

Data Path : Z:\HPCHEM1\BNA F\DATA\BF113017\
 Data File : BF101035.D
 Acq On : 30 Nov 2017 23:19
 Operator : SJ/JU
 Sample : I6630-01 2X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P004-S001-0001-01

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-BF113017.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	5.063	503	506	515	rBV	36808	38405	6.48%	0.582%
2	5.469	571	575	585	rBV	536024	492793	83.17%	7.466%
3	6.480	743	747	758	rBV	618347	539571	91.06%	8.175%
4	6.622	767	771	774	rBV	667985	536151	90.48%	8.123%
5	6.851	807	810	814	rBV	375760	322665	54.45%	4.889%
6	7.010	833	837	840	rBV	489070	409073	69.04%	6.198%
7	7.257	876	879	884	rBB	22292	19488	3.29%	0.295%
8	7.416	902	906	909	rBV	385521	302716	51.09%	4.586%
9	8.133	1025	1028	1032	rBV	460625	395238	66.70%	5.988%
10	9.210	1207	1211	1214	rBV	742899	592542	100.00%	8.977%
11	9.604	1274	1278	1283	rBB	15152	13509	2.28%	0.205%
12	9.810	1308	1313	1318	rBV	11045	11033	1.86%	0.167%
13	9.892	1323	1327	1331	rBV	435626	352121	59.43%	5.335%
14	10.680	1458	1461	1464	rBV	289863	240510	40.59%	3.644%
15	10.786	1476	1479	1483	rBV	8350	9189	1.55%	0.139%
16	10.915	1498	1501	1509	rVB3	4240	8075	1.36%	0.122%
17	11.151	1538	1541	1544	rBV	33261	28681	4.84%	0.435%
18	11.233	1551	1555	1558	rBV	8000	7404	1.25%	0.112%
19	11.380	1576	1580	1583	rBV	353309	291842	49.25%	4.422%
20	11.674	1626	1630	1635	rVB	6860	7861	1.33%	0.119%
21	11.898	1664	1668	1672	rBV	30292	29275	4.94%	0.444%
22	12.068	1693	1697	1701	rBV2	5881	7168	1.21%	0.109%
23	12.680	1796	1801	1805	rBV4	7400	9655	1.63%	0.146%
24	12.962	1845	1849	1852	rBV	549001	449708	75.89%	6.813%
25	13.645	1962	1965	1968	rBV4	7741	9825	1.66%	0.149%
