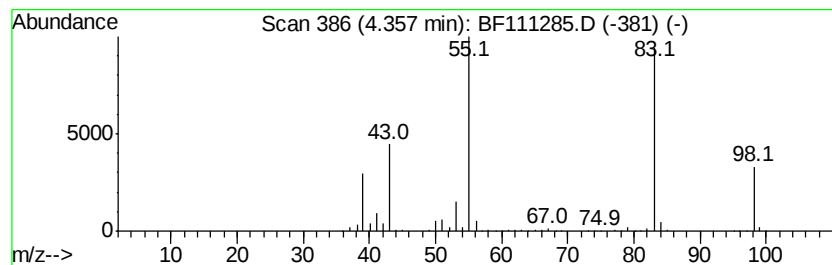
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	18.75 ng	1591230	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72



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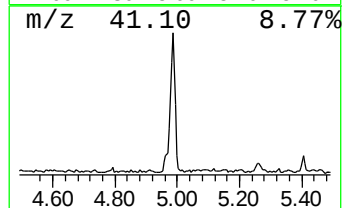
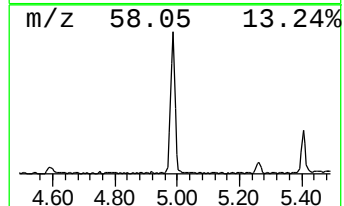
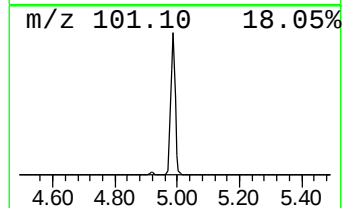
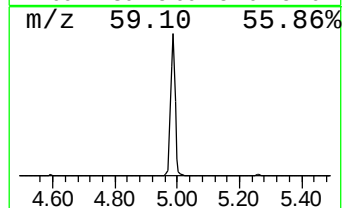
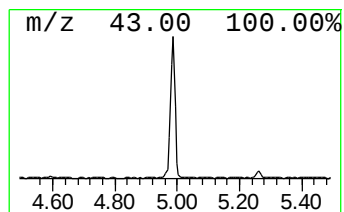
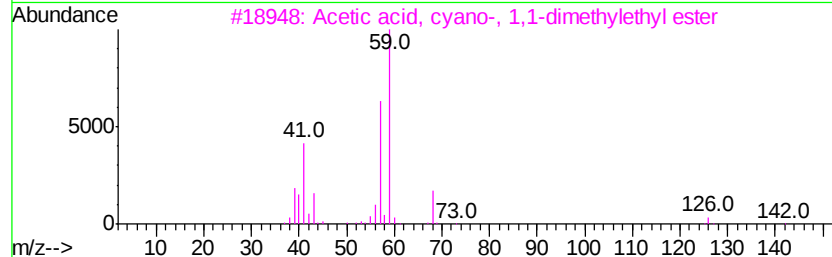
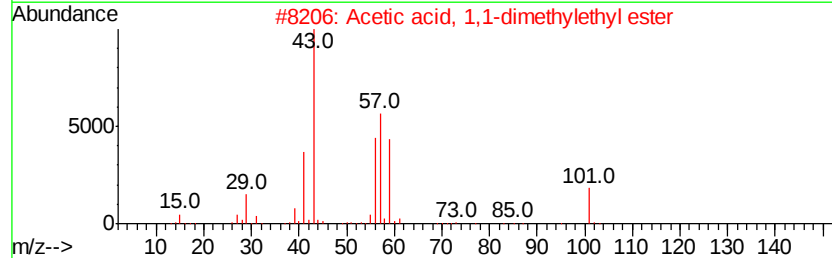
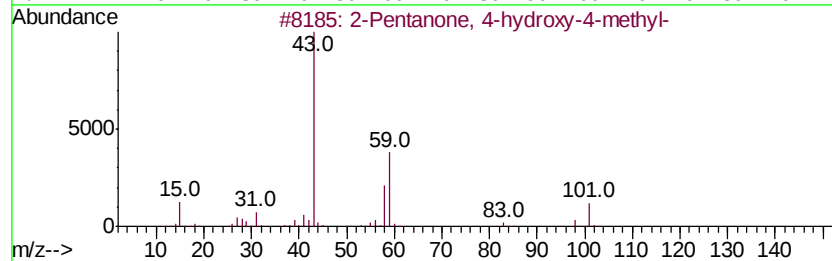
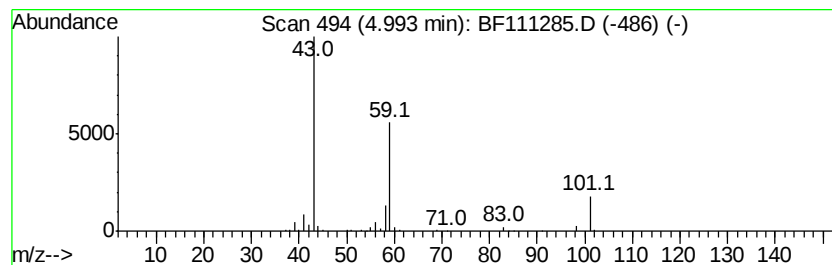
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	8.49 ng	720702	1,4-Dichlorobenzene-d4	6.80

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9



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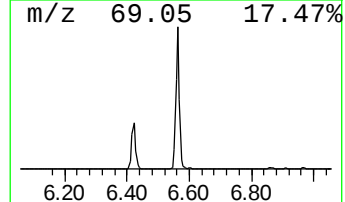
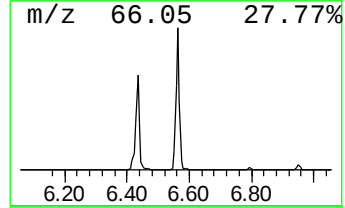
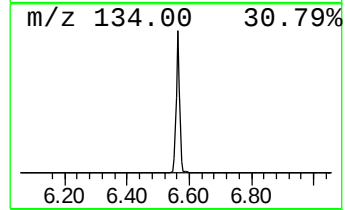
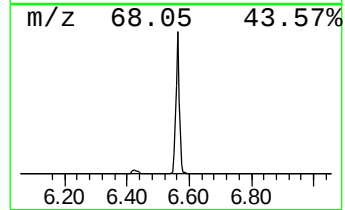
