

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
 Data File : BF110270.D
 Acq On : 29 Oct 2018 19:04
 Operator : JU/SJ
 Sample : J5691-09
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5

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-BF102318.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	2.122	3	6	20	rVB	179118	303042	11.56%	1.225%
2	2.334	35	42	49	rVB	490354	660243	25.18%	2.670%
3	5.216	528	532	538	rBV	86583	116270	4.43%	0.470%
4	5.593	590	596	600	rBV	2297865	2396084	91.38%	9.688%
5	6.592	759	766	774	rBV	2399828	2568125	97.94%	10.384%
6	6.739	786	791	794	rBV	2756853	2521947	96.18%	10.197%
7	6.787	796	799	804	rVB	62785	58086	2.22%	0.235%
8	6.969	826	830	833	rBV	879409	724514	27.63%	2.929%
9	7.022	835	839	845	rVB2	35240	36008	1.37%	0.146%
10	7.122	852	856	860	rBV	1960619	1921783	73.29%	7.770%
11	7.281	880	883	889	rVB2	44855	47836	1.82%	0.193%
12	7.498	915	920	921	rBV	46375	43109	1.64%	0.174%
13	7.534	921	926	929	rBV	1511314	1519227	57.94%	6.143%
14	7.728	956	959	962	rBV	30377	29469	1.12%	0.119%
15	7.757	962	964	970	rVB	43330	38625	1.47%	0.156%
16	8.251	1044	1048	1060	rBV	1067234	1000153	38.14%	4.044%
17	8.963	1165	1169	1176	rBV	70475	73253	2.79%	0.296%
18	9.063	1183	1186	1192	rVB	53054	49086	1.87%	0.198%
19	9.328	1221	1231	1234	rBV	2899888	2622016	100.00%	10.602%
20	9.592	1273	1276	1283	rBV2	29242	33302	1.27%	0.135%
21	9.669	1285	1289	1291	rBV	25649	27962	1.07%	0.113%
22	9.716	1294	1297	1306	rVB	354882	304755	11.62%	1.232%
23	10.010	1343	1347	1359	rVB2	1090935	997370	38.04%	4.033%
24	10.804	1478	1482	1490	rBV	1323952	1261626	48.12%	5.101%
25	11.504	1597	1601	1609	rBV	904308	809640	30.88%	3.274%
26	12.010	1684	1687	1690	rBV	46116	43485	1.66%	0.176%
27	12.969	1843	1850	1855	rBV3	28926	51864	1.98%	0.210%
28	13.086	1866	1870	1874	rBV	1836012	1643877	62.70%	6.647%
29	13.645	1960	1965	1967	rBV3	21093	28529	1.09%	0.115%
30	13.968	2016	2020	2029	rBV	113664	148112	5.65%	0.599%
31	14.151	2047	2051	2055	rBV	653808	659886	25.17%	2.668%
32	14.286	2071	2074	2078	rBV	44042	40665	1.55%	0.164%
33	14.592	2123	2126	2131	rVB	96858	92000	3.51%	0.372%
34	14.915	2177	2181	2186	rVB	176300	188650	7.19%	0.763%

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

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

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35	15.268	2237	2241	2246	rVB	229289	264623	10.09%	1.070%
36	15.680	2305	2311	2318	rBV2	499633	831475	31.71%	3.362%
37	16.133	2383	2388	2395	rBV	166836	266906	10.18%	1.079%
38	16.674	2475	2480	2491	rVB	106099	213003	8.12%	0.861%
39	17.309	2582	2588	2594	rVB4	44291	95537	3.64%	0.386%