26	13.780	1983	1988	1989	rBV5	6308	9493	1.60%	0.144%
27	13.821	1991	1995	1997	rVV	111974	107217	18.09%	1.624%
28	13.851	1997	2000	2005	rVB	39700	46568	7.86%	0.706%
29	13.986	2020	2023	2026	rBV	57075	51346	8.67%	0.778%
30	14.021	2026	2029	2034	rVB	405333	356528	60.17%	5.402%
31	14.103	2040	2043	2045	rBV3	13143	13180	2.22%	0.200%
32	14.145	2047	2050	2053	rVV	90608	84609	14.28%	1.282%
33	14.186	2054	2057	2060	rVV	151004	131641	22.22%	1.994%
34	14.215	2060	2062	2064	rVV	45135	37268	6.29%	0.565%

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ClientSampleId :
P004-S001-0001-01

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.239	2064	2066	2070	rVB	54414	44006	7.43%	0.667%
36	14.474	2104	2106	2109	rBV	23757	27400	4.62%	0.415%
37	14.533	2113	2116	2119	rBV3	23558	25391	4.29%	0.385%
38	14.856	2169	2171	2177	rVB2	20885	23607	3.98%	0.358%
39	15.498	2275	2280	2285	rBV	236621	289076	48.79%	4.380%
40	15.933	2350	2354	2359	rVB2	30706	40630	6.86%	0.616%
41	16.727	2487	2489	2494	rVB5	9306	12310	2.08%	0.187%
42	17.027	2536	2540	2545	rVB2	35378	62898	10.61%	0.953%
43	17.127	2553	2557	2565	rVB9	18260	37733	6.37%	0.572%
44	18.568	2795	2802	2809	rVB10	24962	74902	12.64%	1.135%

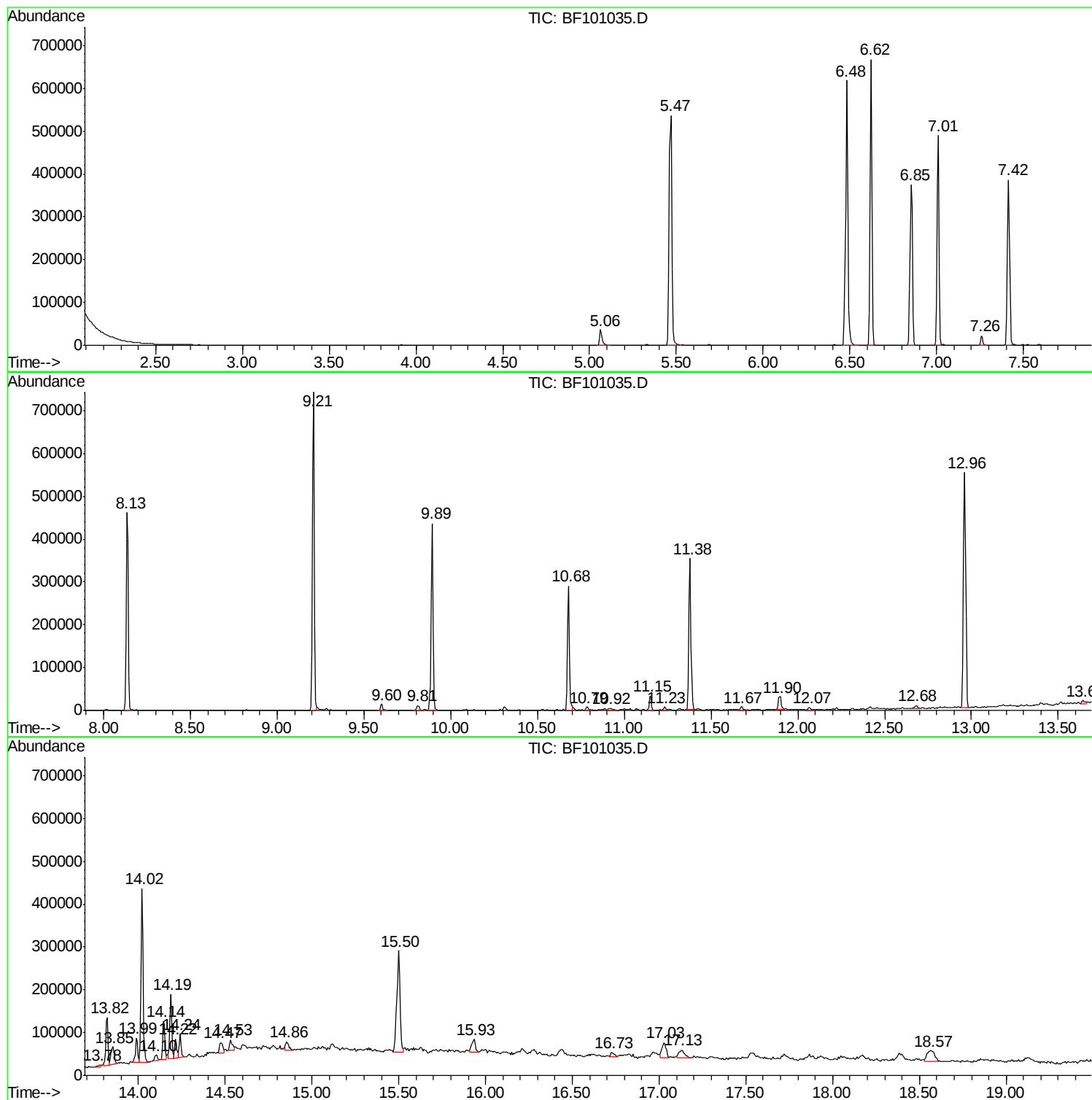
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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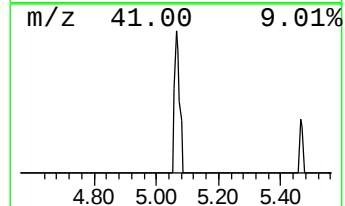
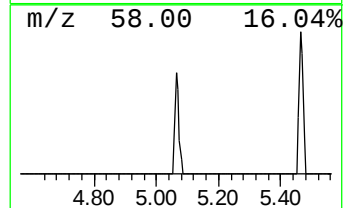
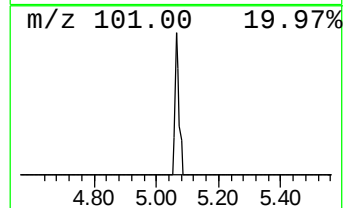
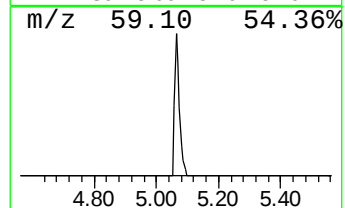
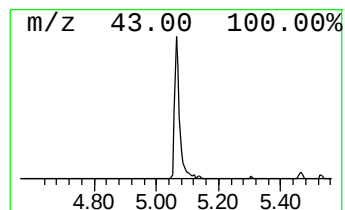
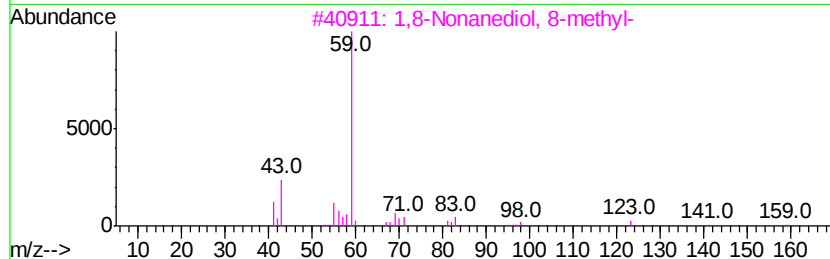
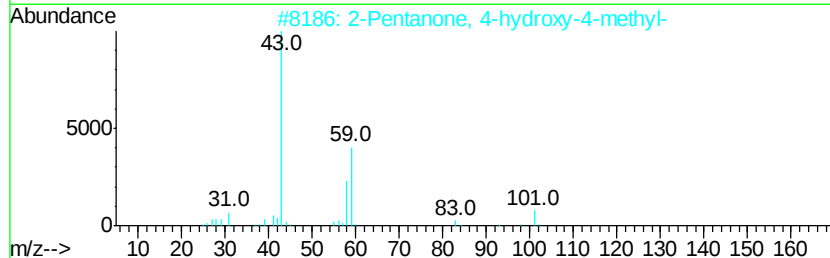
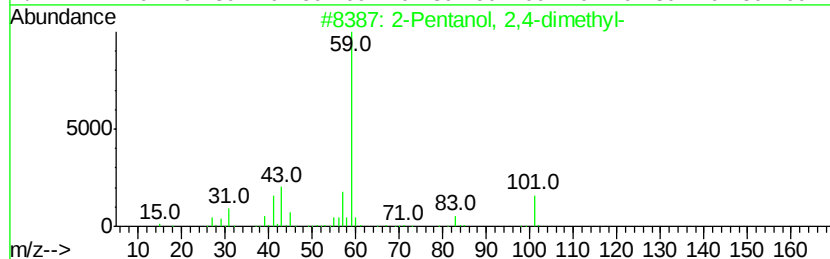
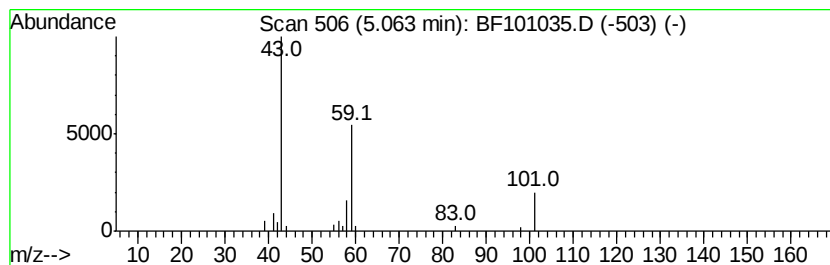