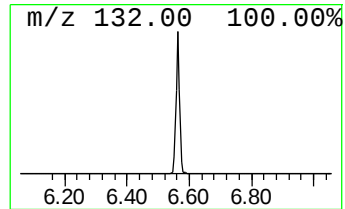
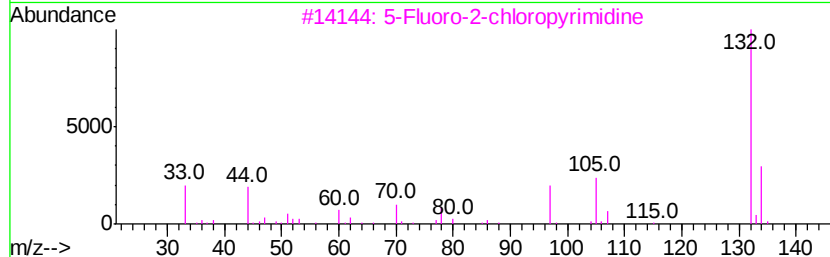
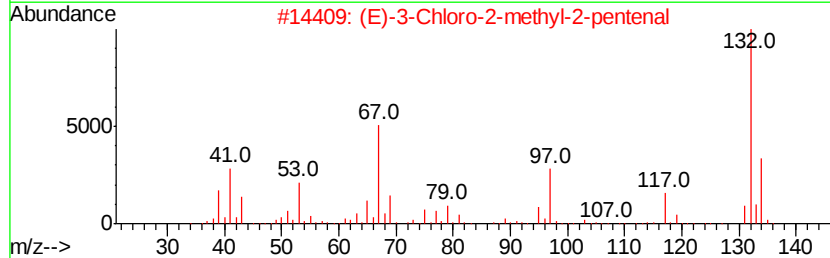
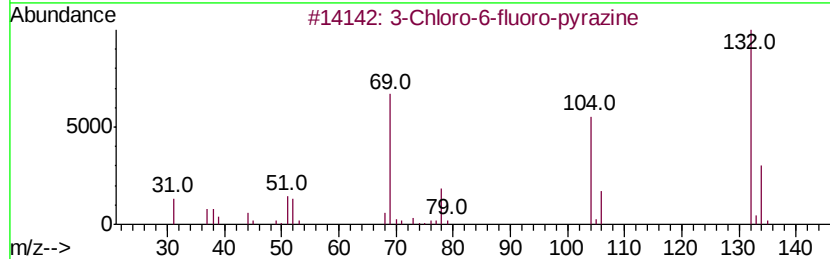
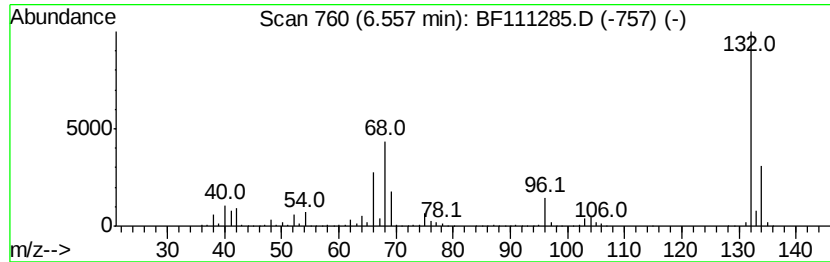
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	35.13 ng	2980890	1,4-Dichlorobenzene-d4	6.80

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	17
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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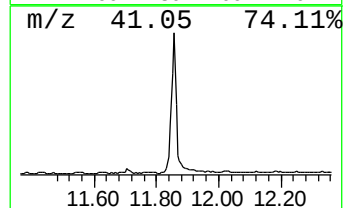
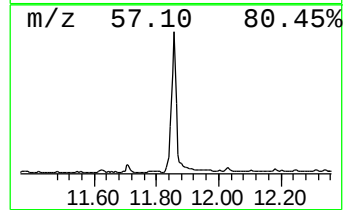
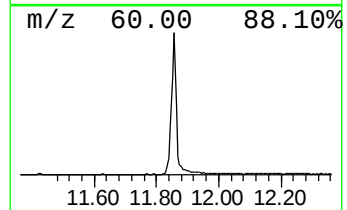
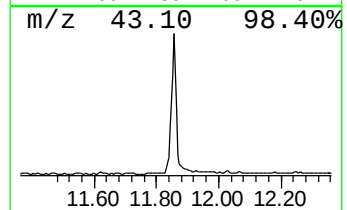
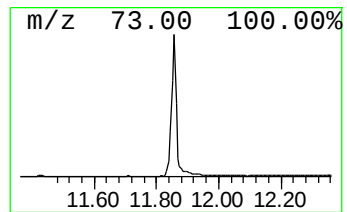
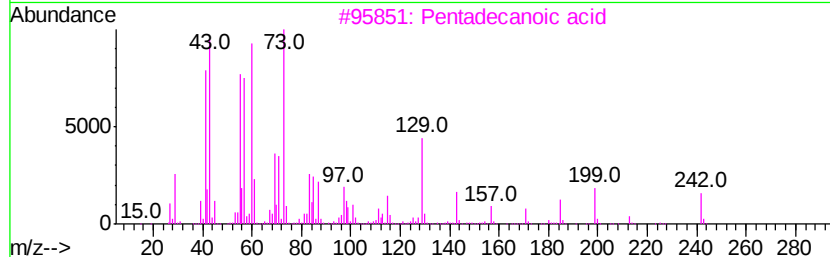
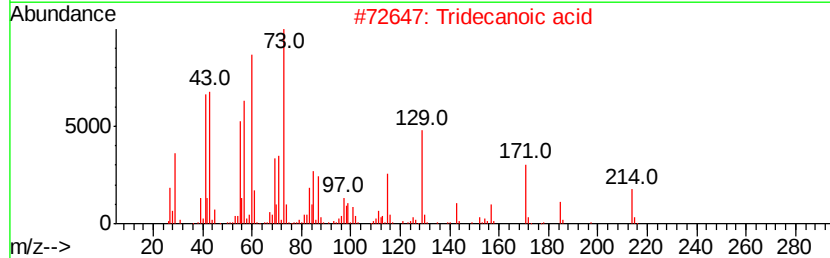
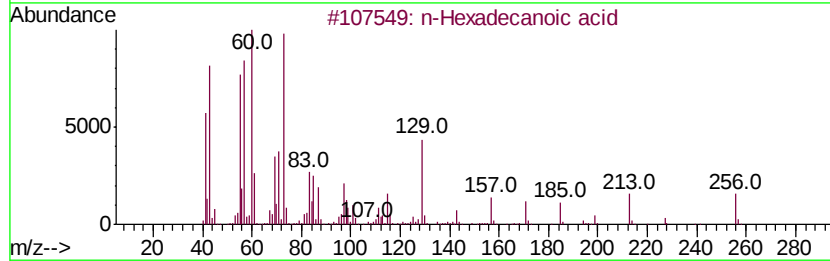
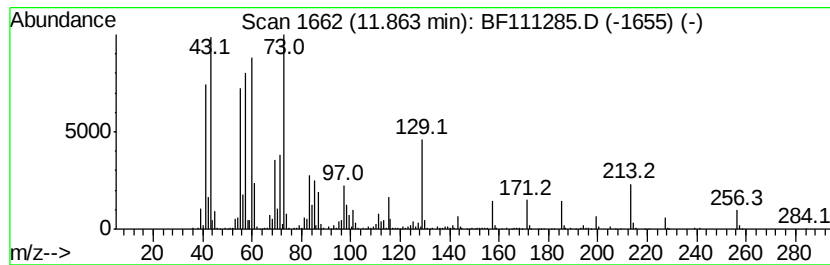
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ClientSampleId :
COMPOSITE-2-TOTAL