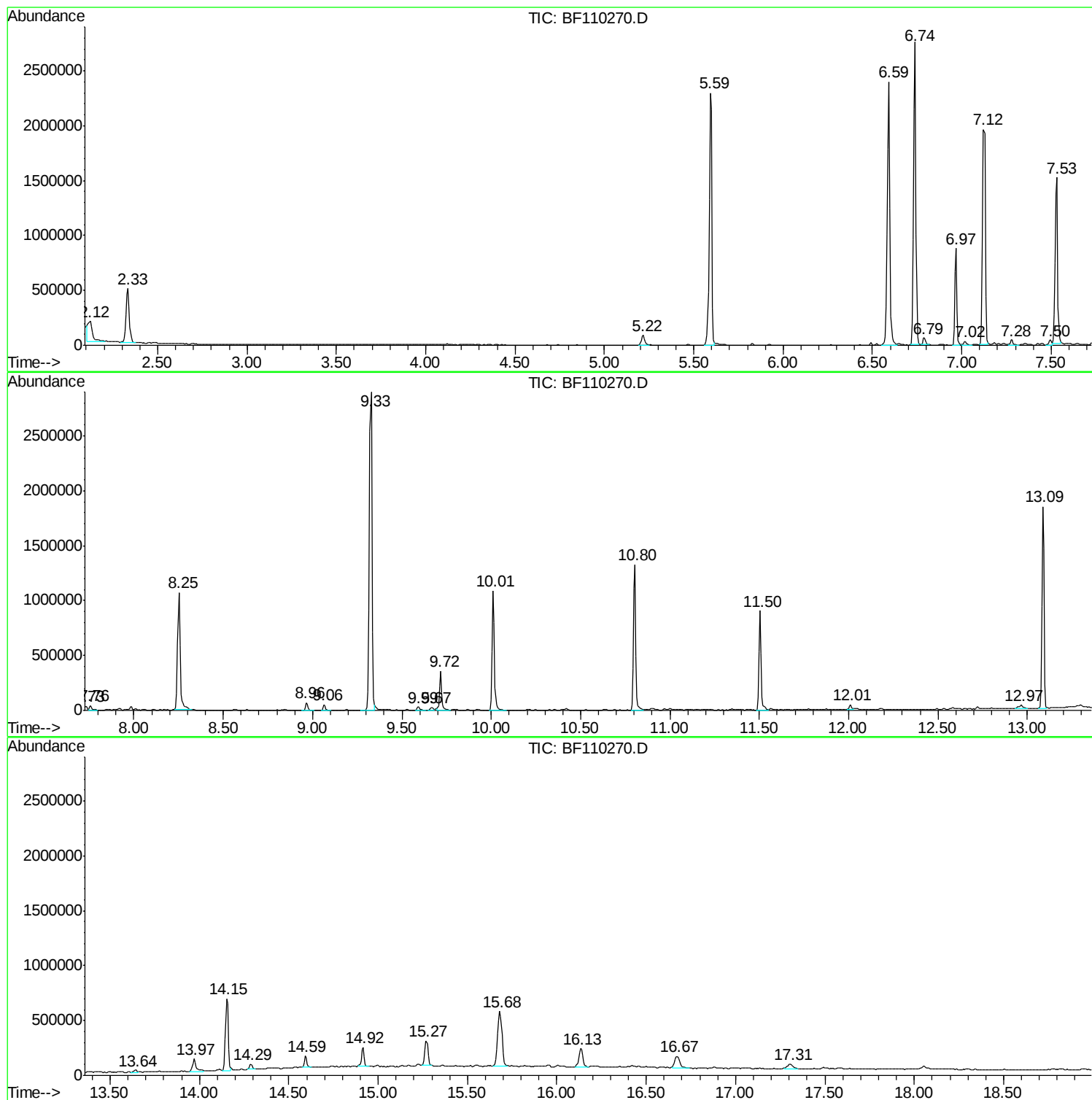
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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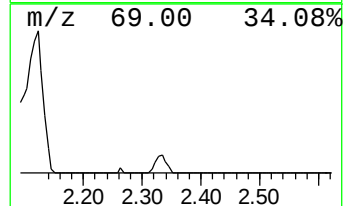
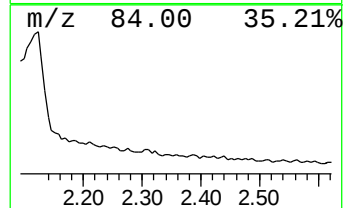
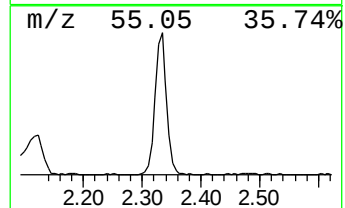
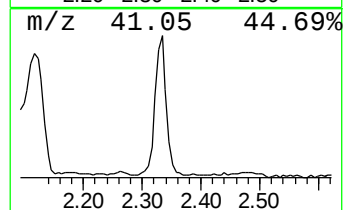
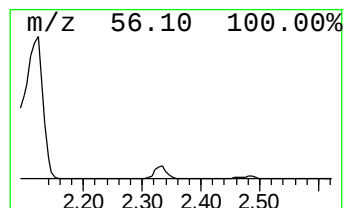
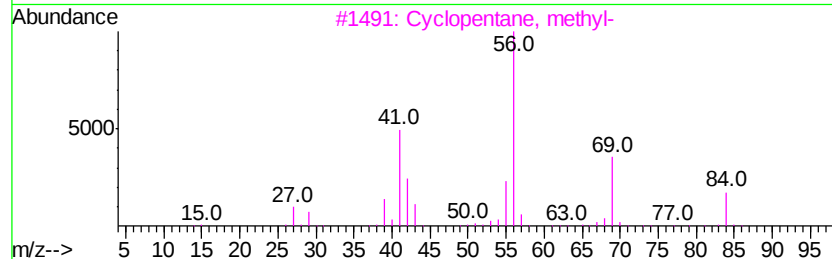
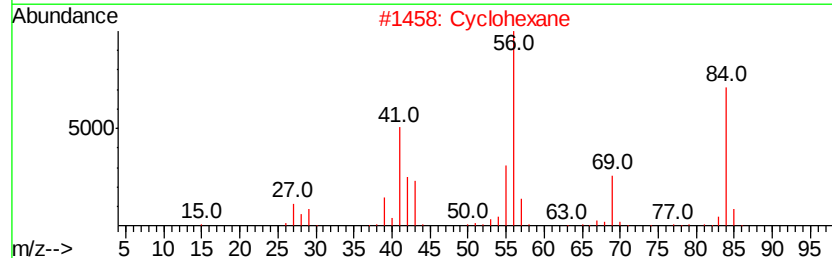
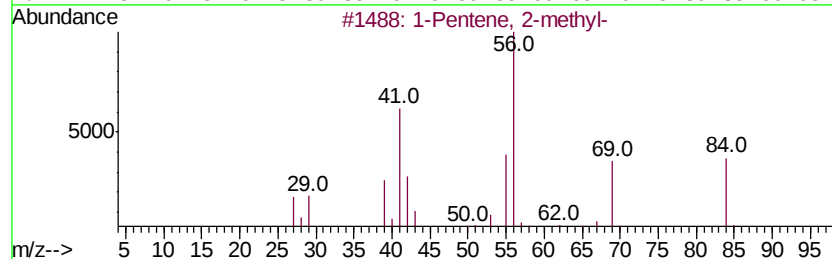
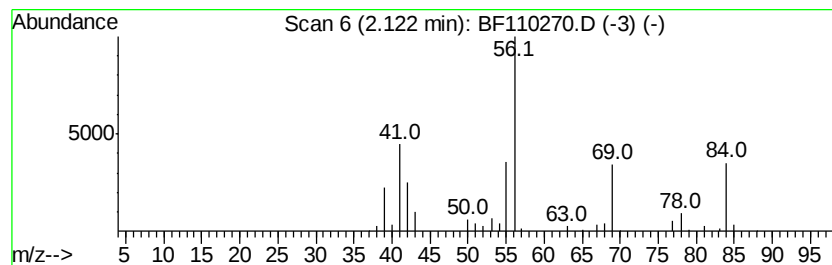
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	8.37 ng	303042	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	87
2		Cyclohexane	84	C6H12	000110-82-7	78
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4		Formic acid, hexyl ester	130	C7H14O2	000629-33-4	59
5		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	47



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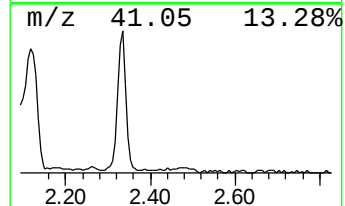
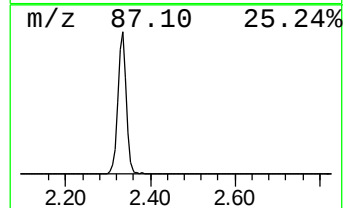
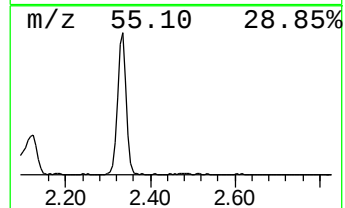
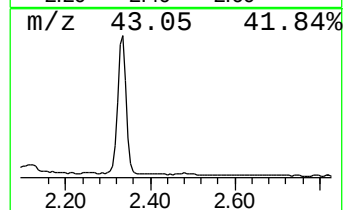
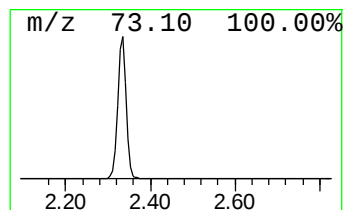
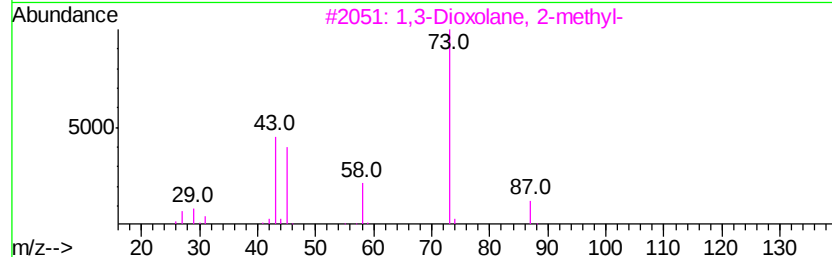
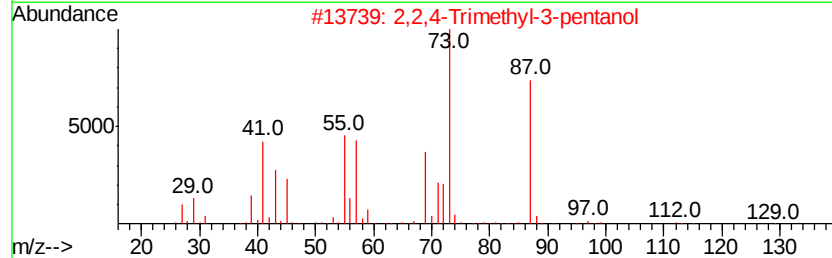
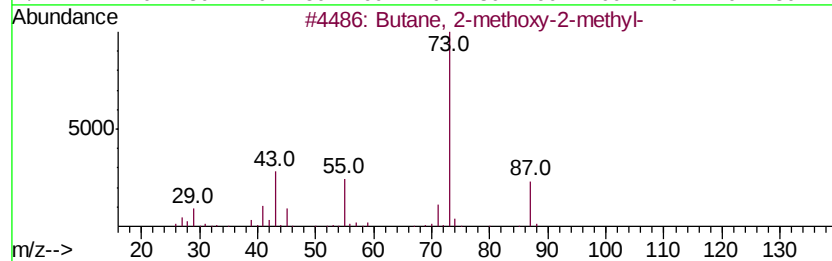
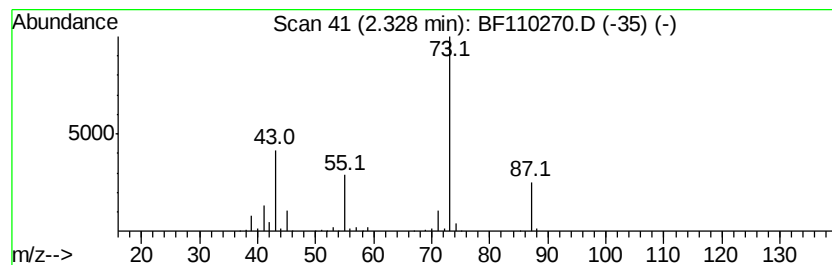
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	18.23 ng	660243	1,4-Dichlorobenzene-d4	6.97

