

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030618\
 Data File : BF103485.D
 Acq On : 7 Mar 2018 4:32
 Operator : SJ/JU
 Sample : J1797-02
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SI-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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	5.098	509	512	520	rBV	53082	85086	2.84%	0.318%
2	5.492	576	579	613	rBV	1842349	2991126	100.00%	11.189%
3	6.510	748	752	771	rBV	1958236	2989152	99.93%	11.182%
4	6.639	771	774	787	rVV	2393526	2714390	90.75%	10.154%
5	6.869	810	813	830	rVB	689661	783977	26.21%	2.933%
6	7.022	836	839	861	rBV	1987937	2207172	73.79%	8.256%
7	7.439	906	910	933	rBV	1259429	1855043	62.02%	6.939%
8	7.592	933	936	946	rVB3	18603	35054	1.17%	0.131%
9	8.157	1028	1032	1053	rBV	664832	1005592	33.62%	3.762%
10	9.028	1177	1180	1182	rBV	35071	32119	1.07%	0.120%
11	9.086	1187	1190	1200	rVB	204810	204516	6.84%	0.765%
12	9.204	1207	1210	1211	rBV	256475	218869	7.32%	0.819%
13	9.228	1211	1214	1223	rVV	2583397	2749036	91.91%	10.283%
14	9.292	1223	1225	1229	rVV2	37641	48520	1.62%	0.181%
15	9.333	1229	1232	1237	rVV2	35166	44565	1.49%	0.167%
16	9.404	1241	1244	1256	rVB2	24924	52090	1.74%	0.195%
17	9.704	1292	1295	1304	rBV3	27033	38181	1.28%	0.143%
18	9.822	1311	1315	1319	rBV	32766	31490	1.05%	0.118%
19	9.910	1326	1330	1343	rVB2	965922	992272	33.17%	3.712%
20	10.298	1393	1396	1398	rBV	89050	74489	2.49%	0.279%
21	10.322	1398	1400	1404	rVB	64902	50854	1.70%	0.190%
22	10.710	1462	1466	1478	rBV	1072889	1435549	47.99%	5.370%
23	10.798	1478	1481	1485	rVB2	44218	56234	1.88%	0.210%
24	10.904	1494	1499	1503	rBV	31788	33565	1.12%	0.126%
25	11.245	1554	1557	1560	rBV	38903	39469	1.32%	0.148%