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 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	25.04 ng	3236300	Phenanthrene-d10	11.32	
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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111285.D
Acq On : 11 Dec 2018 19:02
Operator : JU/SJ
Sample : J6157-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSITE-2-TOTAL

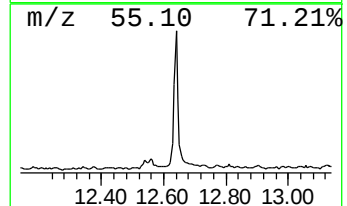
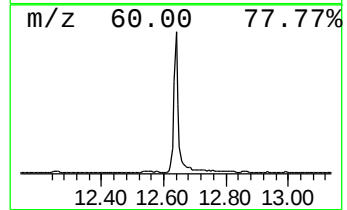
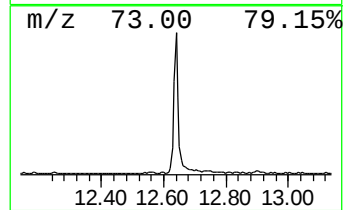
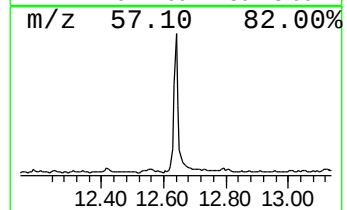
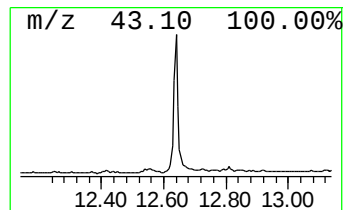
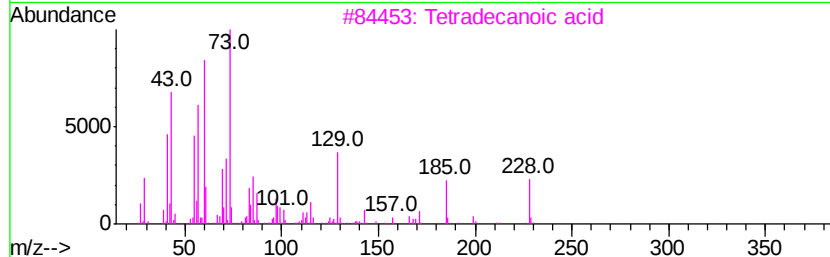
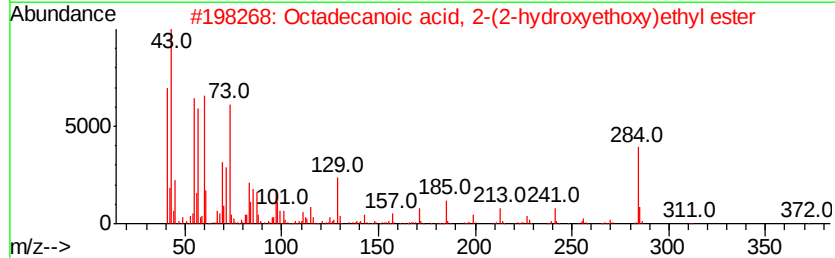
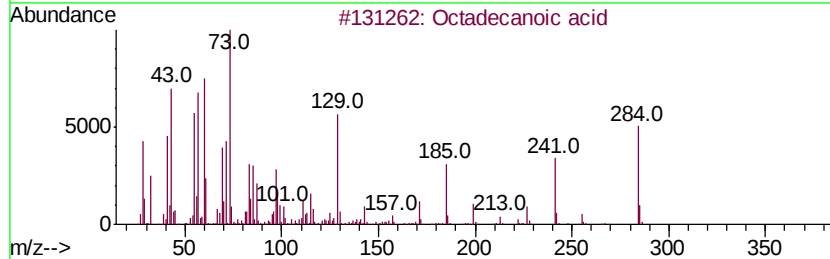
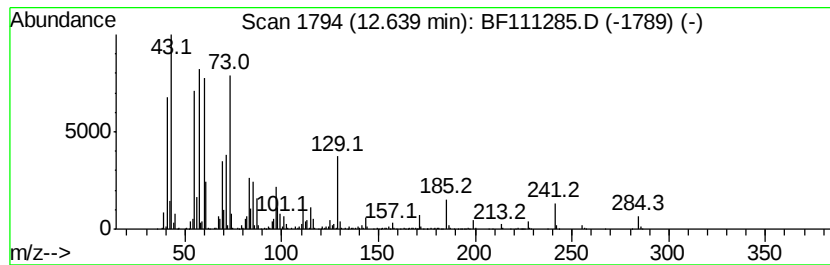
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	16.45 ng	2085250	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	86
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111285.D
Acq On : 11 Dec 2018 19:02
Operator : JU/SJ
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Instrument :