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	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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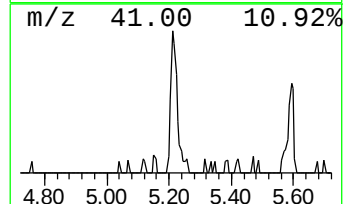
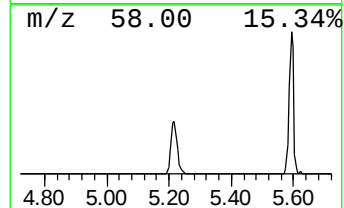
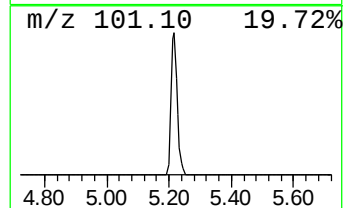
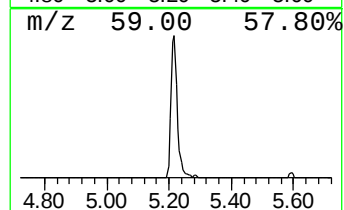
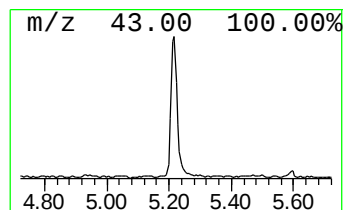
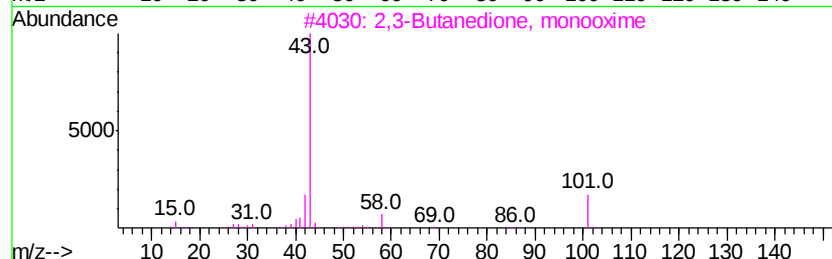
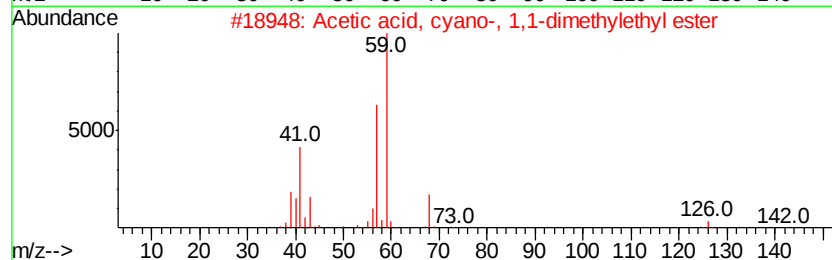
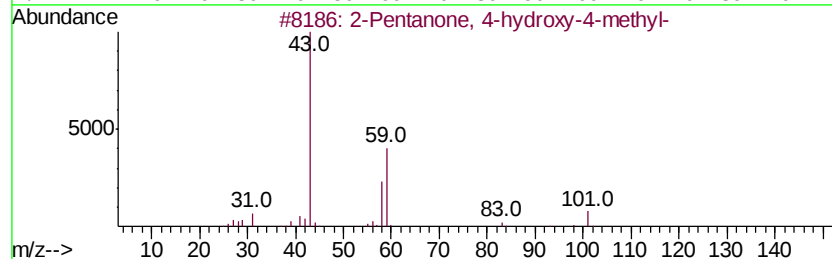
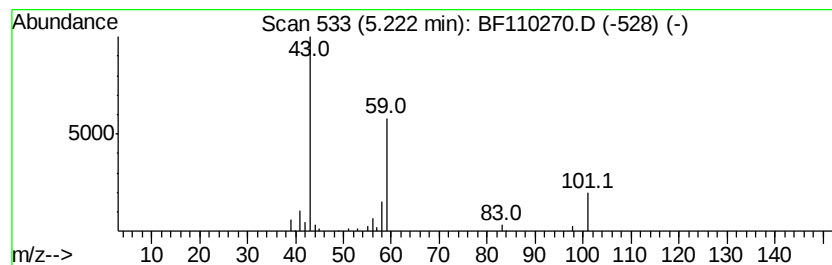
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	3.21 ng	116270	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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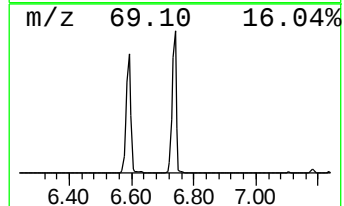
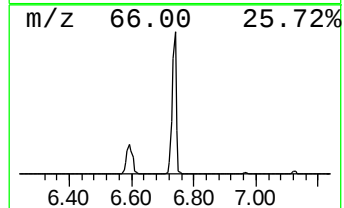
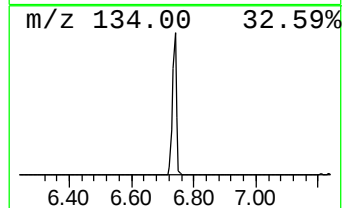
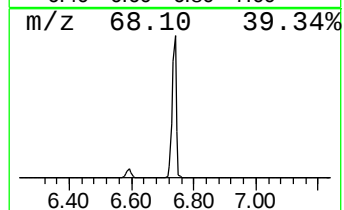
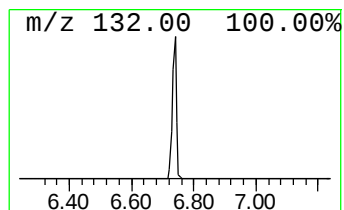
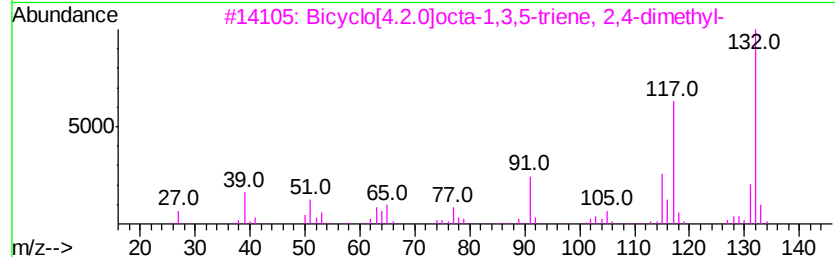
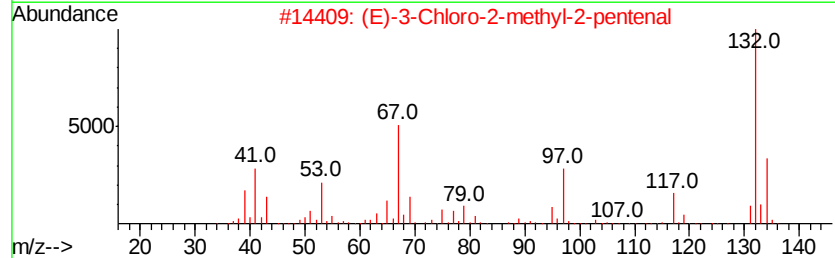
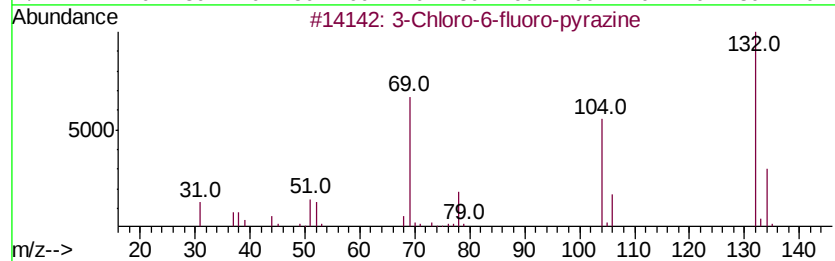
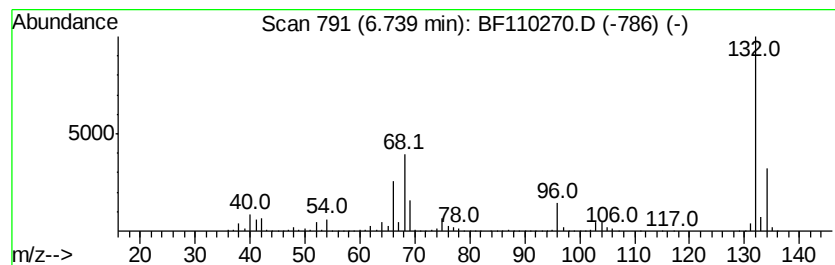
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	69.62 ng	2521950	1,4-Dichlorobenzene-d4	6.97