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanol, 2,4-dimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	2.38 ng	38405	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	59
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	32
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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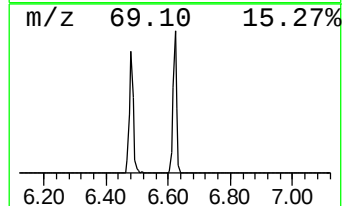
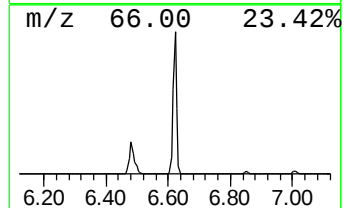
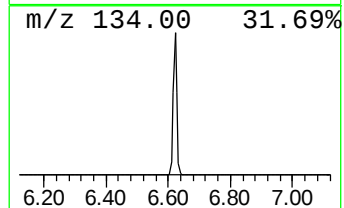
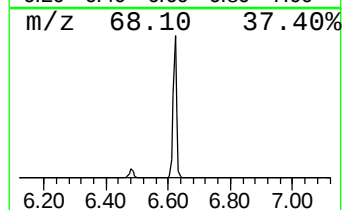
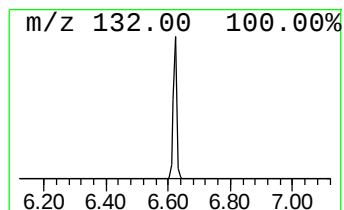
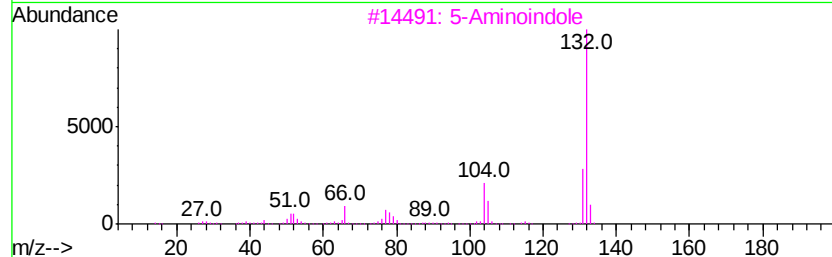
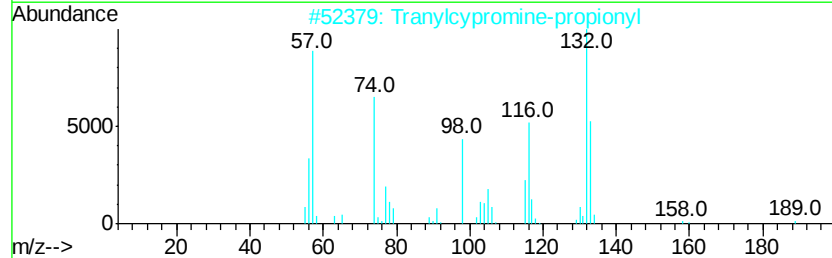
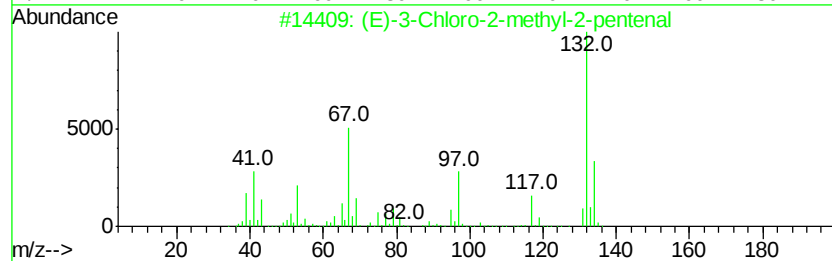
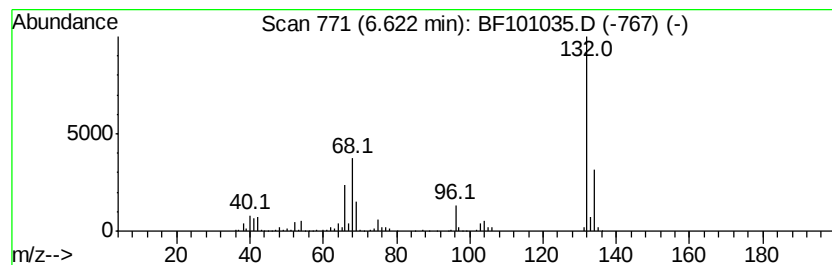
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	33.23 ng	536151	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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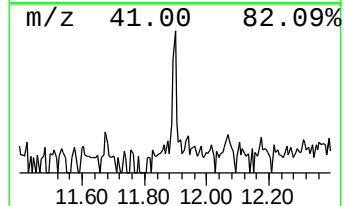
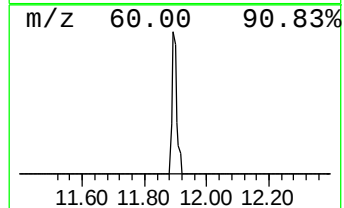
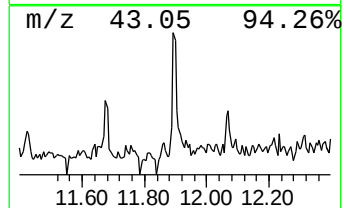
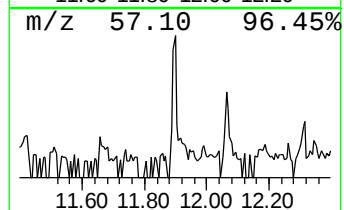
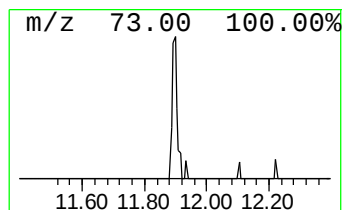
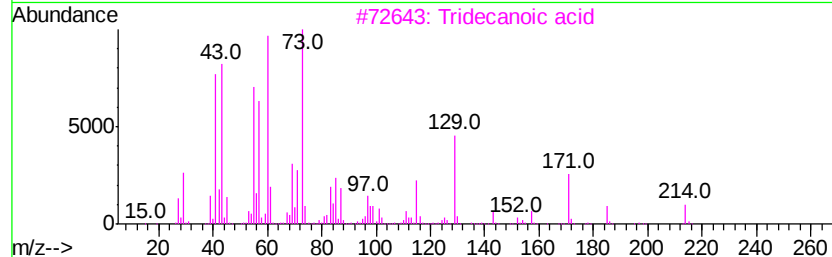
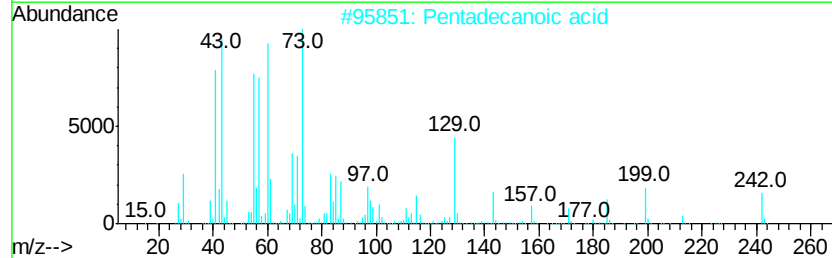
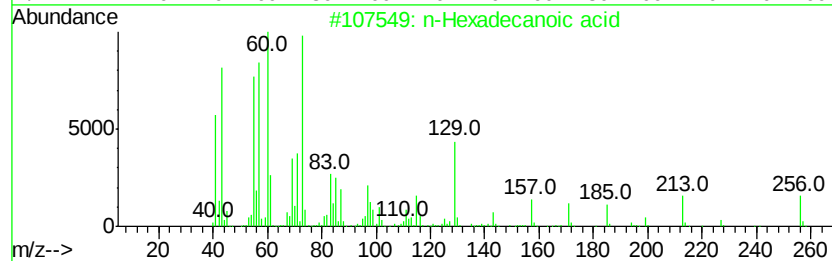
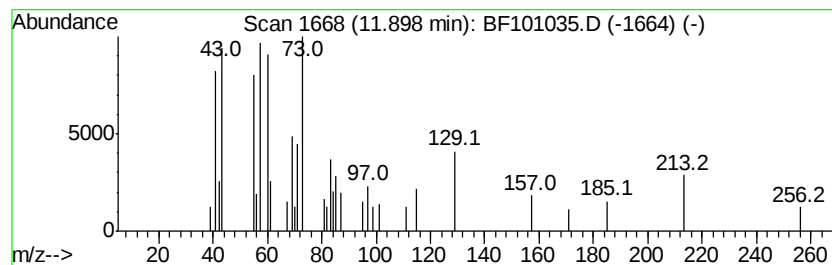
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.01 ng	29275	Phenanthrene-d10	11.38

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14
5		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	14



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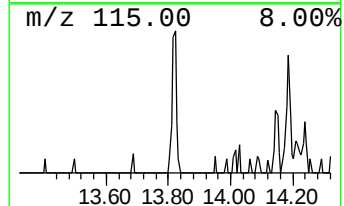
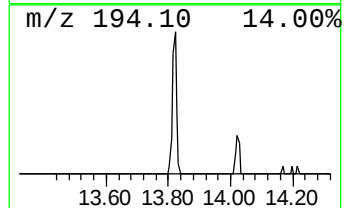
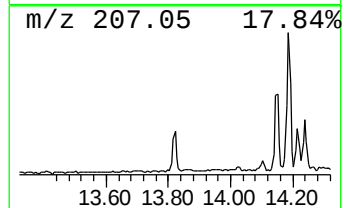
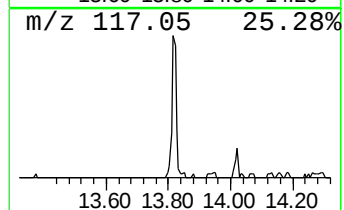