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ClientSampleId :
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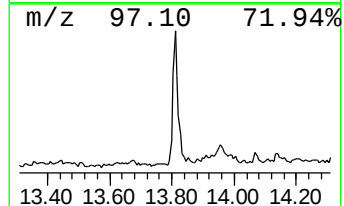
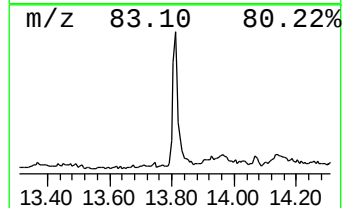
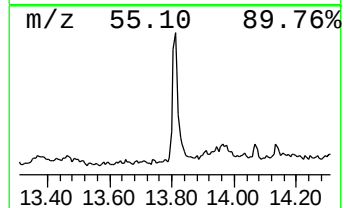
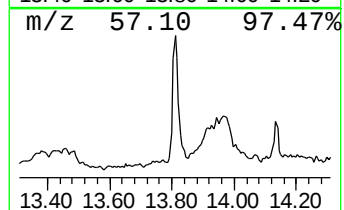
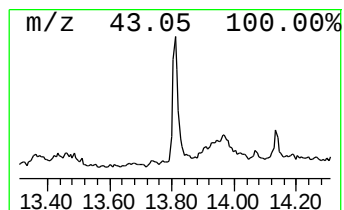
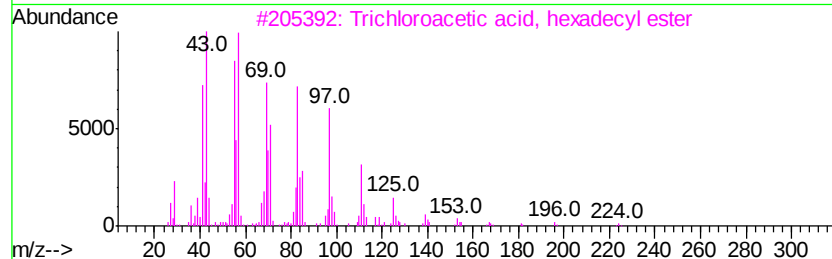
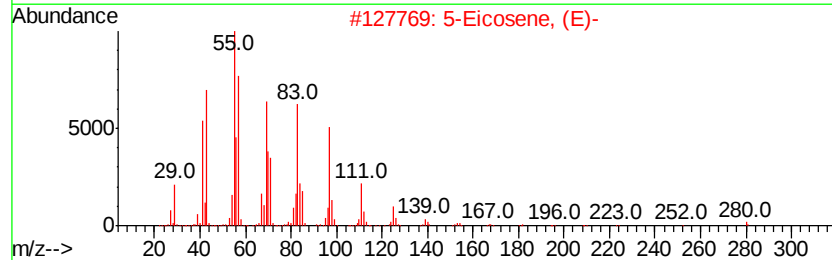
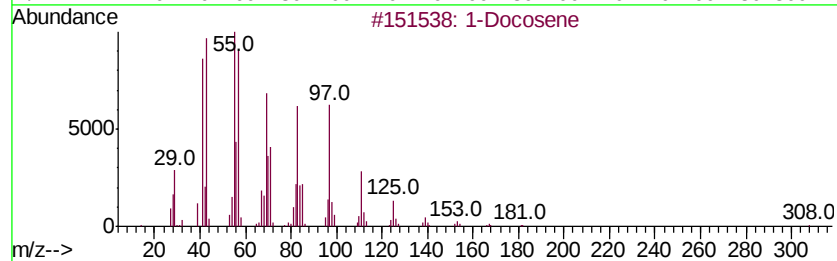
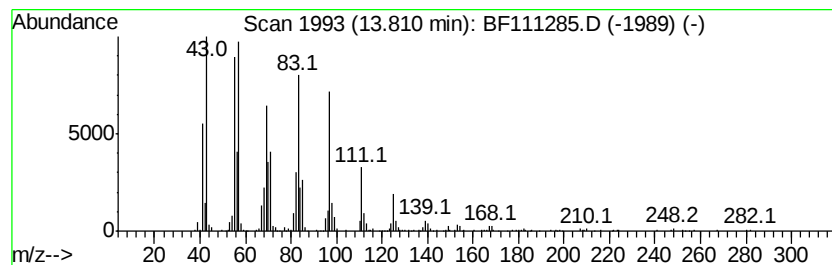
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	7.71 ng	976920	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111285.D
Acq On : 11 Dec 2018 19:02
Operator : JU/SJ
Sample : J6157-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

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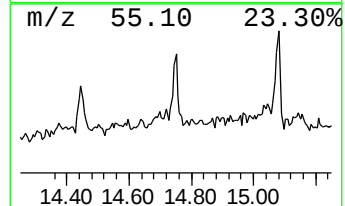
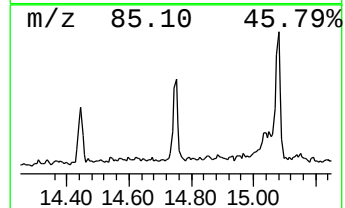
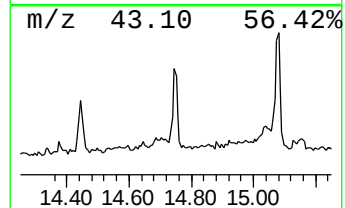
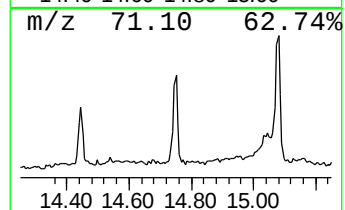