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	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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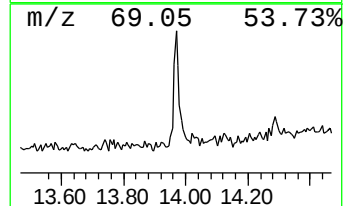
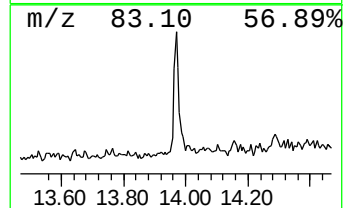
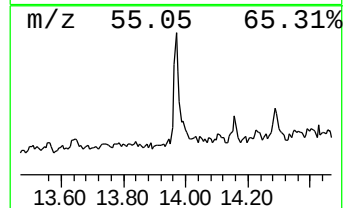
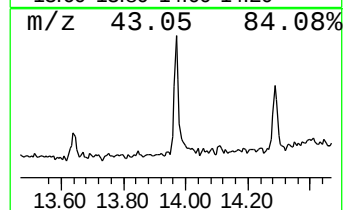
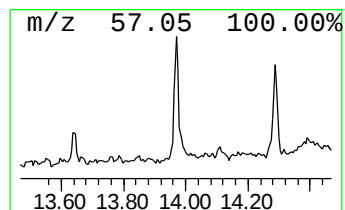
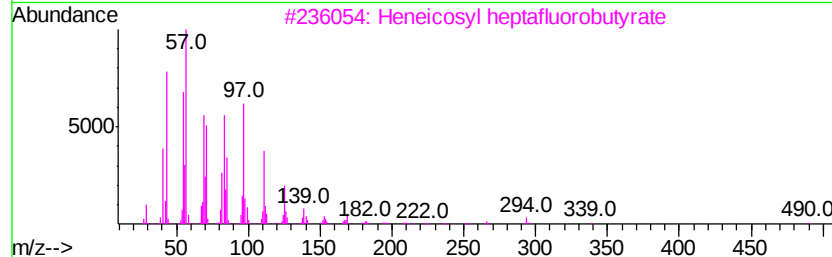
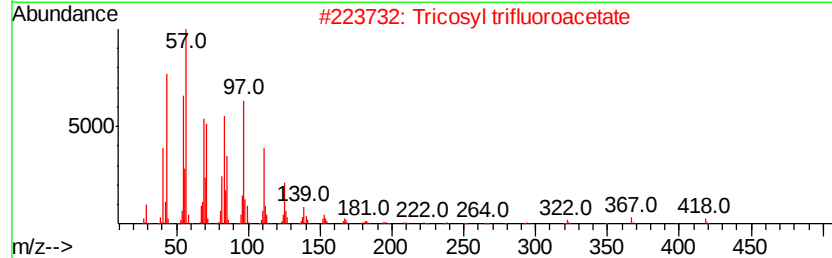
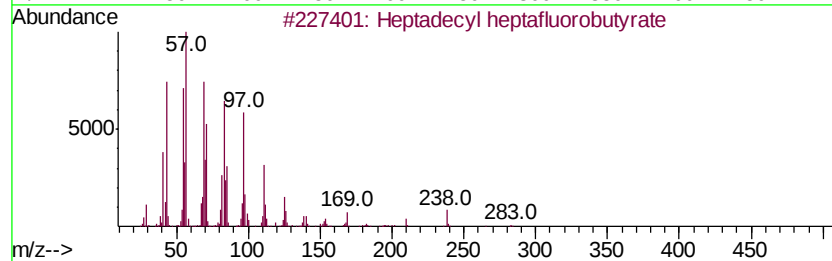
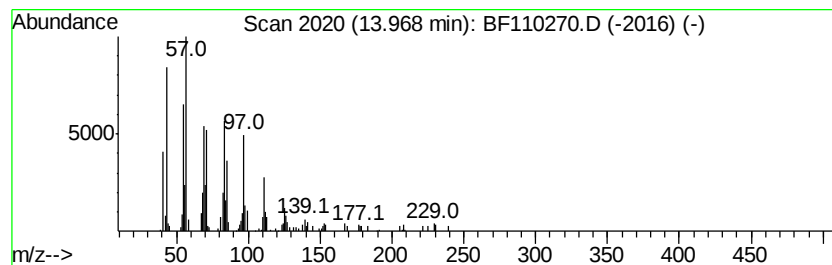
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.49 ng	148112	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	93
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3		Heneicosyl heptafluorobutvrate	508	C25H43F7O2	1000351-83-8	90
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110270.D
Acq On : 29 Oct 2018 19:04
Operator : JU/SJ
Sample : J5691-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