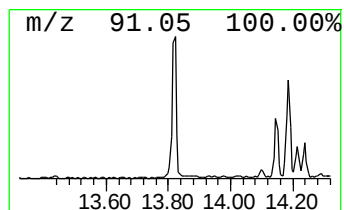
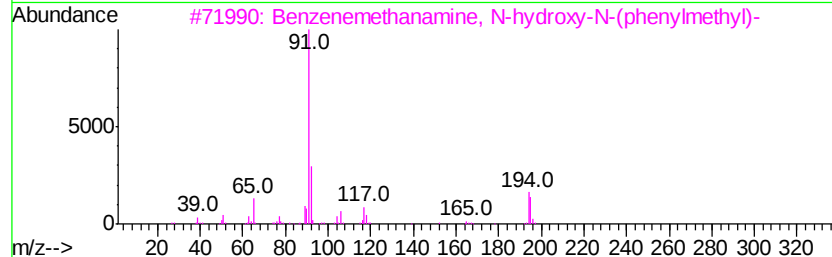
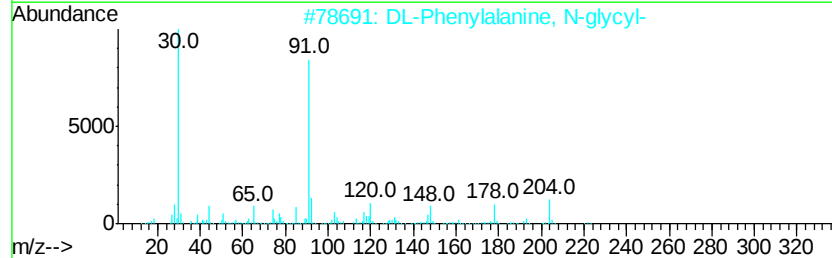
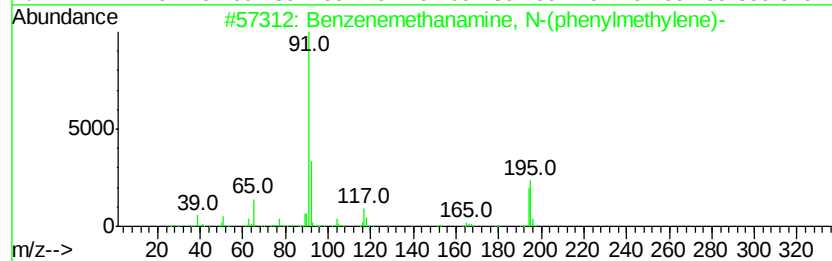
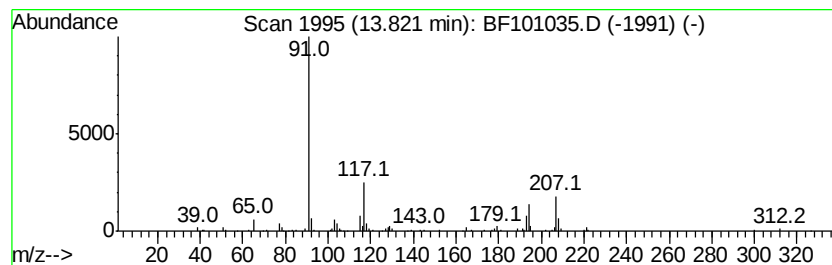
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.82 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	6.01 ng	107217	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenemethanamine, N-(phenylmet...	195	C14H13N	000780-25-6	32
2			DL-Phenylalanine, N-glycyl-	222	C11H14N2O3	000721-66-4	25
3			Benzenemethanamine, N-hydroxy-N-...	213	C14H15NO	000621-07-8	23
4			Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	16
5			N-Benzyl-1H-benzimidazole	208	C14H12N2	004981-92-4	10



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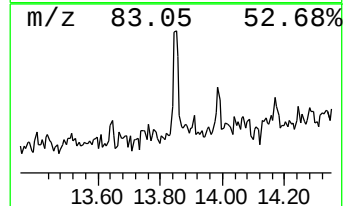
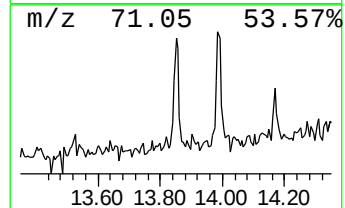
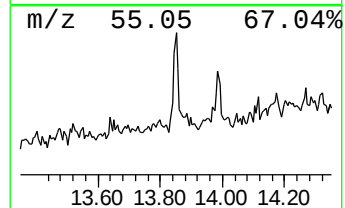
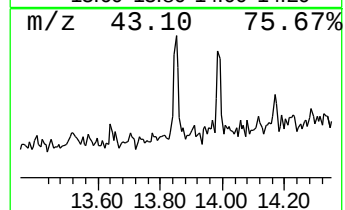
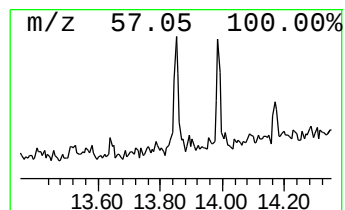
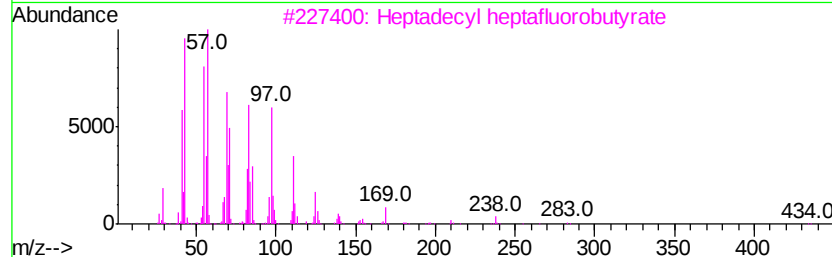
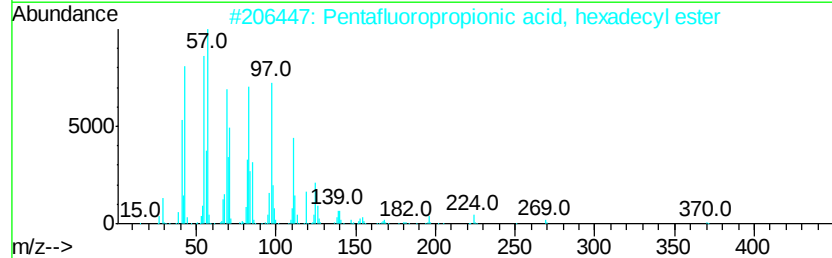
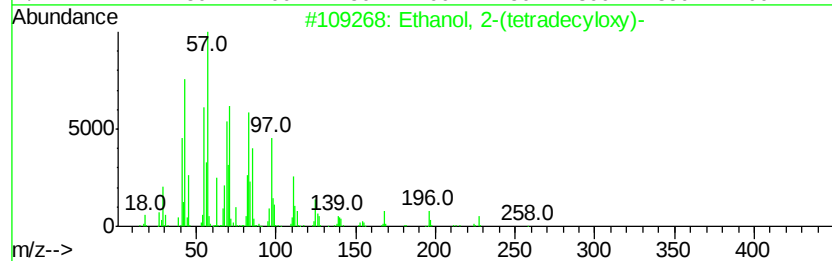
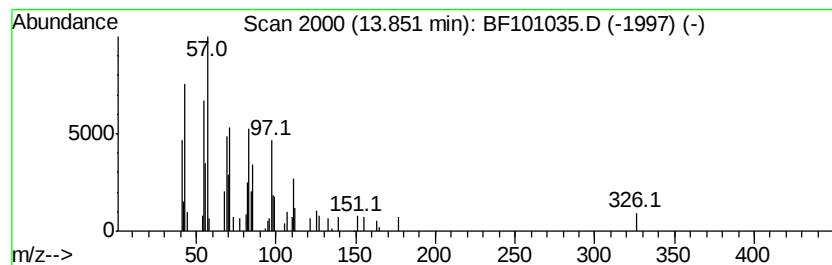
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.85	2.61 ng	46568	Chrysene-d12		14.02		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
2			Pentafluoropropionic acid, hexadecyl-	388	C19H33F5O2	006222-07-7	87
3			Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	83
4			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	80
5			Trichloroacetic acid, tetradecyl-	358	C16H29Cl3O2	074339-52-9	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF113017\
Data File : BF101035.D
Acq On : 30 Nov 2017 23:19
Operator : SJ/JU