26	11.339	1568	1573	1576	rBV4	33044	31388	1.05%	0.117%
27	11.404	1581	1584	1589	rBV	681526	782600	26.16%	2.927%
28	11.551	1606	1609	1615	rBV	188815	153789	5.14%	0.575%
29	11.610	1615	1619	1624	rBV5	21084	33084	1.11%	0.124%
30	11.674	1627	1630	1632	rBV	49498	44617	1.49%	0.167%
31	11.951	1673	1677	1682	rVB	706774	582422	19.47%	2.179%
32	12.080	1696	1699	1702	rBV	48415	41381	1.38%	0.155%
33	12.433	1756	1759	1763	rBV4	21133	31273	1.05%	0.117%
34	12.469	1763	1765	1770	rVB	59598	49178	1.64%	0.184%

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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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35	12.792	1815	1820	1825	rBV2	29143	37686	1.26%	0.141%
36	12.839	1825	1828	1831	rVB	108427	88912	2.97%	0.333%
37	12.992	1849	1854	1861	rBV	1900950	1976385	66.07%	7.393%
38	13.198	1884	1889	1892	rBV	150450	143312	4.79%	0.536%
39	13.539	1944	1947	1954	rVB	143937	135231	4.52%	0.506%
40	13.868	2000	2003	2013	rBV	252885	295167	9.87%	1.104%
41	14.010	2024	2027	2032	rBV	52620	45160	1.51%	0.169%
42	14.063	2032	2036	2045	rVB	582136	622357	20.81%	2.328%
43	14.186	2054	2057	2066	rBV	74543	98775	3.30%	0.369%
44	14.498	2107	2110	2117	rBV	52776	69898	2.34%	0.261%
45	14.804	2158	2162	2167	rBV2	93190	127953	4.28%	0.479%
46	14.886	2173	2176	2179	rVB	149855	132452	4.43%	0.495%
47	15.574	2289	2293	2302	rVB	305081	441520	14.76%	1.652%

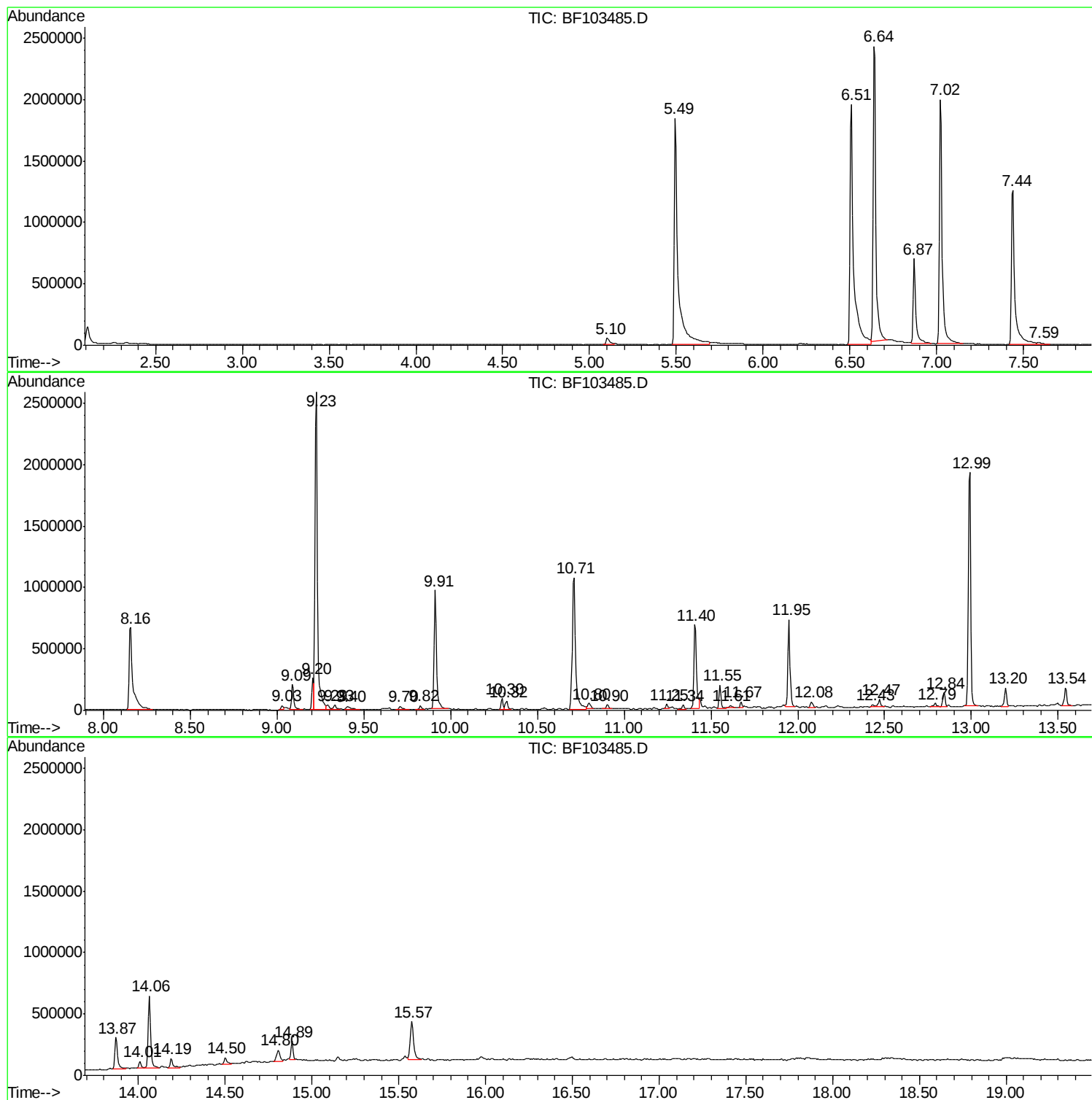
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BNA_F
ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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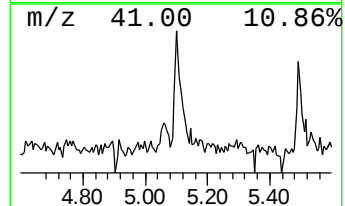
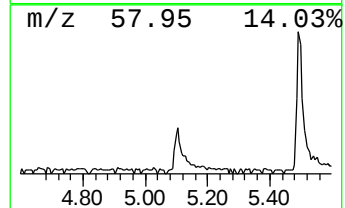