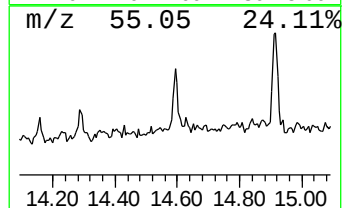
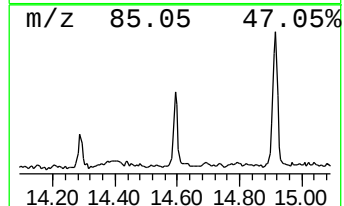
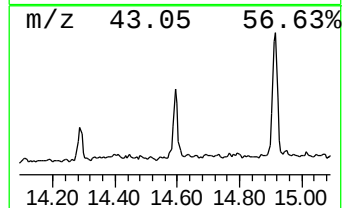
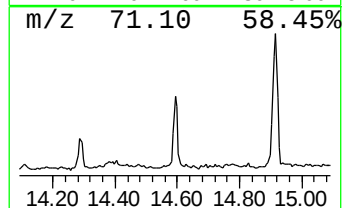
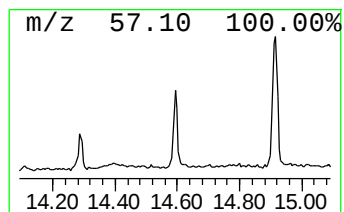
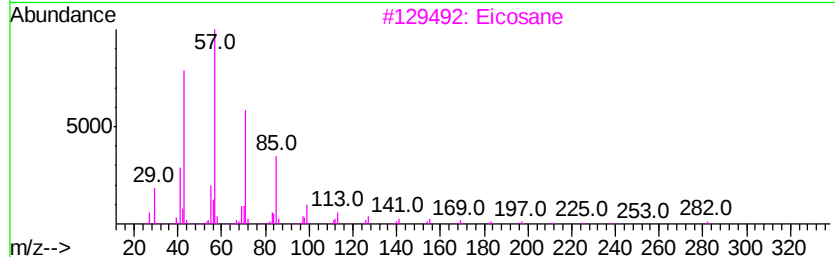
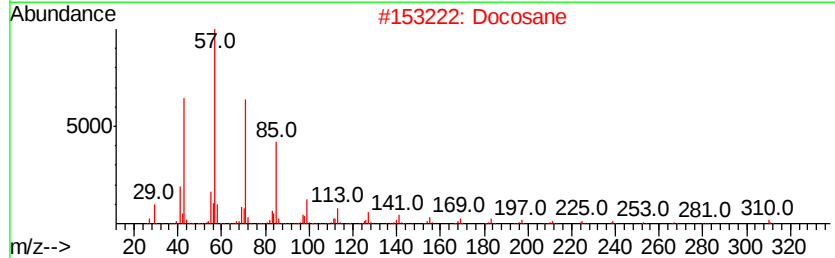
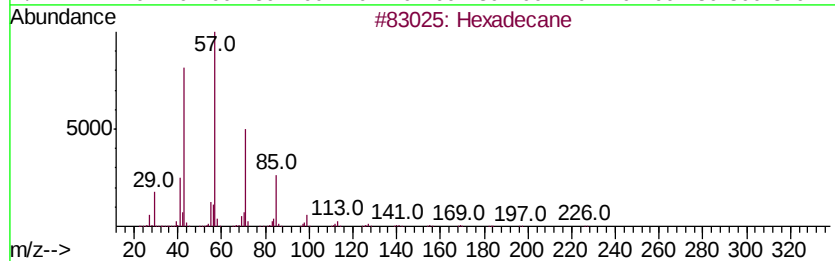
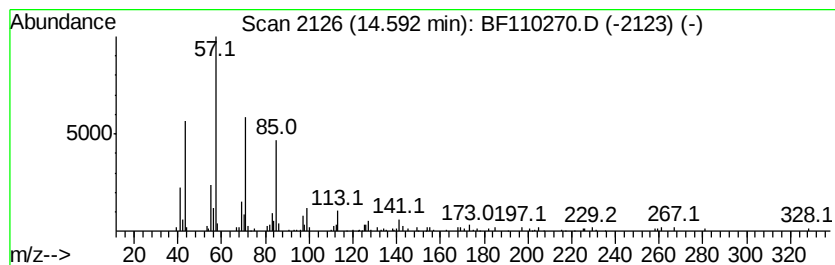
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.59	2.79 ng	92000	Chrysene-d12		14.15		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	95
2			Docosane	310	C22H46	000629-97-0	87
3			Eicosane	282	C20H42	000112-95-8	86
4			Heneicosane	296	C21H44	000629-94-7	83
5			2-Bromo dodecane	248	C12H25Br	013187-99-0	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110270.D
Acq On : 29 Oct 2018 19:04
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Sample : J5691-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-5