Sample : I6630-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-S001-0001-01

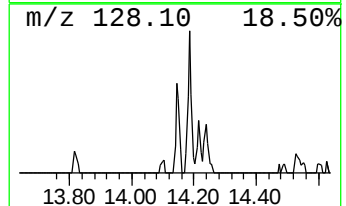
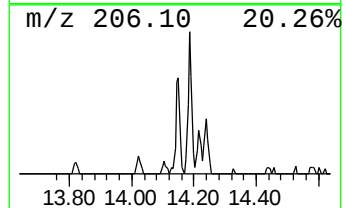
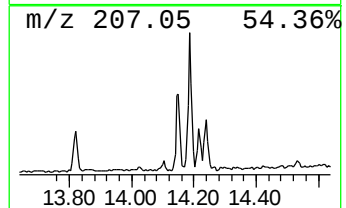
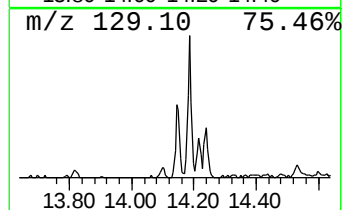
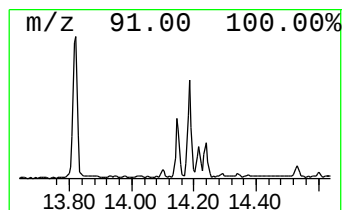
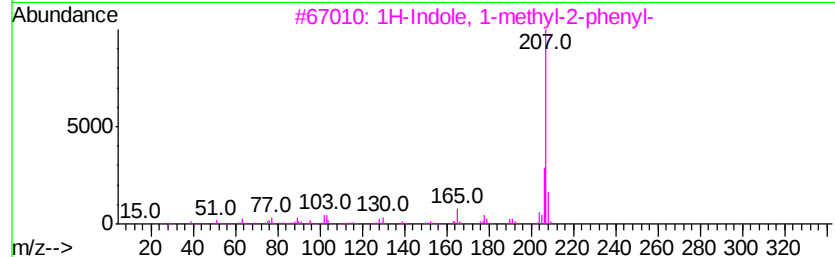
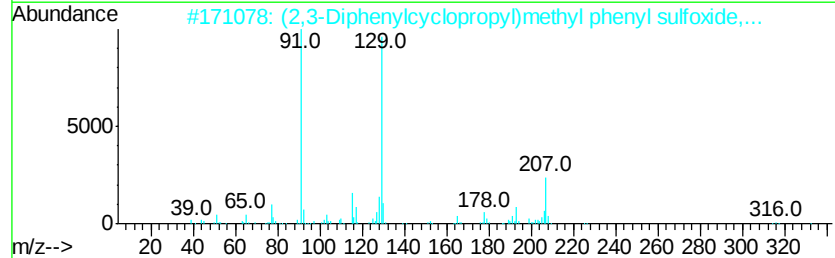
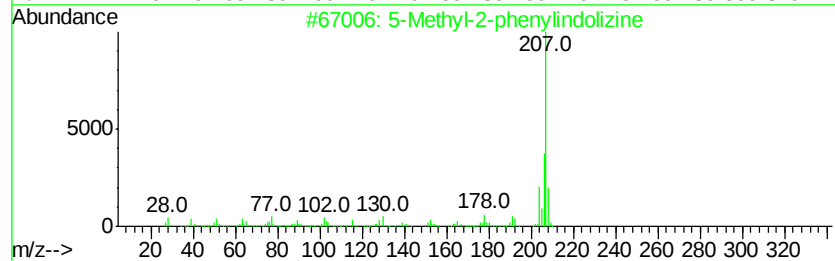
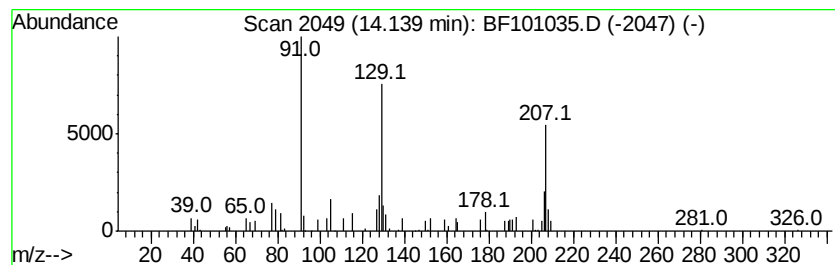
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Methyl-2-phenylindolizine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	4.75 ng	84609	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	60
2			(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	56
3			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	55
4			1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	49
5			1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113017\
Data File : BF101035.D
Acq On : 30 Nov 2017 23:19
Operator : SJ/JU
Sample : I6630-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P004-S001-0001-01

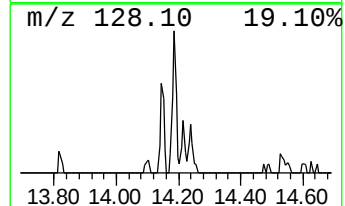
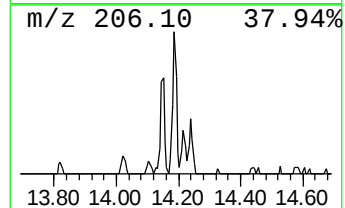
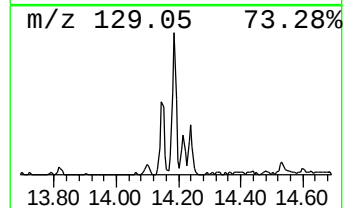
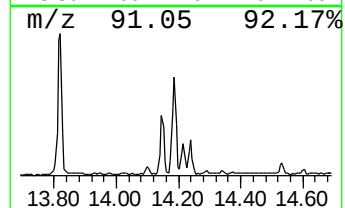
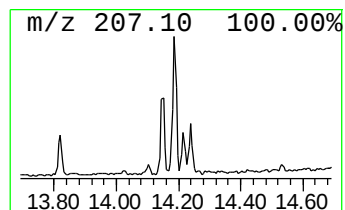
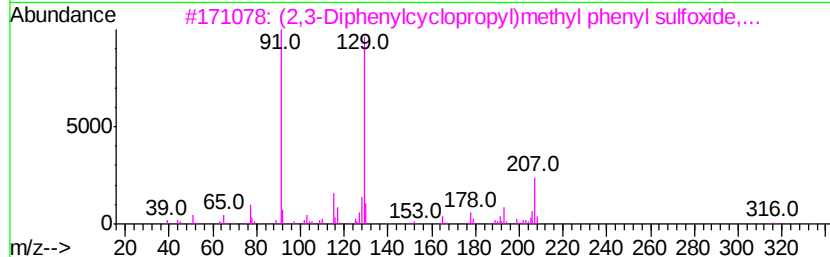
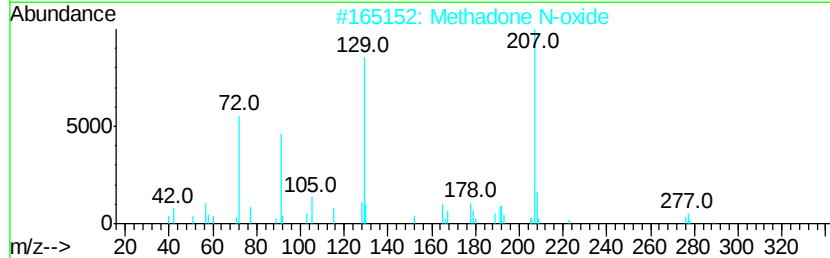
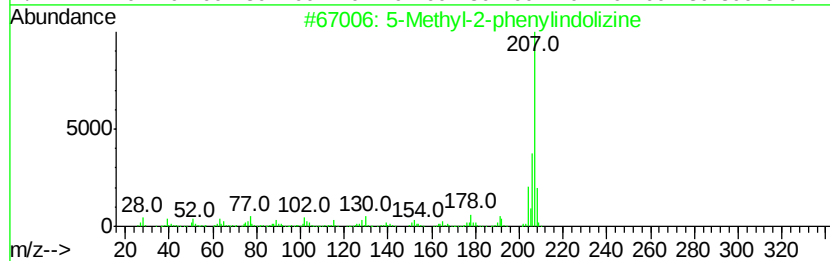
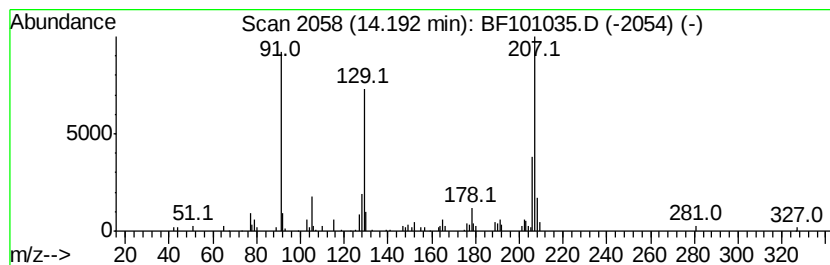
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.19 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	7.38 ng	131641	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	45
2		Methadone N-oxide	325	C21H27NO2	1000120-80-7	45