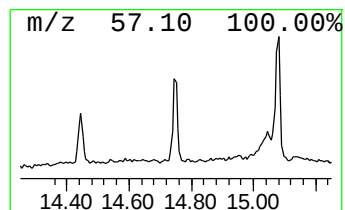
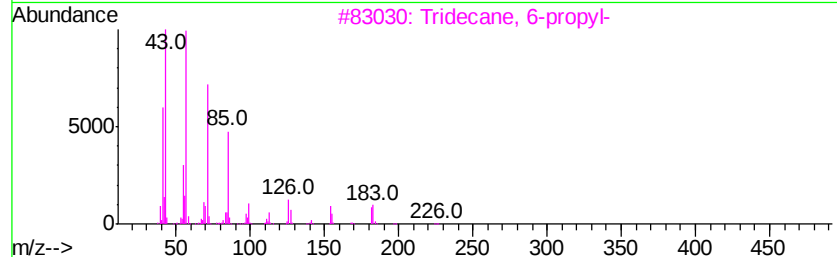
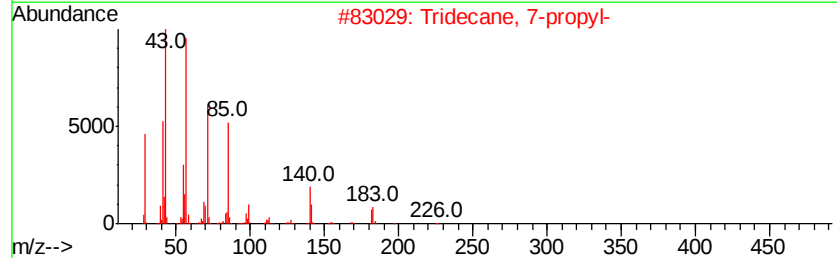
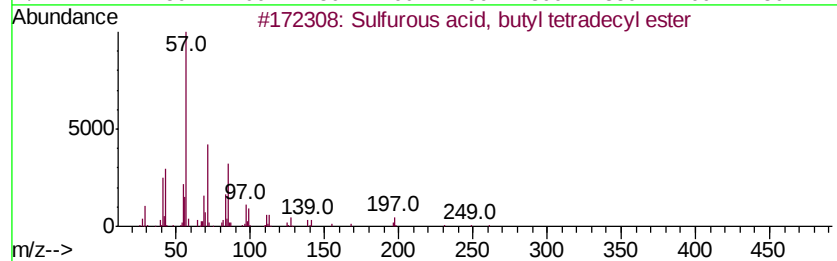
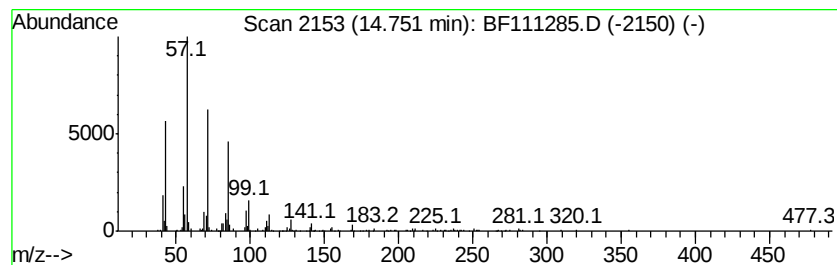
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Sulfurous acid, butyl tetra... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	3.88 ng	371071	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	86
2		Tridecane, 7-propyl-	226	C16H34	055045-09-5	83
3		Tridecane, 6-propyl-	226	C16H34	055045-10-8	80
4		Tridecane, 2-methyl-	198	C14H30	001560-96-9	72
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111285.D
Acq On : 11 Dec 2018 19:02
Operator : JU/SJ
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ALS Vial : 4 Sample Multiplier: 1

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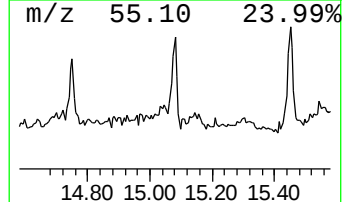
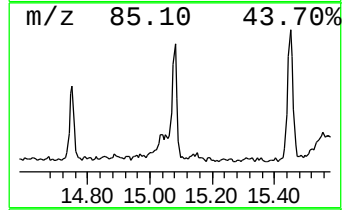
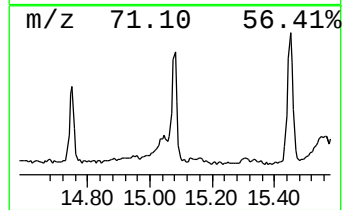
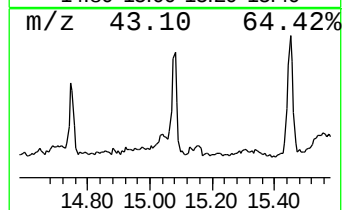