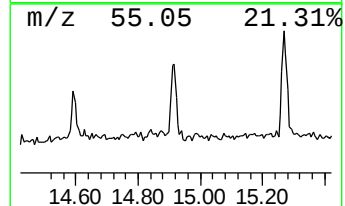
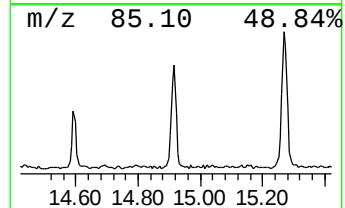
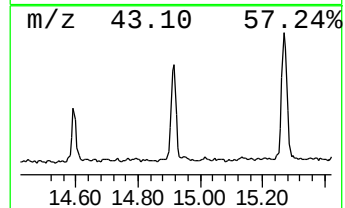
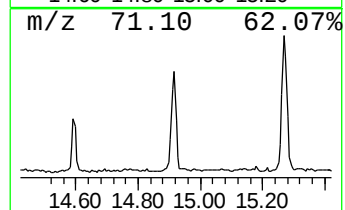
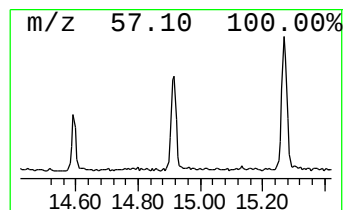
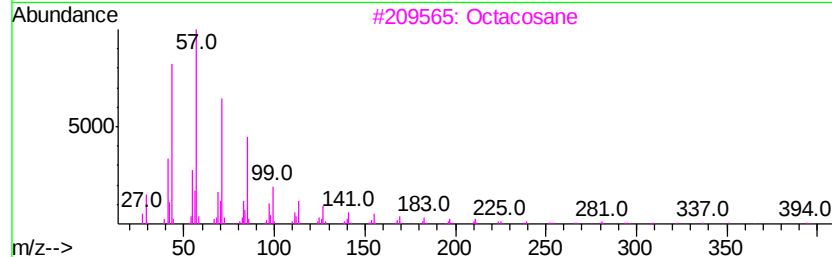
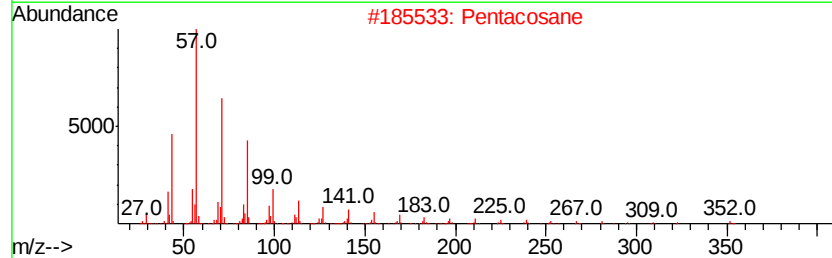
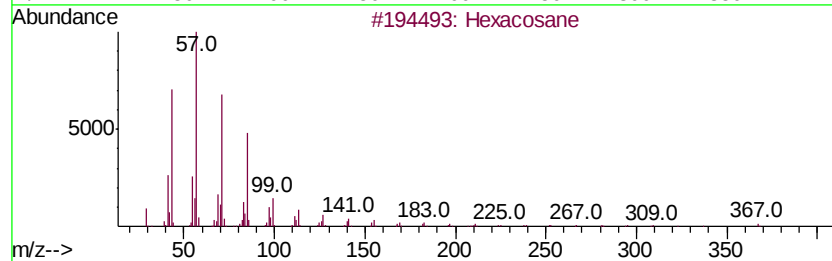
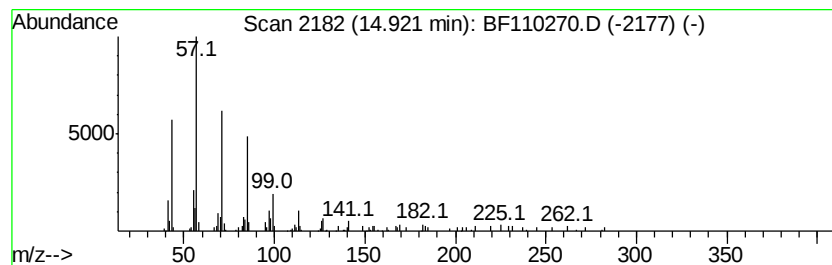
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	5.72 ng	188650	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Pentacosane		352	C25H52	000629-99-2	91
3	Octacosane		394	C28H58	000630-02-4	90
4	Heptadecane		240	C17H36	000629-78-7	87
5	Heneicosane		296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110270.D
Acq On : 29 Oct 2018 19:04
Operator : JU/SJ
Sample : J5691-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

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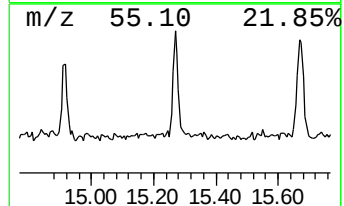
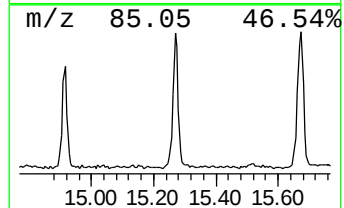
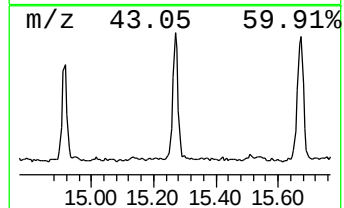
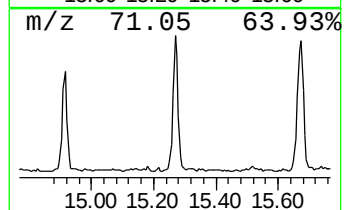
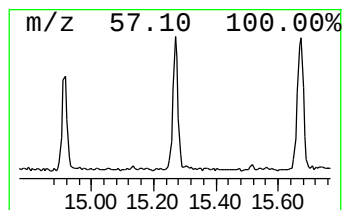
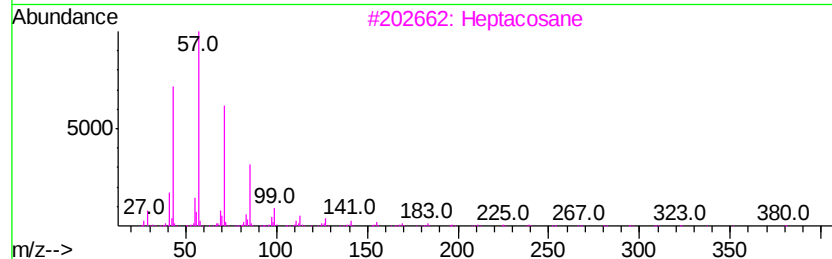
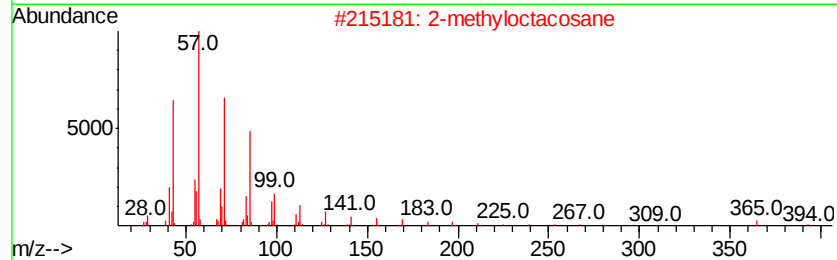
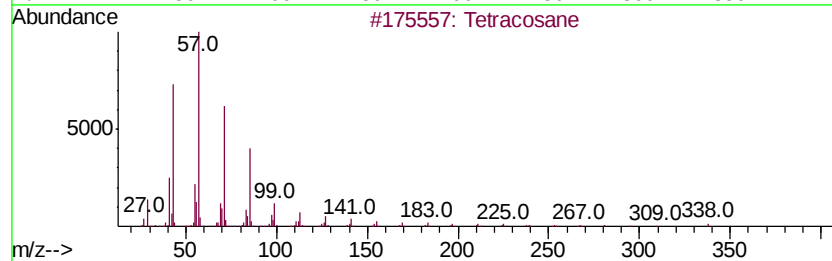
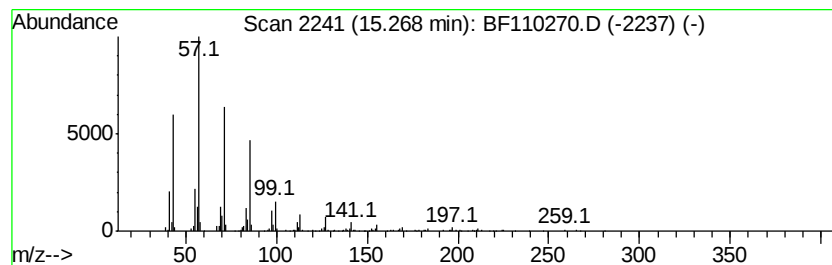
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	6.37 ng	264623	Perylene-d12	15.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110270.D
Acq On : 29 Oct 2018 19:04
Operator : JU/SJ
Sample : J5691-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