3		(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	43
4		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
5		1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF113017\
Data File : BF101035.D
Acq On : 30 Nov 2017 23:19
Operator : SJ/JU
Sample : I6630-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

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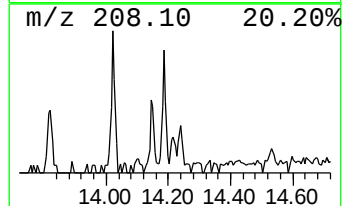
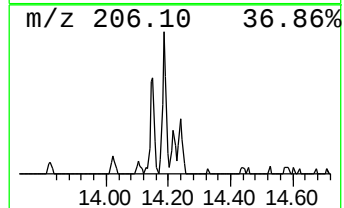
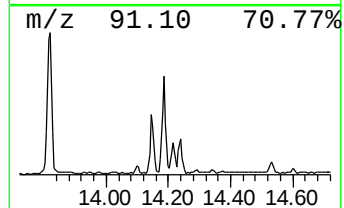
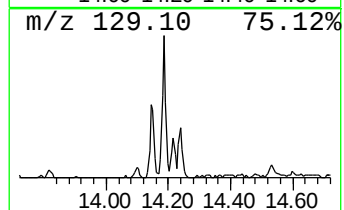
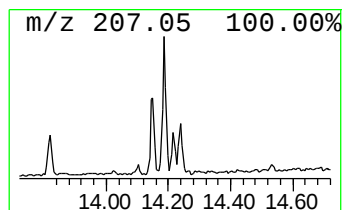
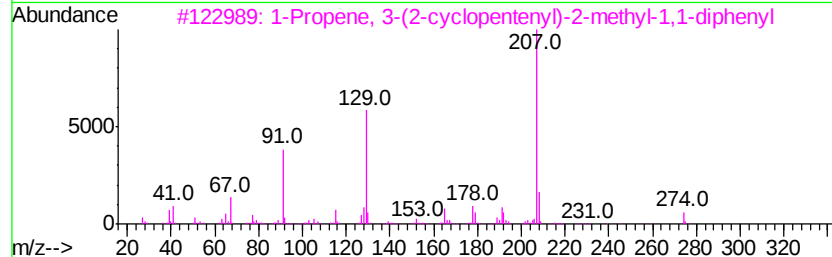
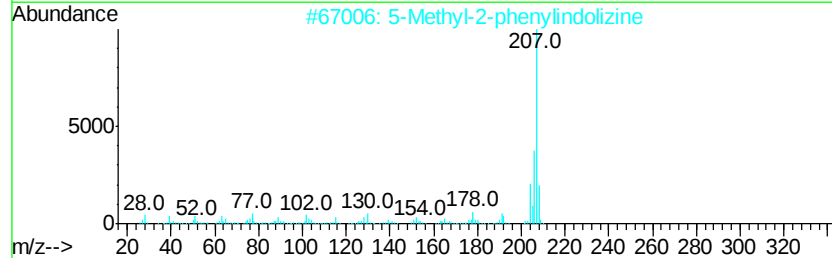
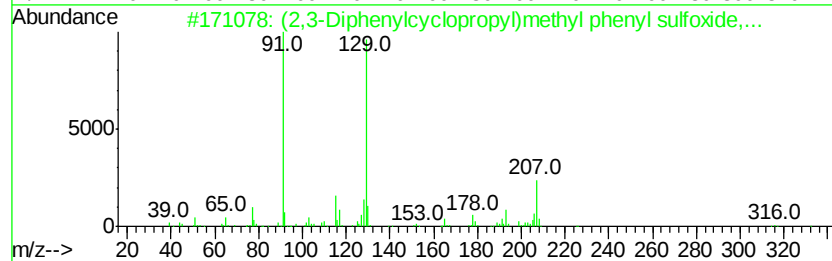
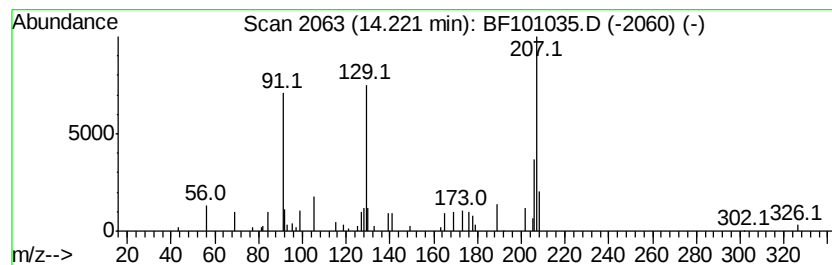
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 (2,3-Diphenylcyclopropyl)me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.22	2.09 ng	37268	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	78
2		5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	60
3		1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	53
4		1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	49
5		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113017\
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Acq On : 30 Nov 2017 23:19
Operator : SJ/JU
Sample : I6630-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

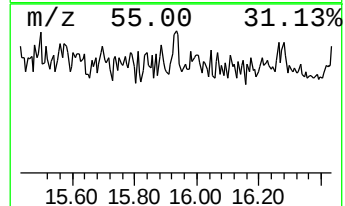
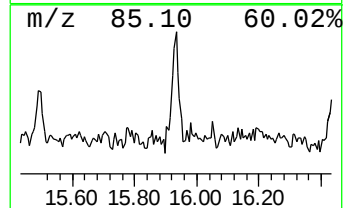
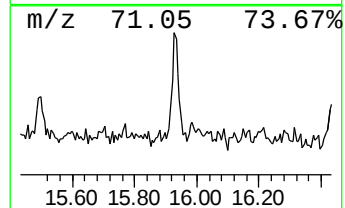
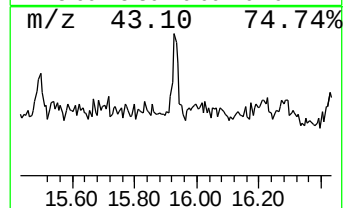
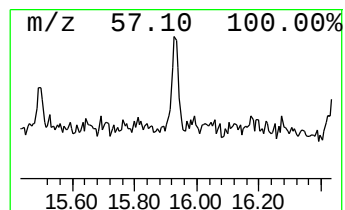
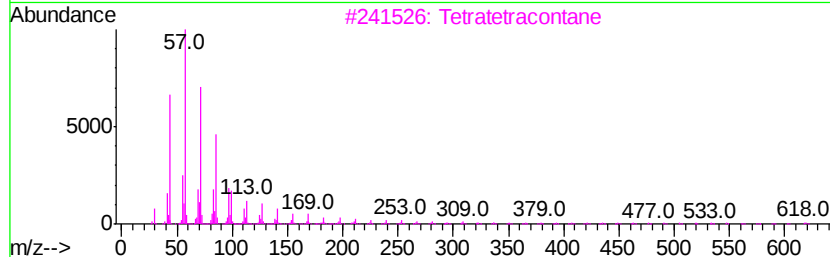
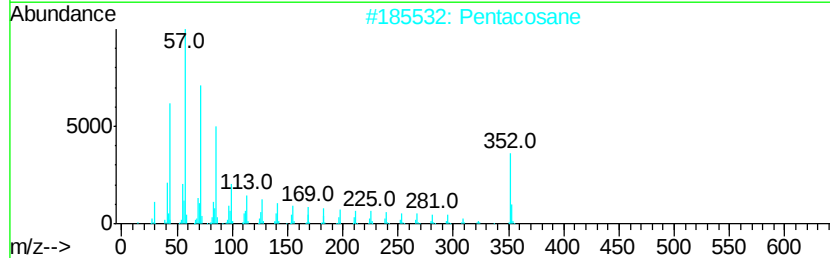
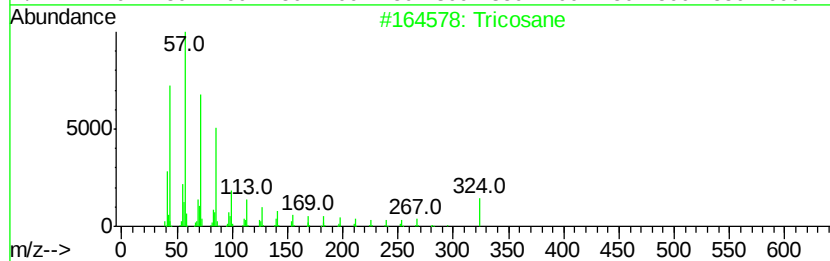