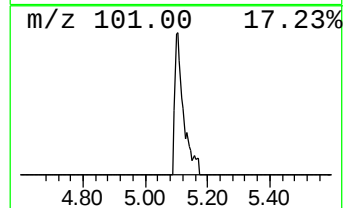
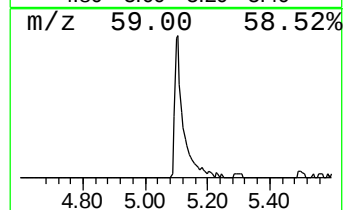
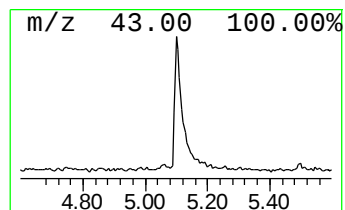
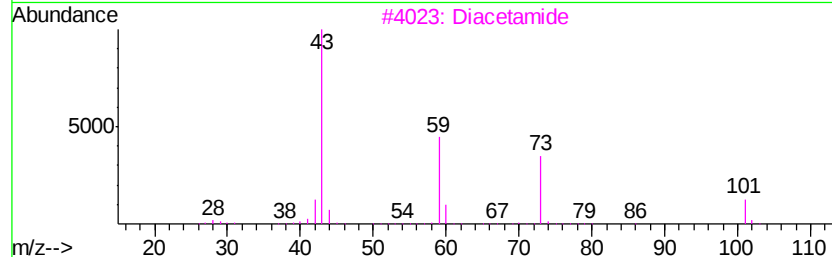
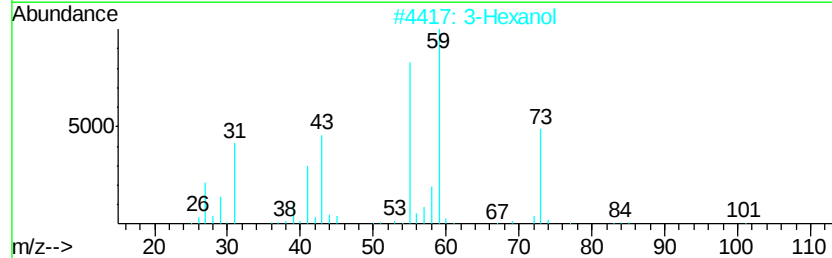
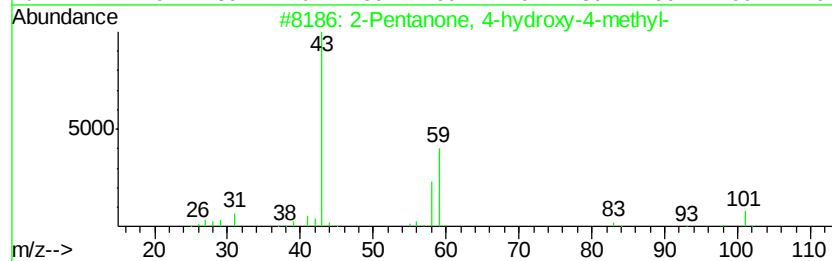
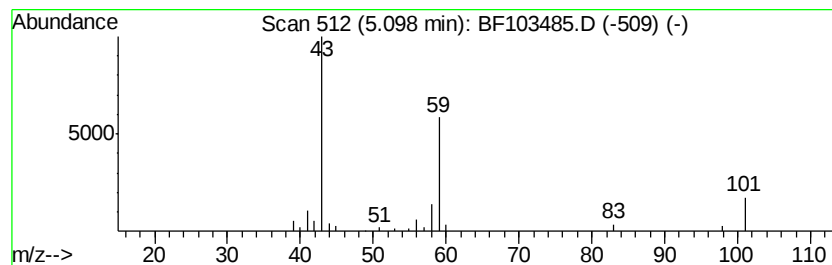
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.10 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.17 ng	85086	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2			3-Hexanol	102	C6H14O	000623-37-0	33
3			Diacetamide	101	C4H7NO2	000625-77-4	9
4			Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5			Propylamine	59	C3H9N	000107-10-8	9



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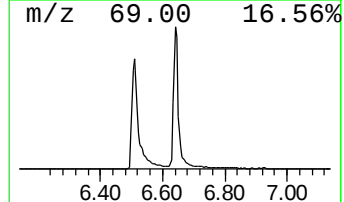
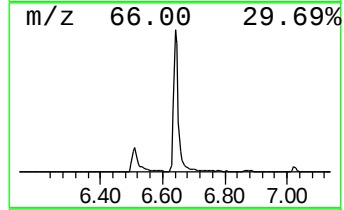
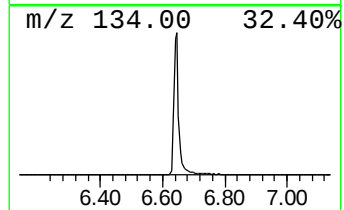
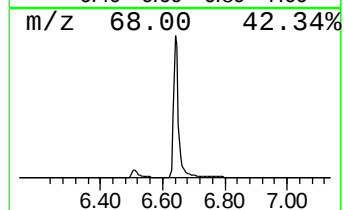
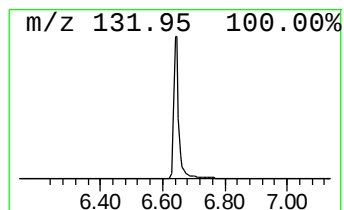
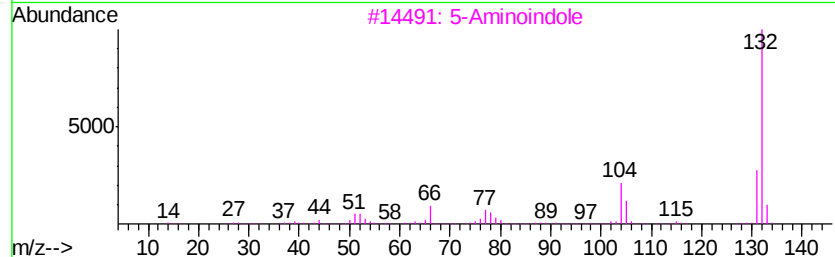
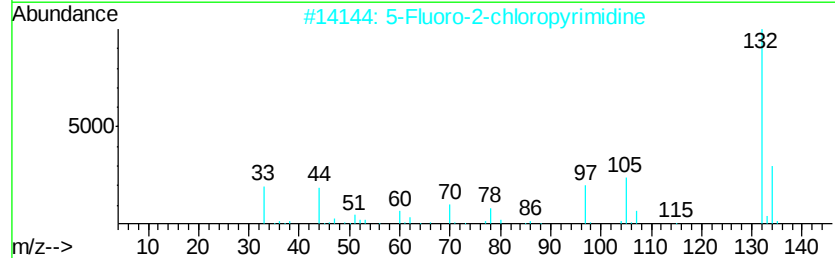
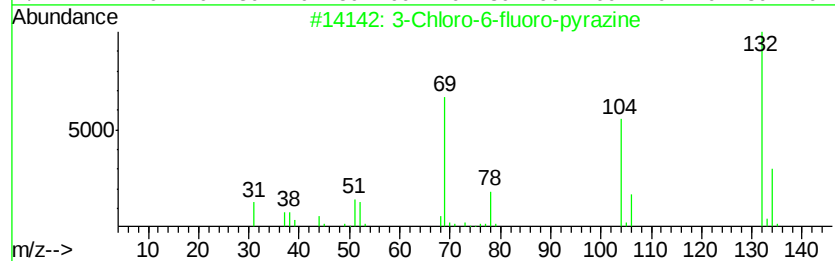
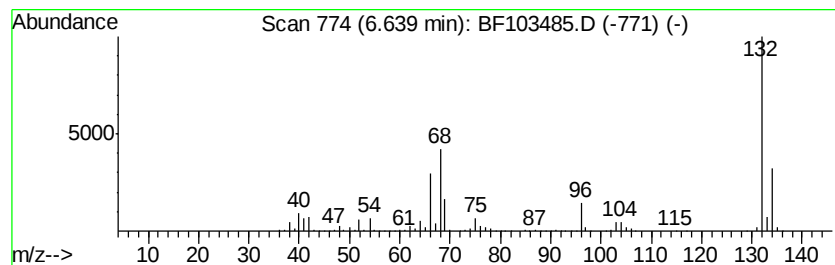
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	69.25 ng	2714390	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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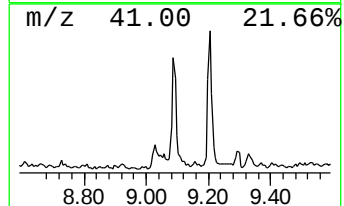
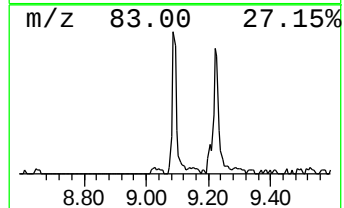
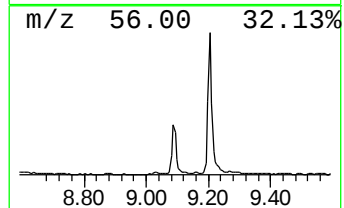
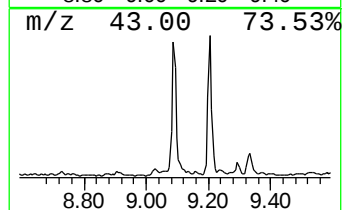
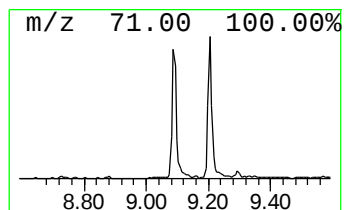
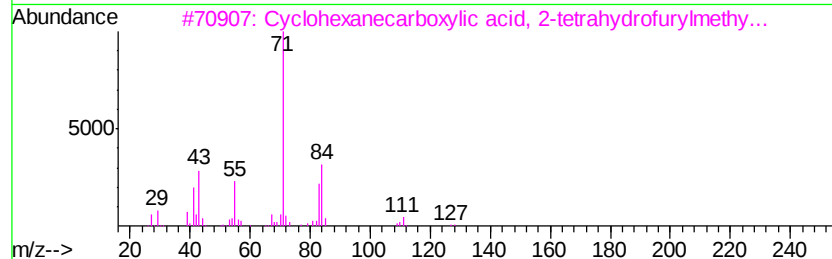
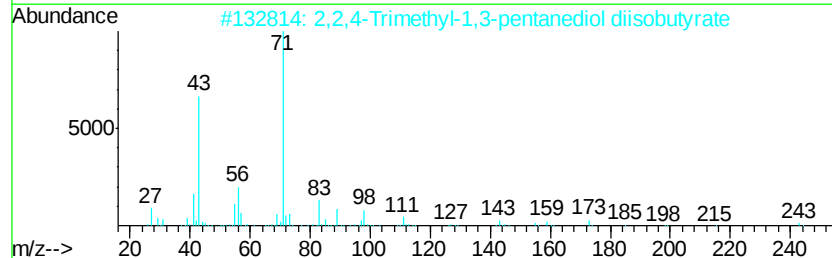
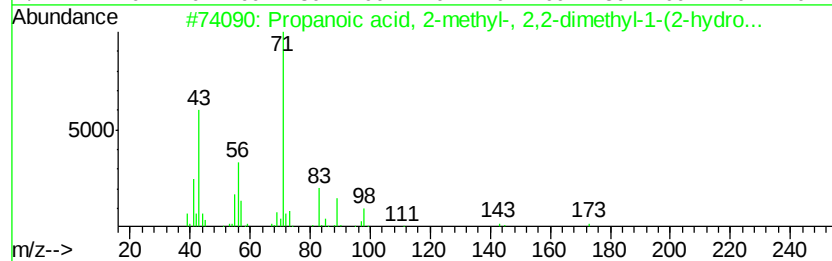
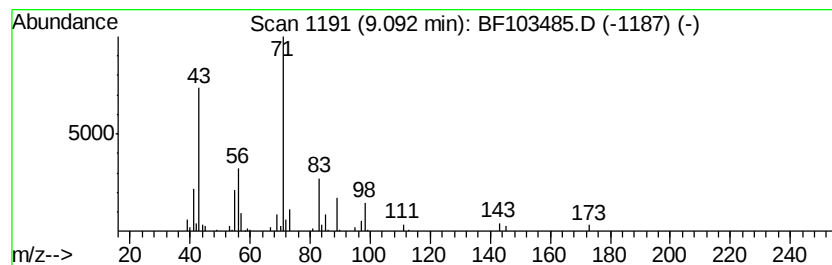
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.		