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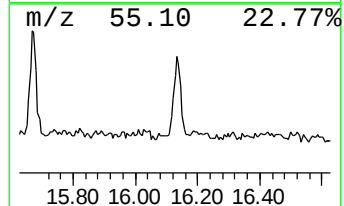
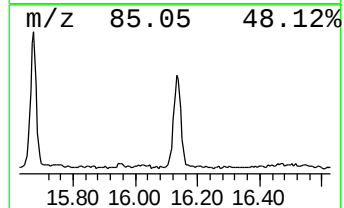
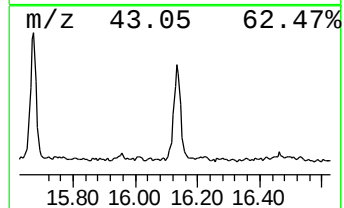
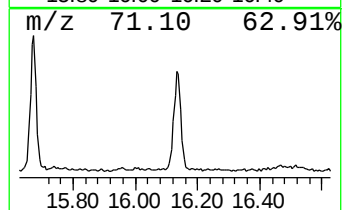
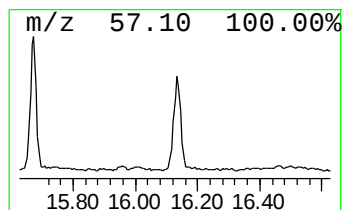
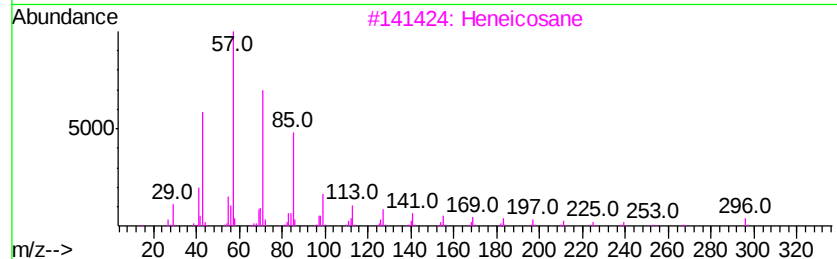
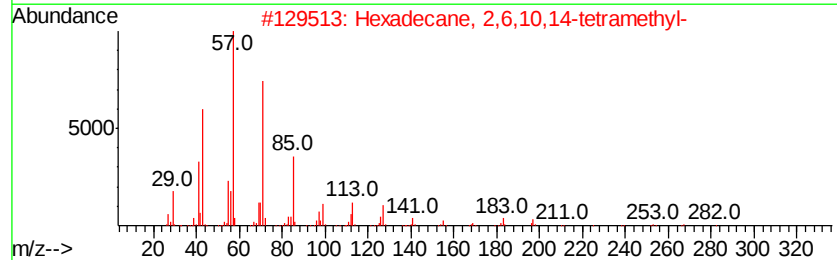
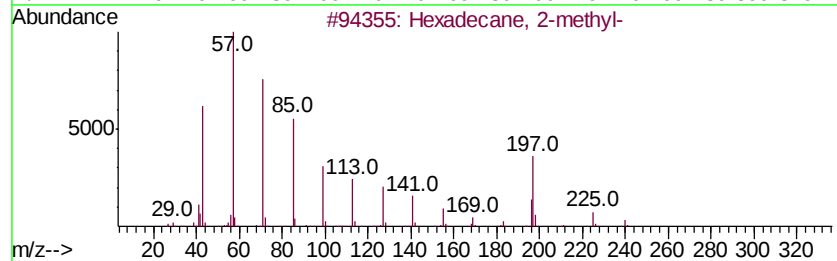
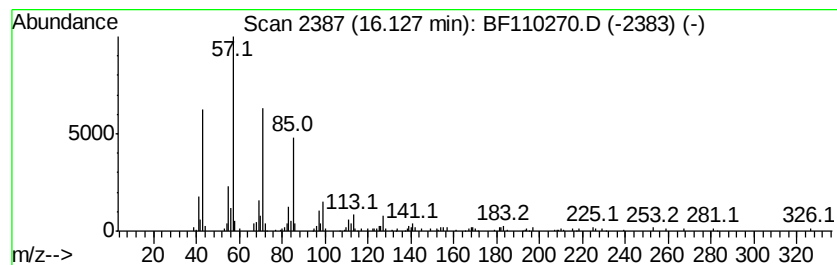
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	6.42 ng	266906	Perylene-d12	15.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	91
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Tetracosane	338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110270.D
Acq On : 29 Oct 2018 19:04
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Sample : J5691-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

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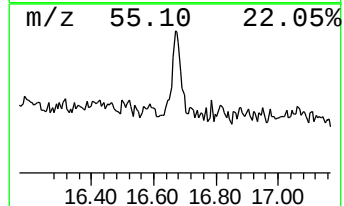
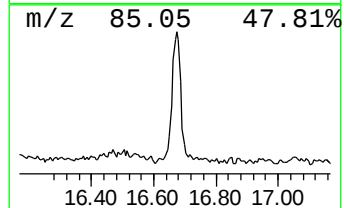
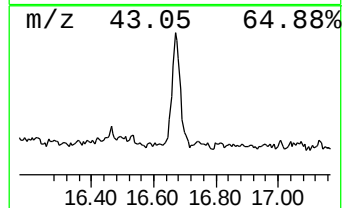
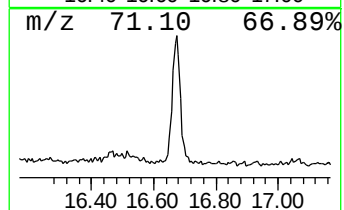
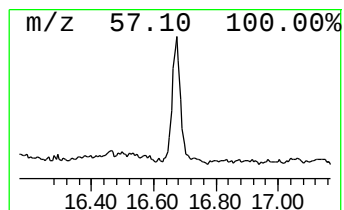
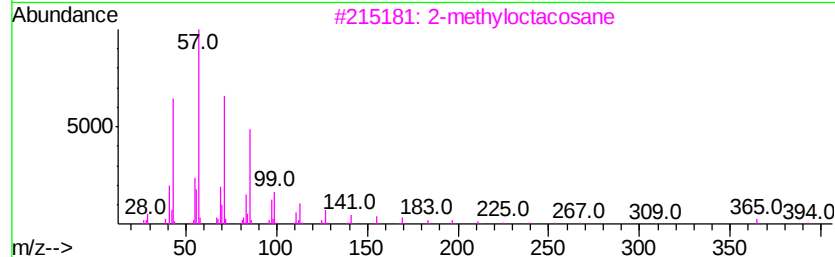
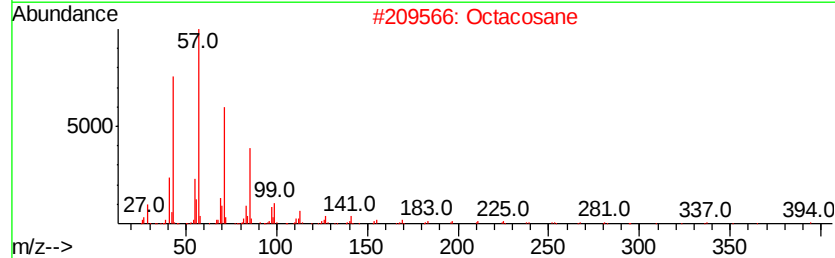
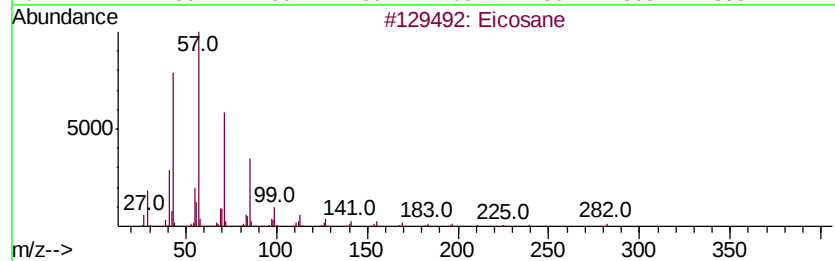
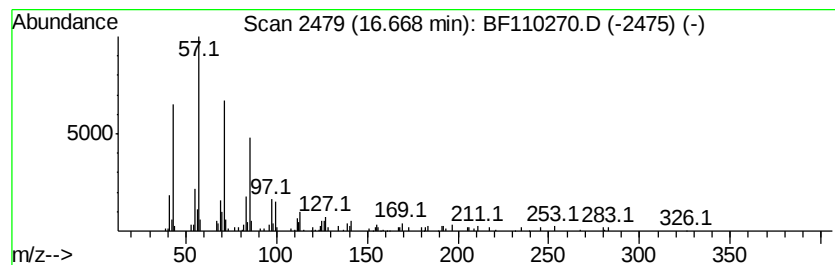
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	5.12 ng	213003	Perylene-d12	15.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Octacosane	394	C28H58	000630-02-4	87
3			2-methyloctacosane	408	C29H60	1000376-72-8	86
4			Heptacosane	380	C27H56	000593-49-7	86
5			2-methyltetracosane	352	C25H52	1000376-72-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102918\
Data File : BF110270.D
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Sample : J5691-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