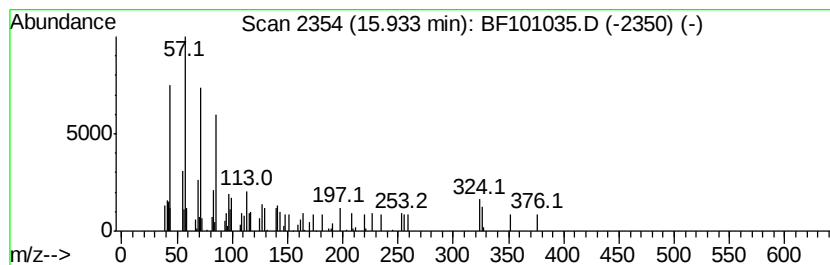
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.81 ng	40630	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Tricosane	324 C23H48	000638-67-5	76
2	Pentacosane	352 C25H52	000629-99-2	59
3	Tetratetracontane	619 C44H90	007098-22-8	53
4	Docosane, 11-butyl-	366 C26H54	013475-76-8	53
5	Octadecane, 3-ethyl-5-(2-ethylbu...	366 C26H54	055282-12-7	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF113017\
Data File : BF101035.D
Acq On : 30 Nov 2017 23:19
Operator : SJ/JU
Sample : I6630-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P004-S001-0001-01

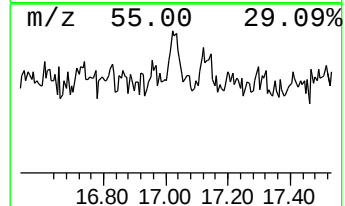
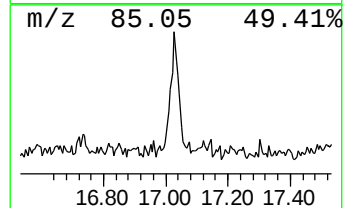
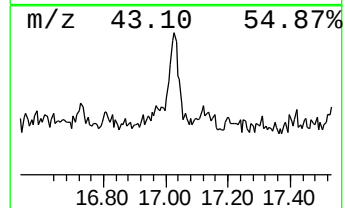
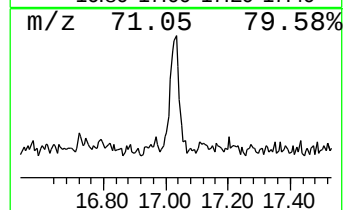
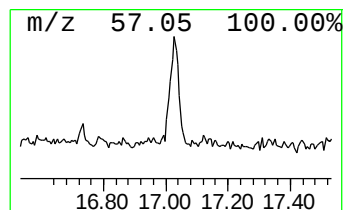
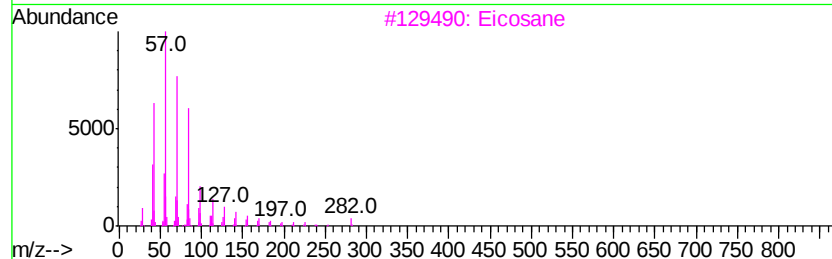
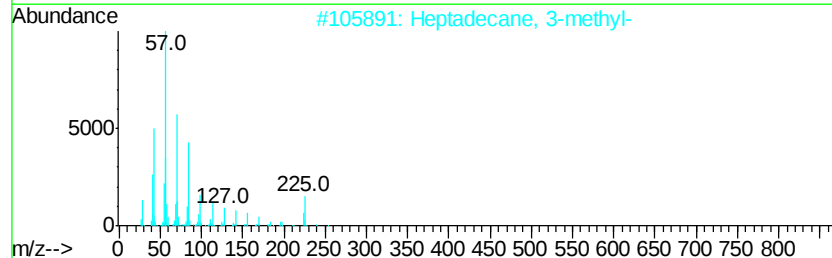
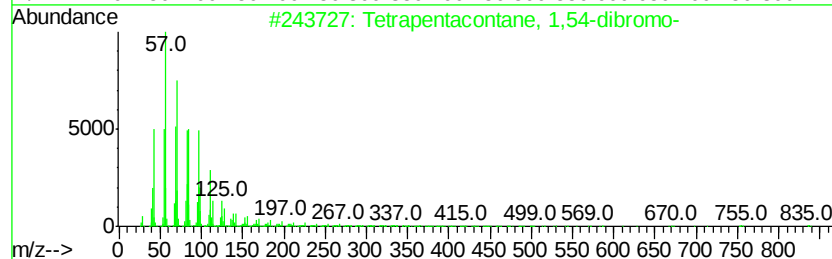
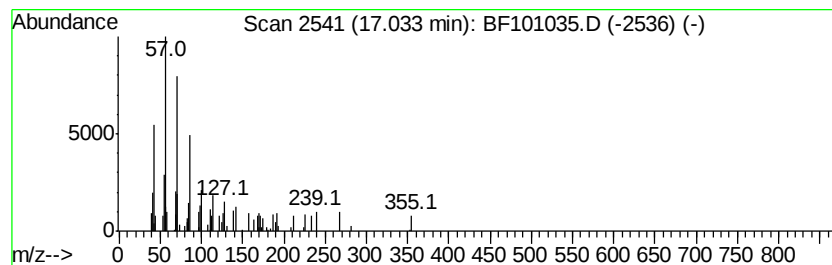
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetrapentacontane, 1,54-dib... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.03	4.35 ng	62898	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	59
2			Heptadecane, 3-methyl-	254	C18H38	006418-44-6	58
3			Eicosane	282	C20H42	000112-95-8	58
4			Tetracosane	338	C24H50	000646-31-1	58
5			Pentacosane	352	C25H52	000629-99-2	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113017\
Data File : BF101035.D
Acq On : 30 Nov 2017 23:19
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Sample : I6630-01 2X
Misc :
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ClientSampleId :
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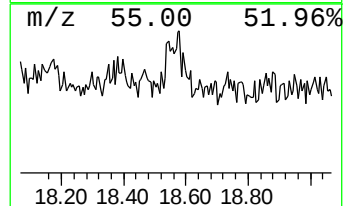