9.09	4.12 ng	204516	Acenaphthene-d10		9.91		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	91
2			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	59
3			Cyclohexanecarboxylic acid, 2-te...	212	C12H20O3	1000279-85-7	50
4			Butanoic acid, decyl ester	228	C14H28O2	005454-09-1	50
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50



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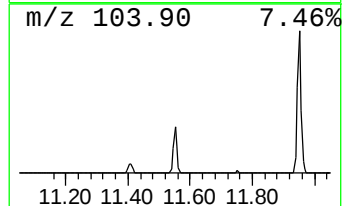
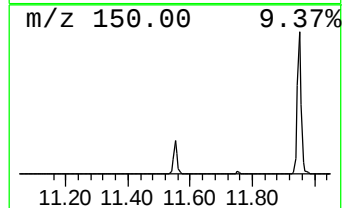
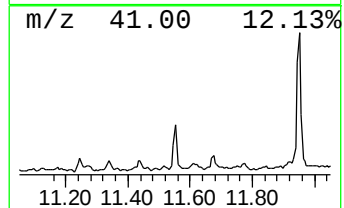
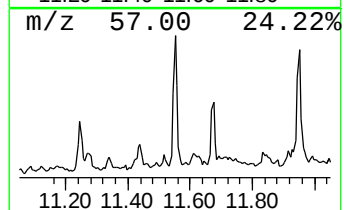
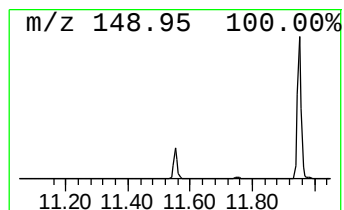
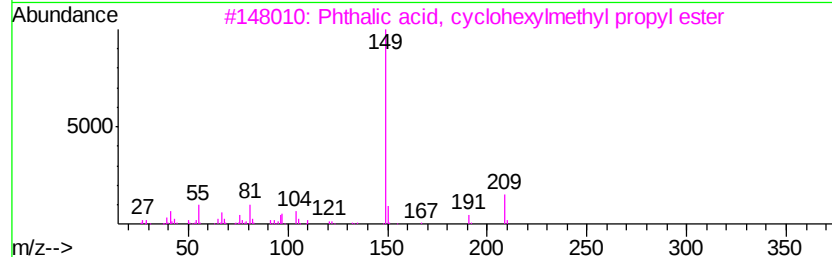
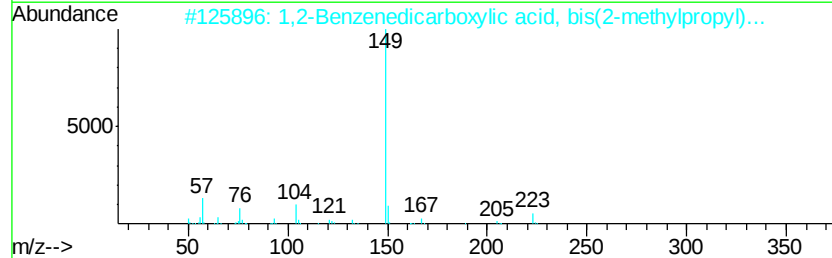
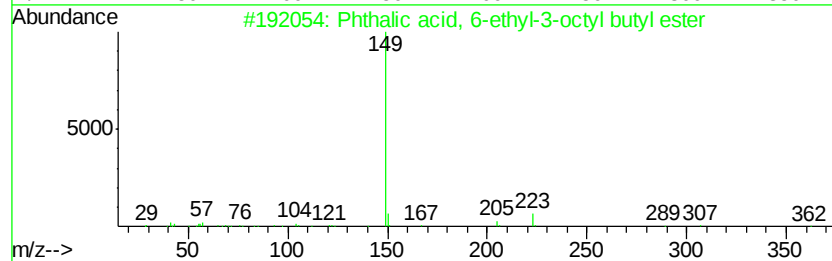
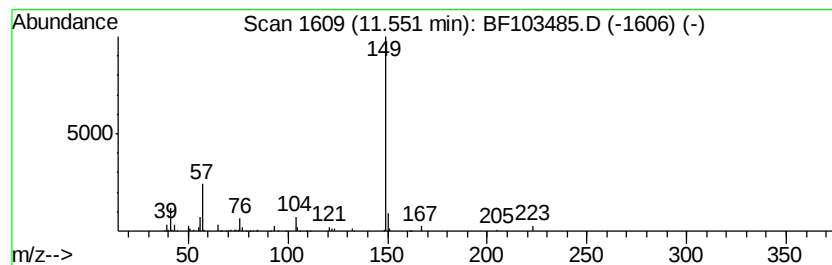
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Phthalic acid, 6-ethyl-3-oc... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	3.93 ng	153789	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phthalic acid, 6-ethyl-3-octyl b...	362	C22H34O4	1000315-17-4	83
2		1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	83
3		Phthalic acid, cyclohexylmethyl ...	304	C18H24O4	1000309-08-7	78
4		Phthalic acid, 2-ethoxyethyl pro...	280	C15H20O5	1000322-87-0	78
5		1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	78



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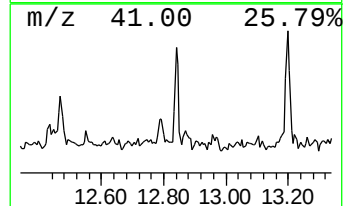
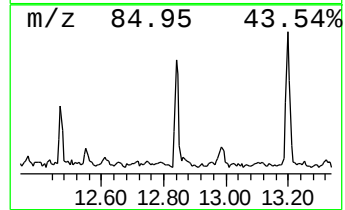
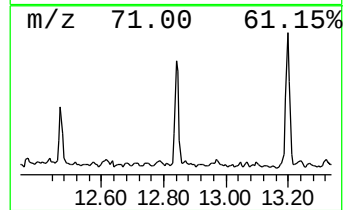
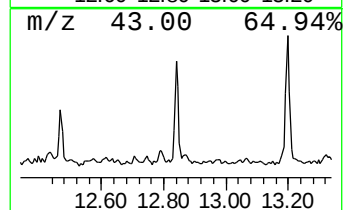
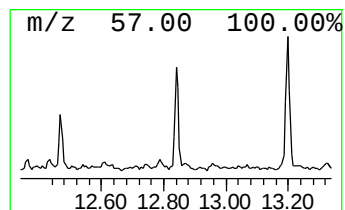
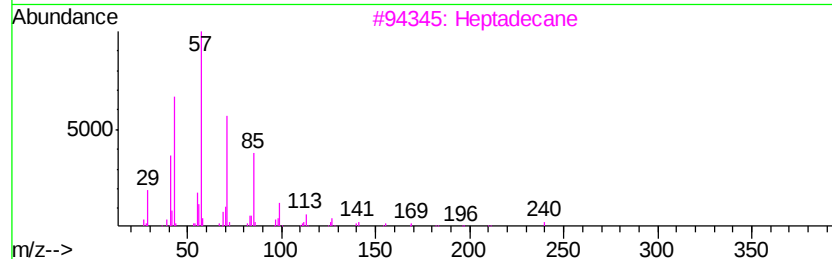
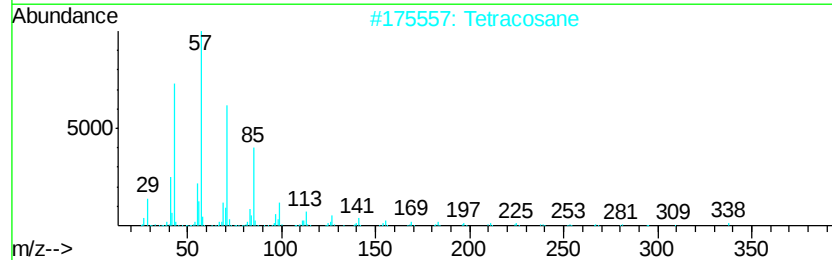