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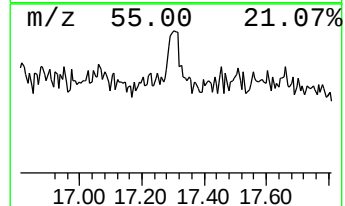
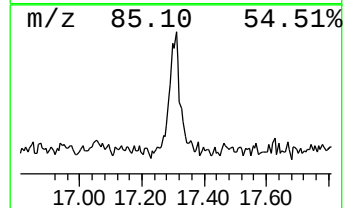
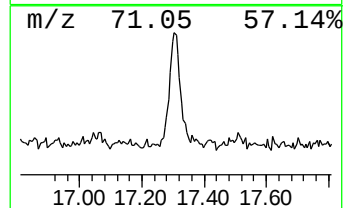
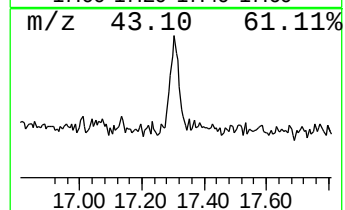
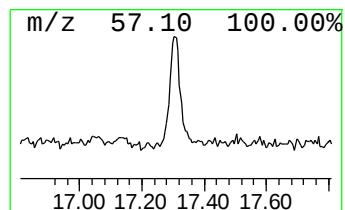
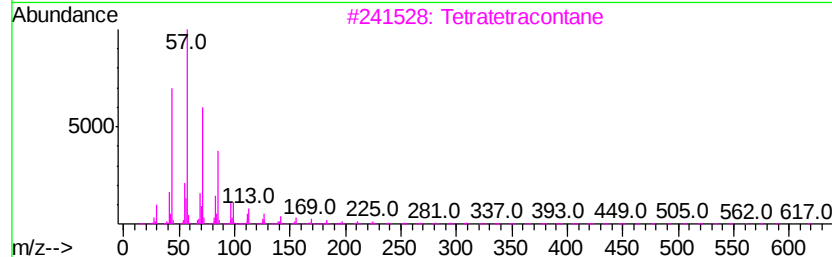
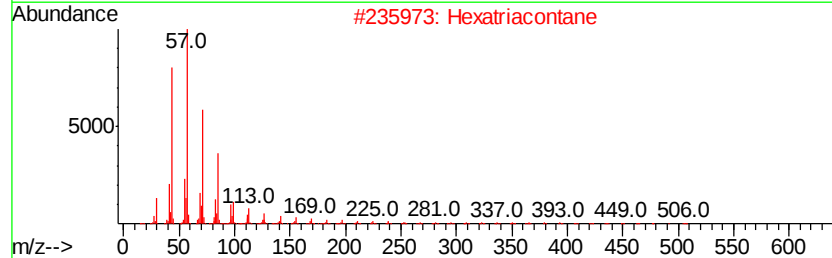
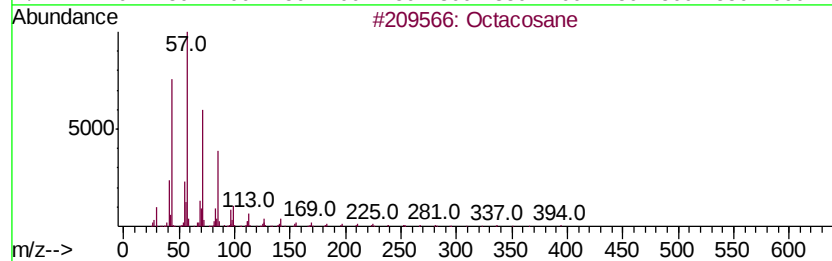
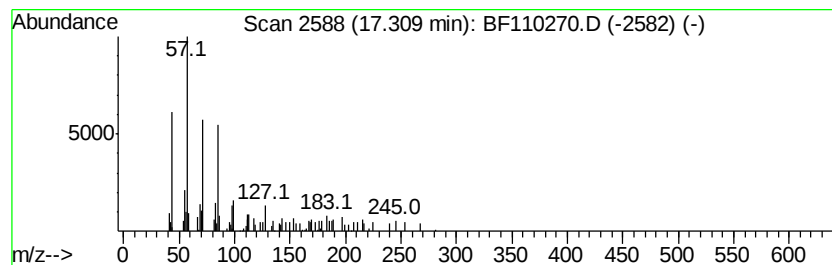
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.31	2.30 ng	95537	Perylene-d12	15.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	72
2			Hexatriacontane	507	C36H74	000630-06-8	58
3			Tetratetracontane	619	C44H90	007098-22-8	58
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	50
5			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102918\
 Data File : BF110270.D
 Acq On : 29 Oct 2018 19:04
 Operator : JU/SJ
 Sample : J5691-09
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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Butane, 2-methoxy...	2.33	18.2	ng	660243	1	6.97	724514	20.0
2-Pentanone, 4-hy...	5.22	3.2	ng	116270	1	6.97	724514	20.0
unknown6.74	6.74	69.6	ng	2521950	1	6.97	724514	20.0
Heptadecyl heptaf...	13.97	4.5	ng	148112	5	14.15	659886	20.0
Hexadecane	14.59	2.8	ng	92000	5	14.15	659886	20.0
Hexacosane	14.92	5.7	ng	188650	5	14.15	659886	20.0
Tetracosane	15.27	6.4	ng	264623	6	15.69	831475	20.0
Hexadecane, 2-met...	16.13	6.4	ng	266906	6	15.69	831475	20.0
Eicosane	16.67	5.1	ng	213003	6	15.69	831475	20.0
Octacosane	17.31	2.3	ng	95537	6	15.69	831475	20.0