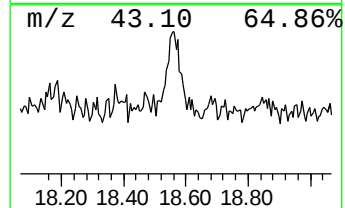
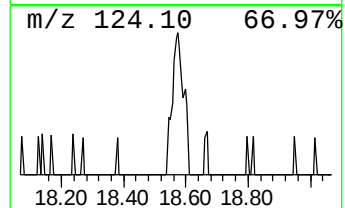
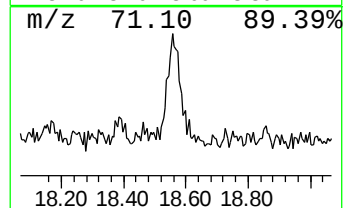
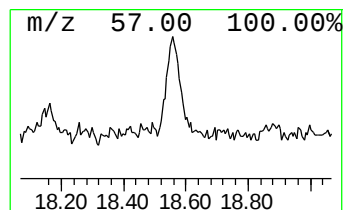
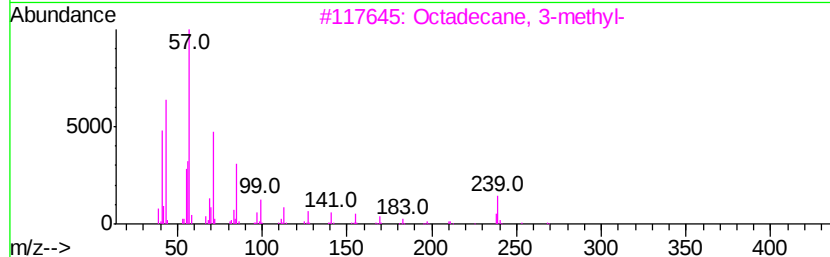
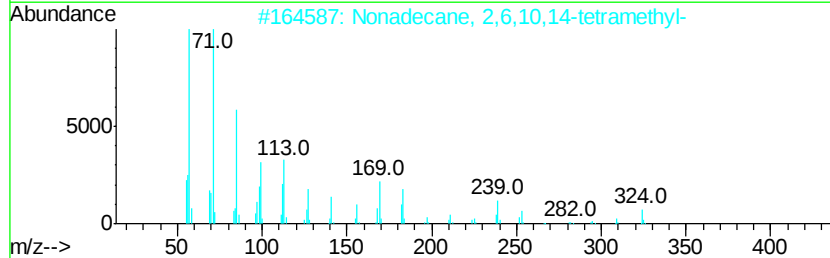
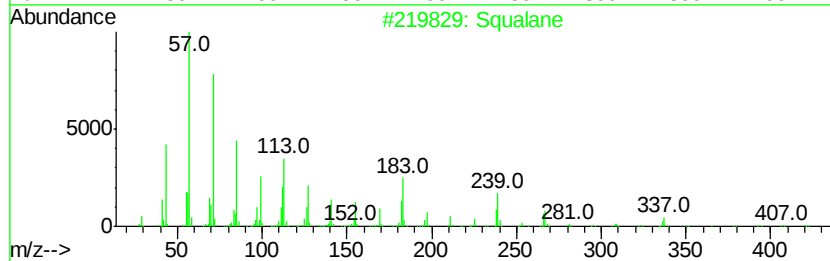
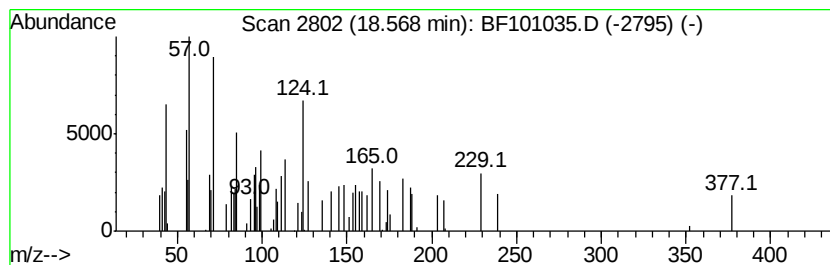
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown18.57 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	5.18 ng	74902	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalane	422	C30H62	000111-01-3	46
2		Nonadecane, 2,6,10,14-tetramethyl-	324	C23H48	055124-80-6	43
3		Octadecane, 3-methyl-	268	C19H40	006561-44-0	38
4		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	35
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF113017\
Data File : BF101035.D
Acq On : 30 Nov 2017 23:19
Operator : SJ/JU
Sample : I6630-01 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P004-S001-0001-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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unknown6.62	6.62	33.2	ng	536151	1	6.85	322665	20.0
n-Hexadecanoic acid	11.90	2.0	ng	29275	4	11.38	291842	20.0
unknown13.82	13.82	6.0	ng	107217	5	14.02	356528	20.0
Ethanol, 2-(tetra...	13.85	2.6	ng	46568	5	14.02	356528	20.0
5-Methyl-2-phenyl...	14.14	4.8	ng	84609	5	14.02	356528	20.0
unknown14.19	14.19	7.4	ng	131641	5	14.02	356528	20.0
(2,3-Diphenylcycl...	14.22	2.1	ng	37268	5	14.02	356528	20.0
Tricosane	15.93	2.8	ng	40630	6	15.50	289076	20.0
Tetrapentacontane...	17.03	4.3	ng	62898	6	15.50	289076	20.0
unknown17.13	17.13	2.6	ng	37733	6	15.50	289076	20.0
unknown18.57	18.57	5.2	ng	74902	6	15.50	289076	20.0