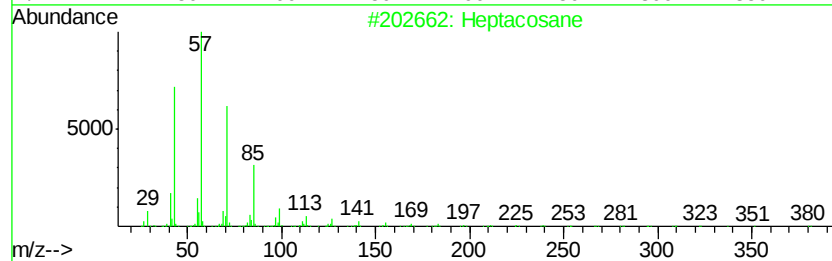
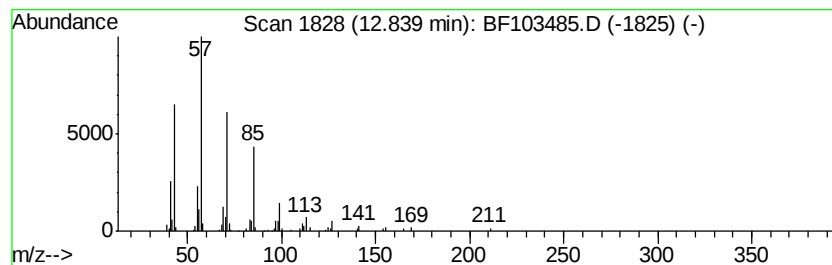
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.86 ng	88912	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Heptadecane	240	C17H36	000629-78-7	90
4		Octadecane	254	C18H38	000593-45-3	90
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030618\
Data File : BF103485.D
Acq On : 7 Mar 2018 4:32
Operator : SJ/JU
Sample : J1797-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SI-2

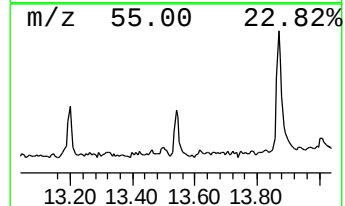
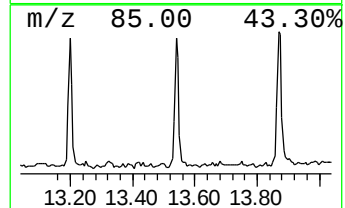
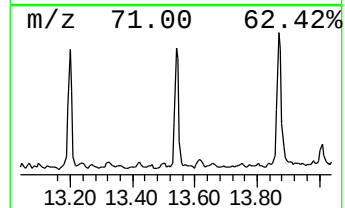
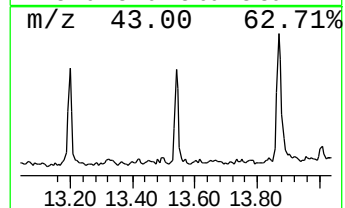
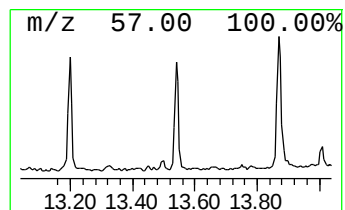
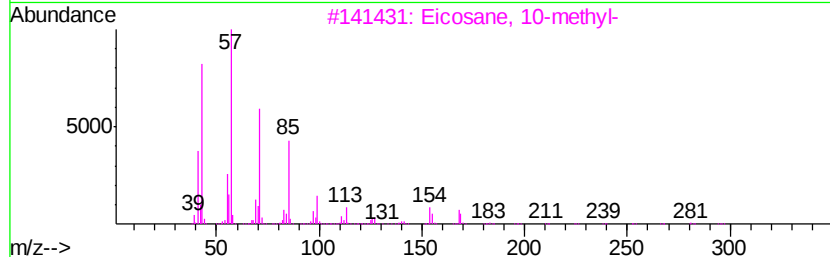
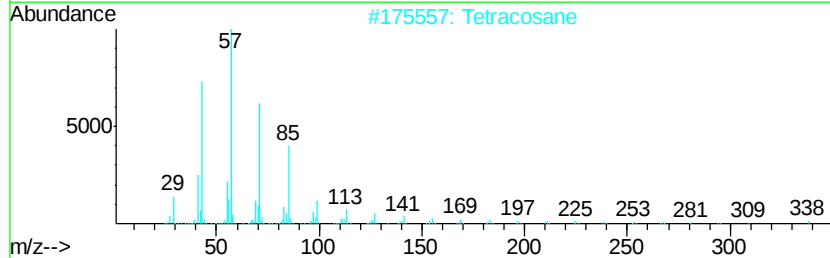
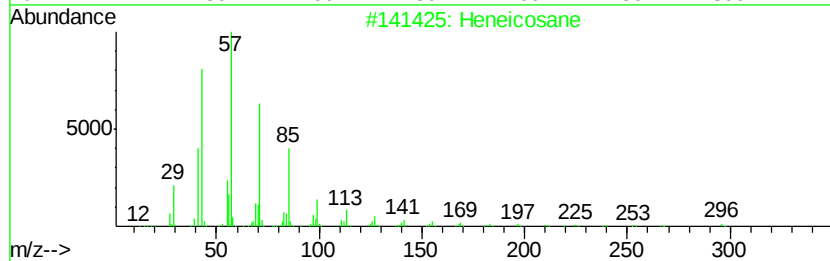
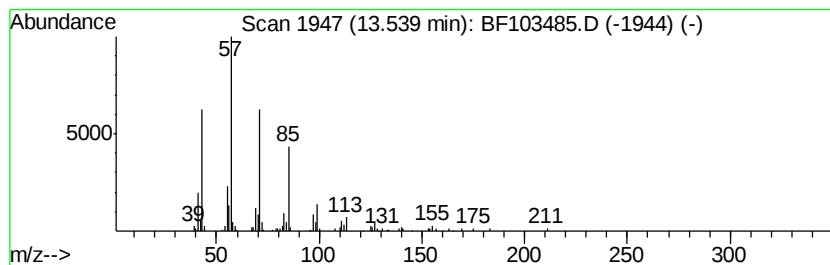
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	4.35 ng	135231	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Tetracosane		338	C24H50	000646-31-1	90
3	Eicosane, 10-methyl-		296	C21H44	054833-23-7	90
4	Octadecane		254	C18H38	000593-45-3	90
5	Hexadecane		226	C16H34	000544-76-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030618\
Data File : BF103485.D
Acq On : 7 Mar 2018 4:32
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Sample : J1797-02
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SI-2

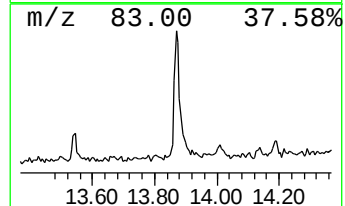
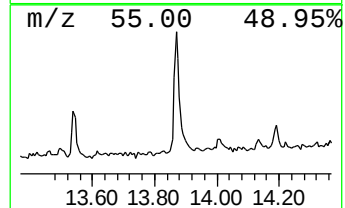
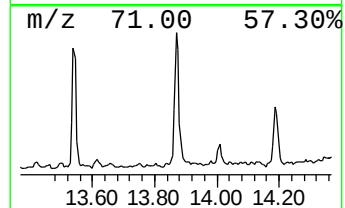
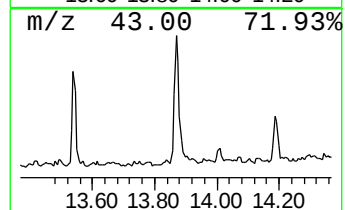
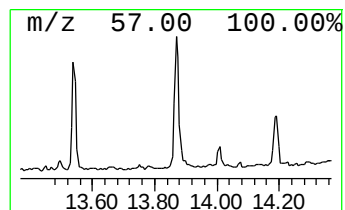
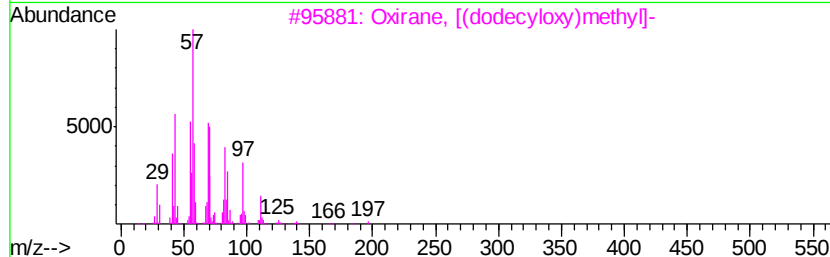
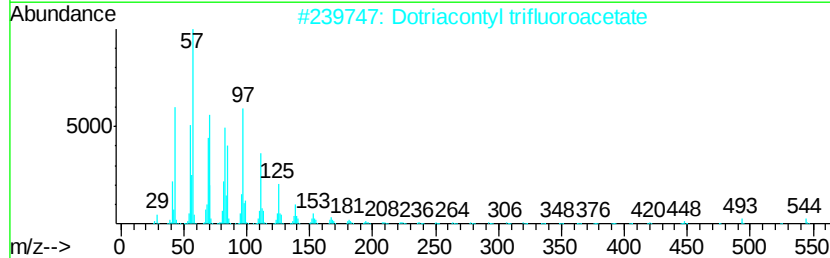