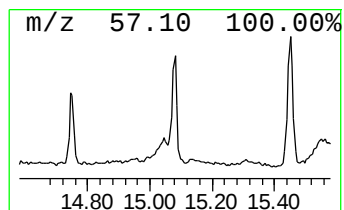
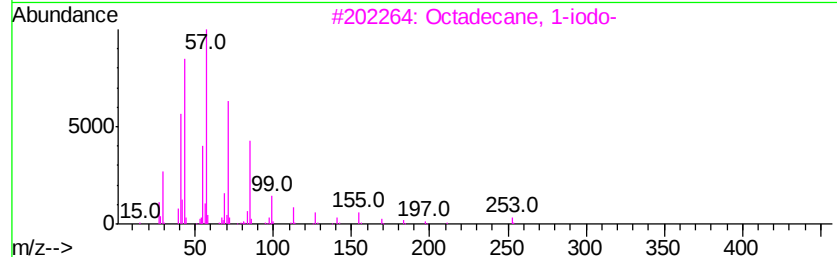
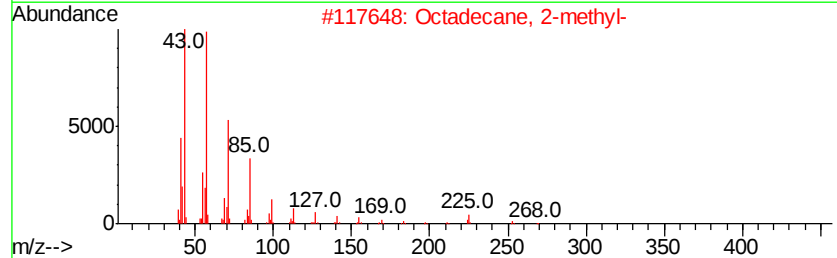
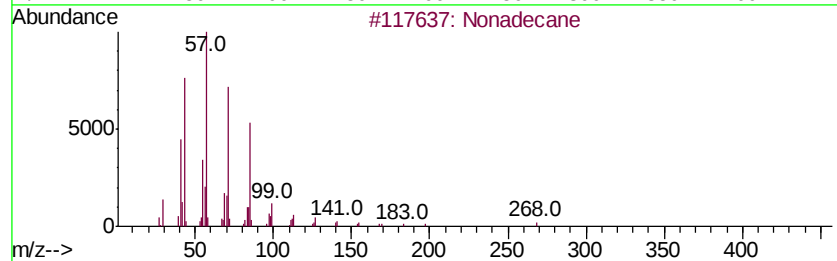
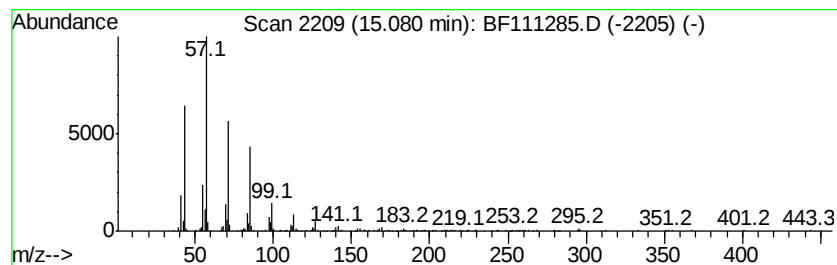
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	5.11 ng	487778	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	90
2			Octadecane, 2-methyl-	268	C19H40	001560-88-9	87
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111285.D
Acq On : 11 Dec 2018 19:02
Operator : JU/SJ
Sample : J6157-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSITE-2-TOTAL

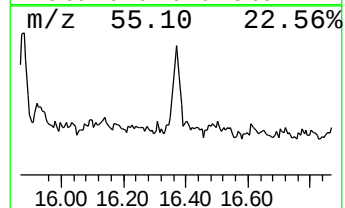
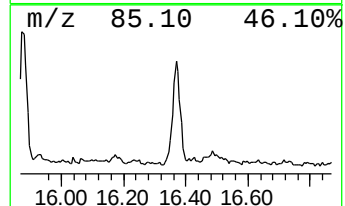
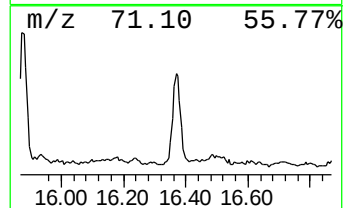
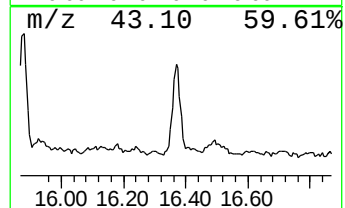
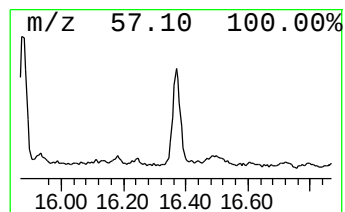
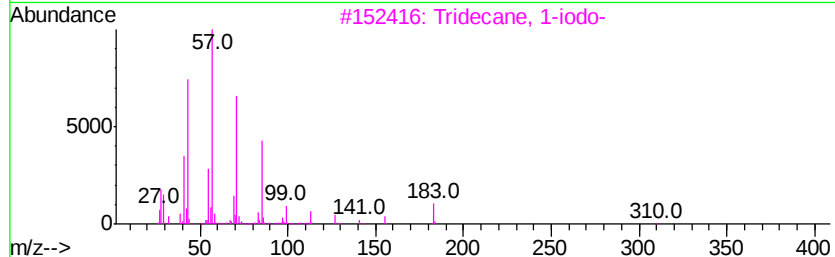
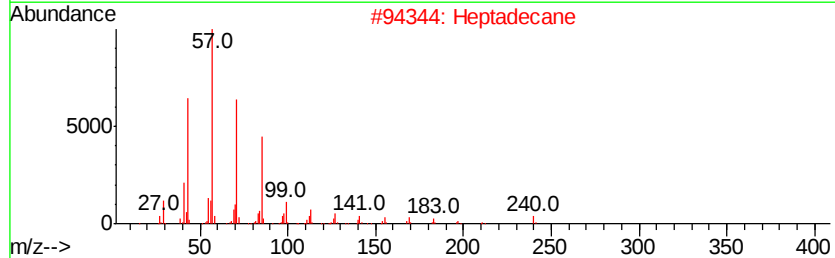
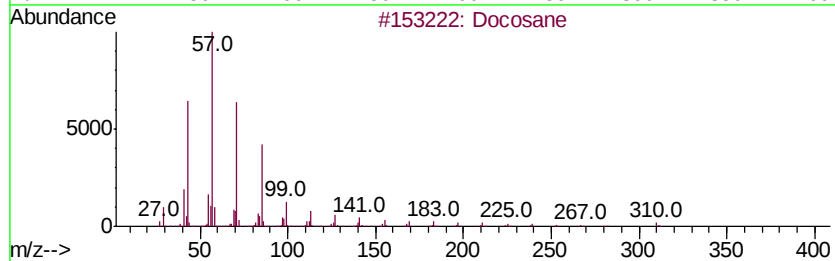
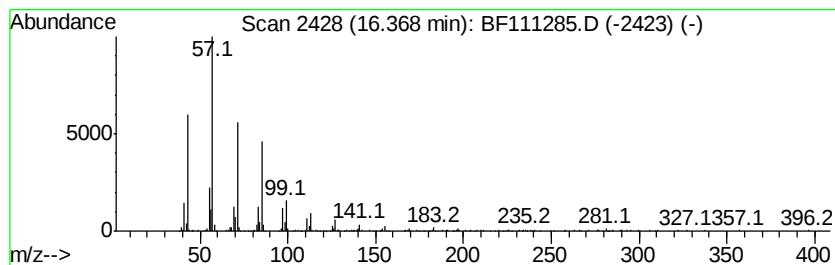