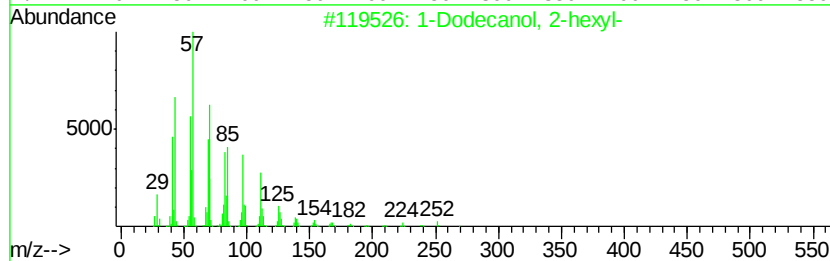
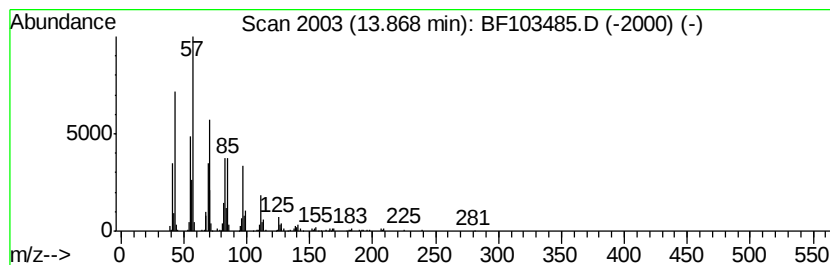
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Dodecanol, 2-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	9.49 ng	295167	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91
2		Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	91
3		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	90
4		Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	90
5		Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030618\
Data File : BF103485.D
Acq On : 7 Mar 2018 4:32
Operator : SJ/JU
Sample : J1797-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SI-2

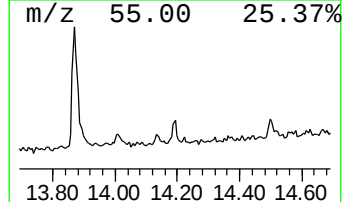
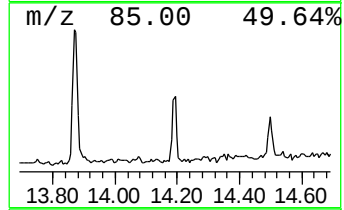
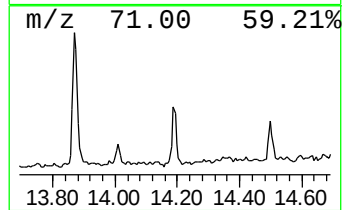
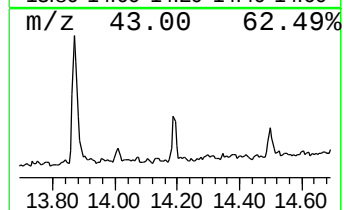
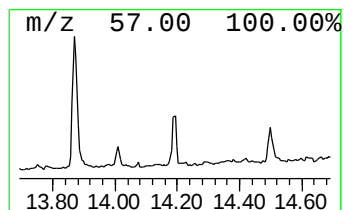
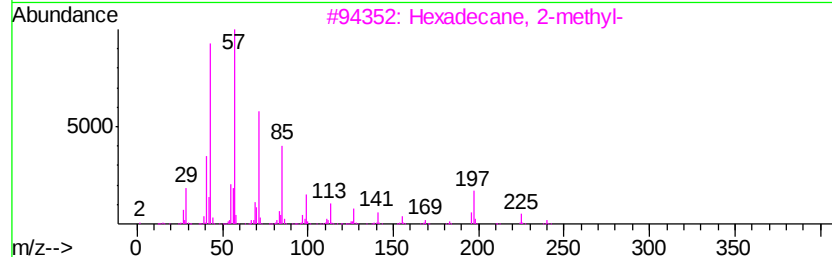
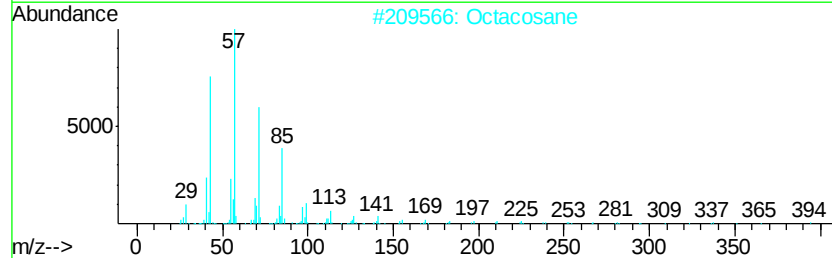
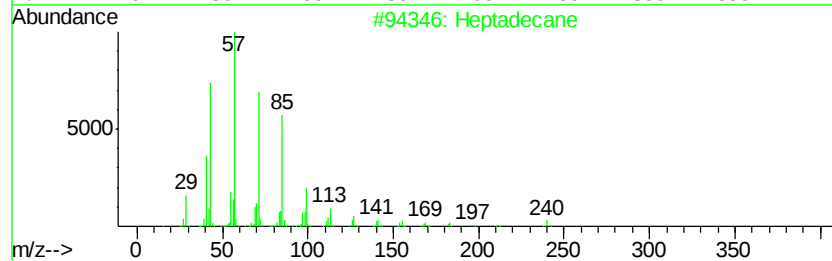
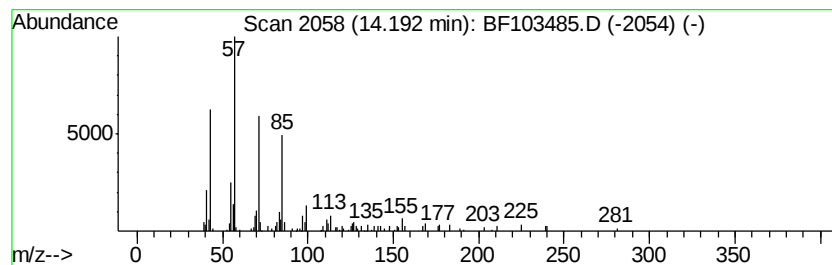
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	3.17 ng	98775	Chrysene-d12	14.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	93
2	Octacosane		394	C28H58	000630-02-4	87
3	Hexadecane, 2-methyl-		240	C17H36	001560-92-5	86
4	1-Iodo-2-methylnonane		268	C10H21I	1000101-47-9	64
5	Eicosane		282	C20H42	000112-95-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030618\
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Operator : SJ/JU
Sample : J1797-02
Misc :
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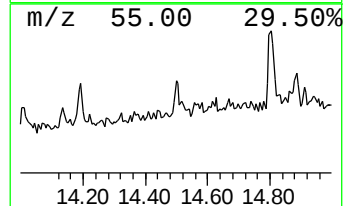
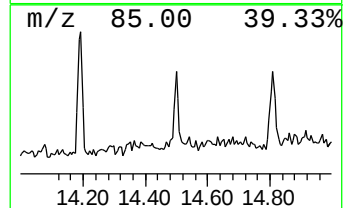