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Docosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	6.76 ng	646072	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	90
2		Heptadecane	240	C17H36	000629-78-7	87
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
4		Heneicosane	296	C21H44	000629-94-7	83
5		Hexatriacontane	507	C36H74	000630-06-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111285.D
Acq On : 11 Dec 2018 19:02
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMPOSITE-2-TOTAL

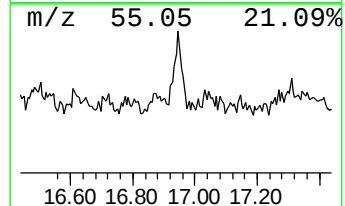
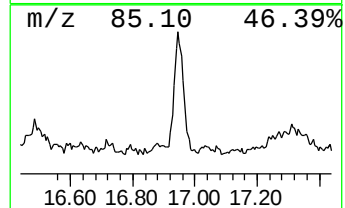
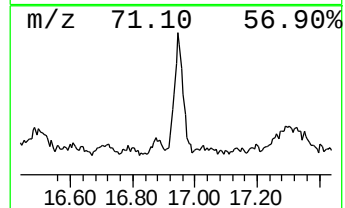
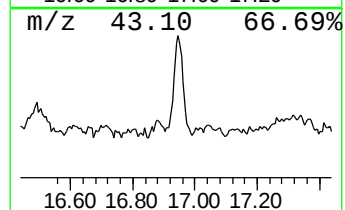
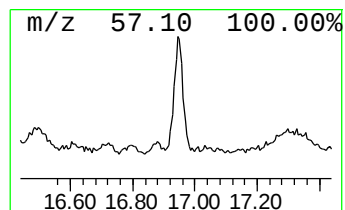
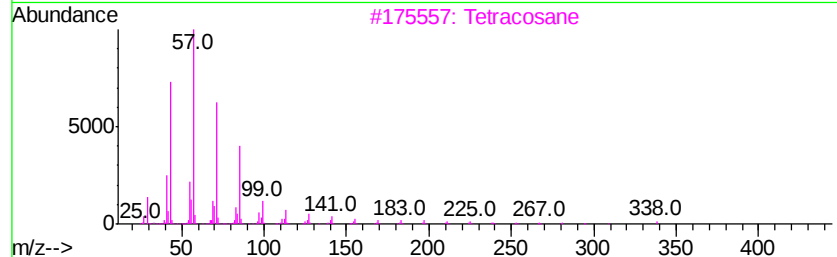
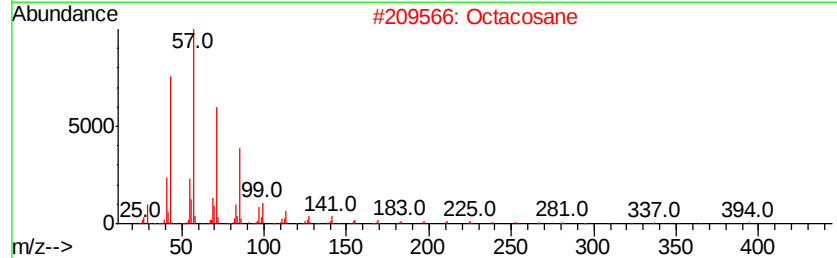
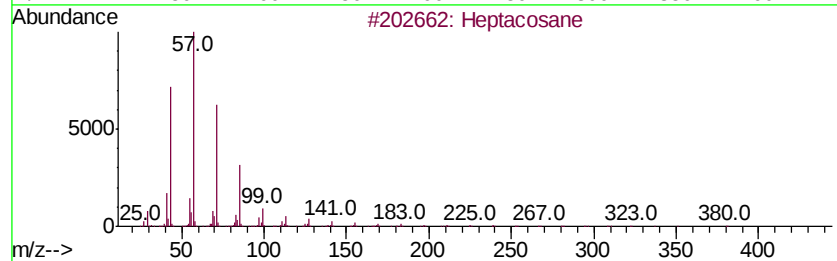
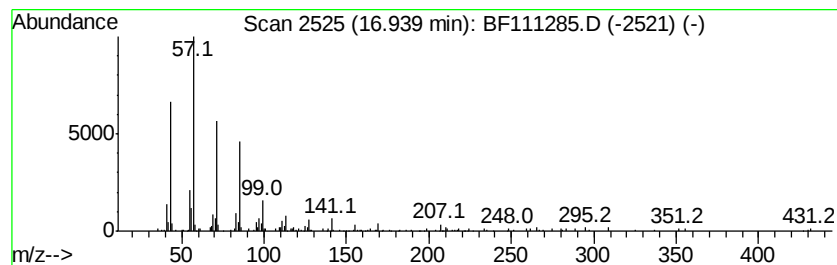
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.94	4.47 ng	427120	Perylene-d12	15.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Tetracosane	338	C24H50	000646-31-1	87
4			Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	87
5			Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
 Data File : BF111285.D
 Acq On : 11 Dec 2018 19:02
 Operator : JU/SJ
 Sample : J6157-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-2-TOTAL

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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3-Penten-2-one, 4...	4.36	18.8 ng		1591230	1	6.80	1696990	20.0
2-Pentanone, 4-hy...	4.99	8.5 ng		720702	1	6.80	1696990	20.0
unknown6.56	6.56	35.1 ng		2980890	1	6.80	1696990	20.0
n-Hexadecanoic acid	11.86	25.0 ng		3236300	4	11.32	2584900	20.0
Octadecanoic acid	12.64	16.4 ng		2085250	5	13.96	2534970	20.0
1-Docosene	13.81	7.7 ng		976920	5	13.96	2534970	20.0
Sulfurous acid, b...	14.75	3.9 ng		371071	6	15.40	1910660	20.0
Nonadecane	15.08	5.1 ng		487778	6	15.40	1910660	20.0
Docosane	16.37	6.8 ng		646072	6	15.40	1910660	20.0
Heptacosane	16.94	4.5 ng		427120	6	15.40	1910660	20.0