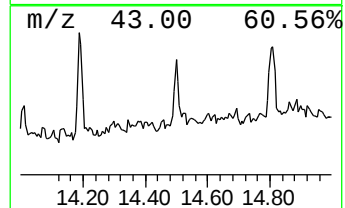
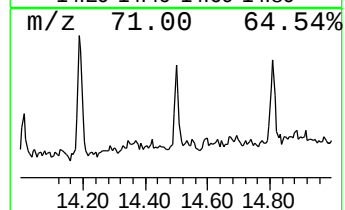
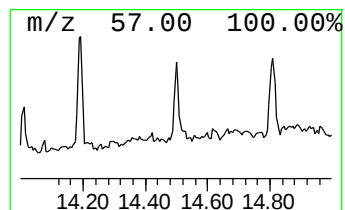
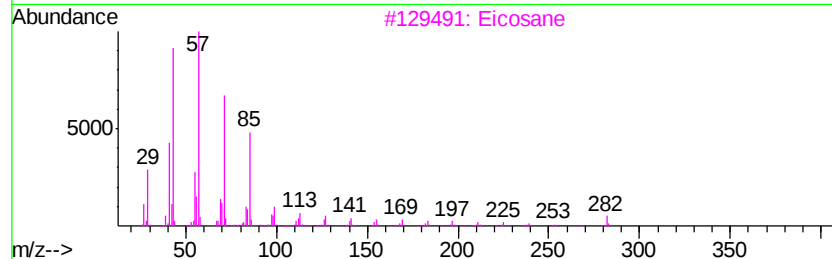
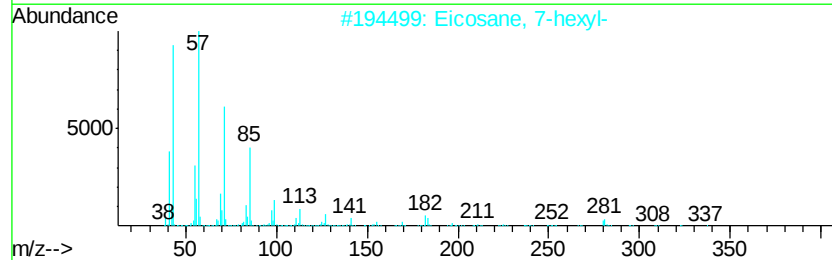
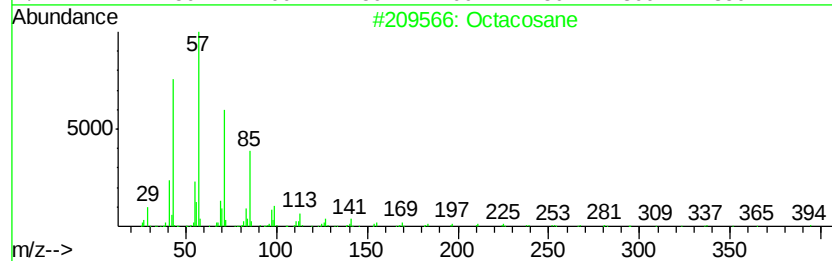
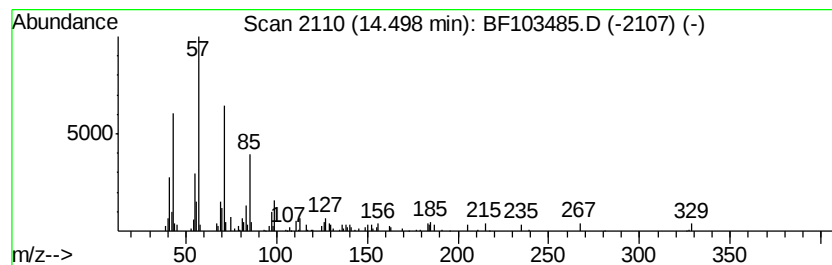
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.25 ng	69898	Chrysene-d12	14.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394 C28H58	000630-02-4	74
2	Eicosane, 7-hexyl-	366 C26H54	055333-99-8	72
3	Eicosane	282 C20H42	000112-95-8	72
4	Hexatriacontane	507 C36H74	000630-06-8	72
5	10-Methylnonadecane	282 C20H42	056862-62-5	68



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103485.D
Acq On : 7 Mar 2018 4:32
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Sample : J1797-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

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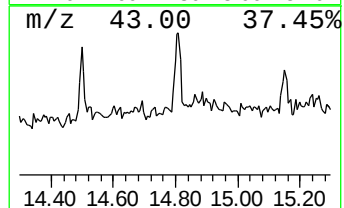
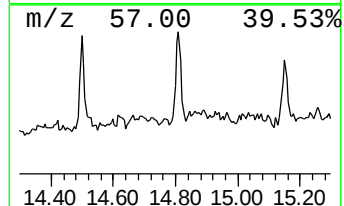
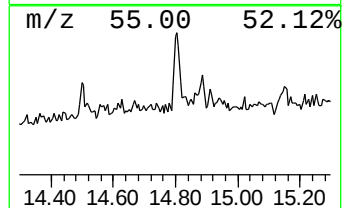
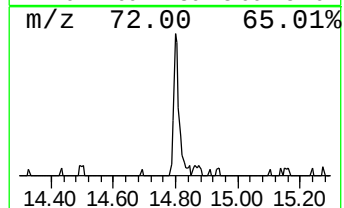
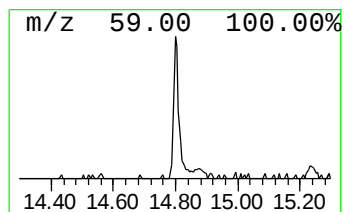
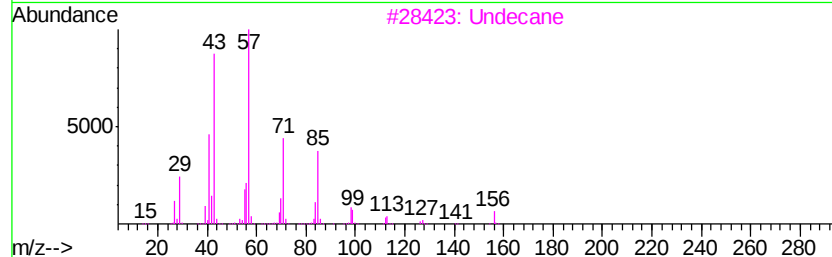
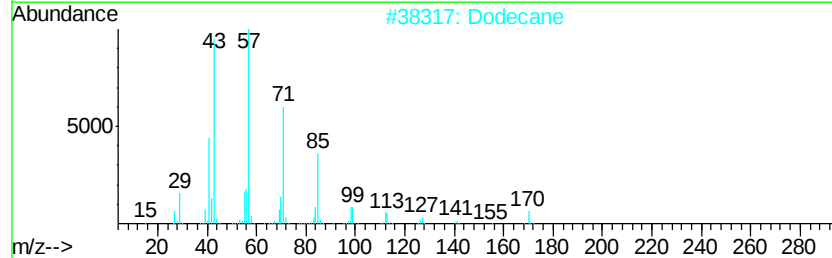
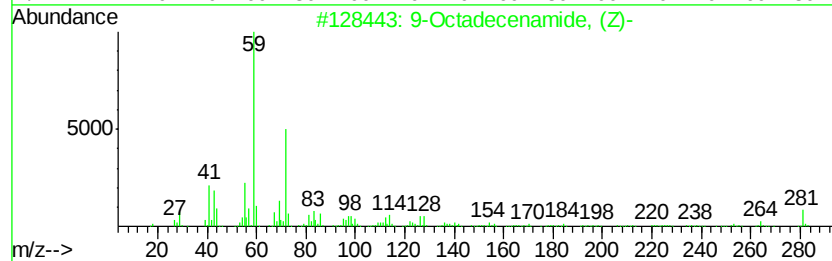
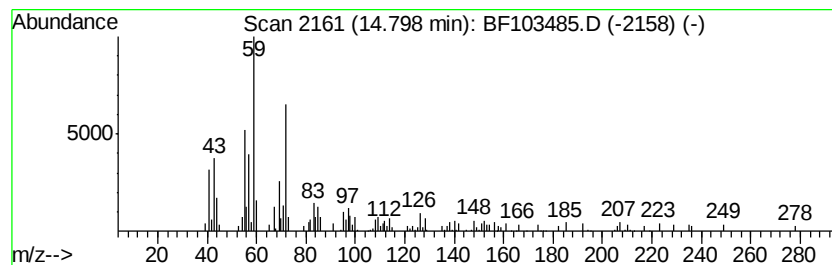
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown14.80 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.11 ng	127953	Chrysene-d12	14.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	49
2			Dodecane	170	C12H26	000112-40-3	40
3			Undecane	156	C11H24	001120-21-4	25
4			Tridecane	184	C13H28	000629-50-5	25
5			Carbonic acid, 2-methoxyethyl ph...	196	C10H12O4	1000357-86-8	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030618\
Data File : BF103485.D
Acq On : 7 Mar 2018 4:32
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Sample : J1797-02
Misc :
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ClientSampleId :
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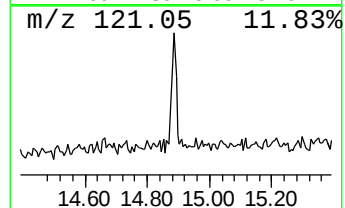
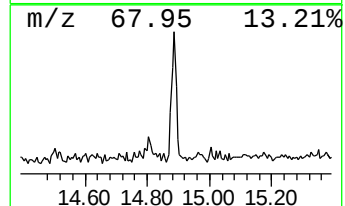
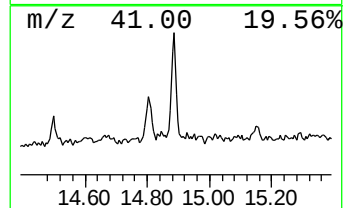
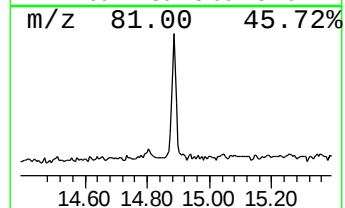
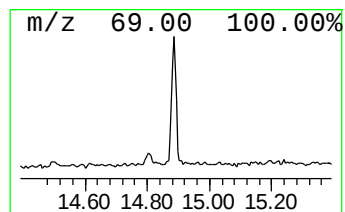
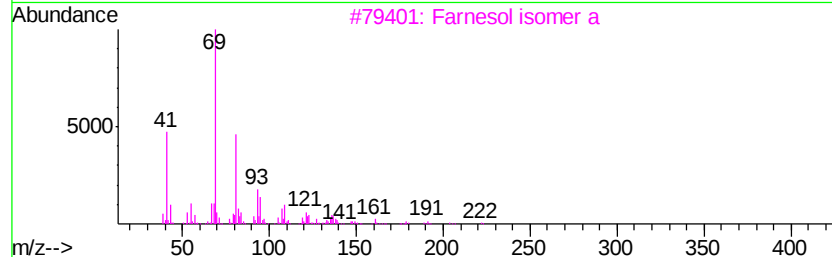
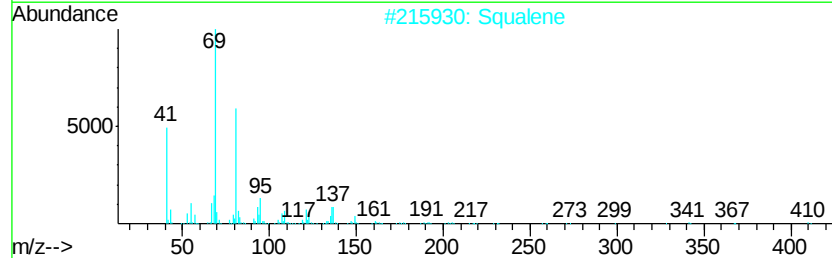
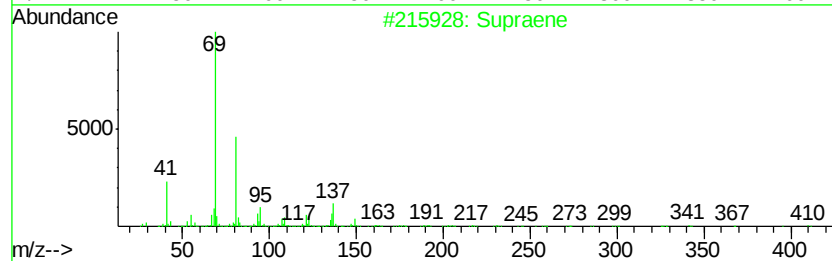
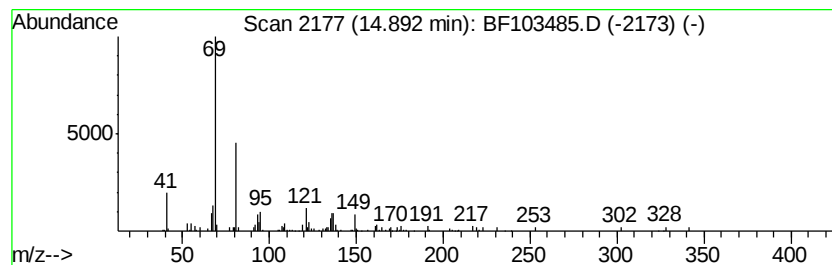
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	6.00 ng	132452	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	90
2		Squalene	410	C30H50	000111-02-4	90
3		Farnesol isomer a	222	C15H26O	1000108-92-4	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030618\
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Sample : J1797-02
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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unknown6.64	6.64	69.3	ng	2714390	1	6.87	783977	20.0
Propanoic acid, 2...	9.09	4.1	ng	204516	3	9.91	992272	20.0
Phthalic acid, 6-...	11.55	3.9	ng	153789	4	11.40	782600	20.0
Heptacosane	12.84	2.9	ng	88912	5	14.06	622357	20.0
Heneicosane	13.54	4.3	ng	135231	5	14.06	622357	20.0
1-Dodecanol, 2-he...	13.87	9.5	ng	295167	5	14.06	622357	20.0
Heptadecane	14.19	3.2	ng	98775	5	14.06	622357	20.0
Octacosane	14.50	2.3	ng	69898	5	14.06	622357	20.0
unknown14.80	14.80	4.1	ng	127953	5	14.06	622357	20.0
Supraene	14.89	6.0	ng	132452	6	15.57	441520	20.0