LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106616.D
Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.189	482	485	492	rBV	63647	65081	2.41%	0.361%
2	5.601	552	555	562	rBV	1072409	925299	34.27%	5.133%
3	6.595	721	724	732	rVB	714020	622744	23.07%	3.455%
4	6.736	744	748	751	rBV	1821693	1571730	58.22%	8.719%
5	6.960	782	786	789	rBV	783654	593807	22.00%	3.294%
6	7.118	809	813	816	rBV	2273979	2090909	77.45%	11.599%
7	7.524	877	882	885	rBV	1572636	1770860	65.60%	9.823%
8	8.242	1000	1004	1008	rBV	819810	679367	25.16%	3.769%
9	8.795	1095	1098	1102	rBV	46829	38333	1.42%	0.213%
10	9.318	1182	1187	1190	rBV	2804499	2699672	100.00%	14.976%
11	9.707	1250	1253	1261	rBV	188276	155687	5.77%	0.864%
12	10.001	1300	1303	1311	rVB2	734092	631082	23.38%	3.501%
13	10.712	1421	1424	1429	rVB	114342	90269	3.34%	0.501%
14	10.795	1434	1438	1445	rBV	1088461	939214	34.79%	5.210%
15	11.495	1553	1557	1566	rBV	661301	543698	20.14%	3.016%
16	13.083	1822	1827	1830	rBV	2623896	2426574	89.88%	13.461%
17	13.636	1917	1921	1924	rBV2	48142	43941	1.63%	0.244%
18	13.965	1972	1977	1982	rBV	91481	85482	3.17%	0.474%
19	14.147	2004	2008	2011	rBV	728397	678099	25.12%	3.762%
20	14.289	2028	2032	2036	rBV	93140	92175	3.41%	0.511%
21	14.600	2081	2085	2090	rBV	141312	126483	4.69%	0.702%
22	14.918	2135	2139	2143	rBV	153482	149010	5.52%	0.827%
23	15.277	2195	2200	2206	rBV	142663	167154	6.19%	0.927%
24	15.683	2263	2269	2279	rBV	467127	643774	23.85%	3.571%
25	16.141	2342	2347	2352	rVB	80785	120794	4.47%	0.670%
26	16.677	2433	2438	2445	rVB2	43490	75596	2.80%	0.419%

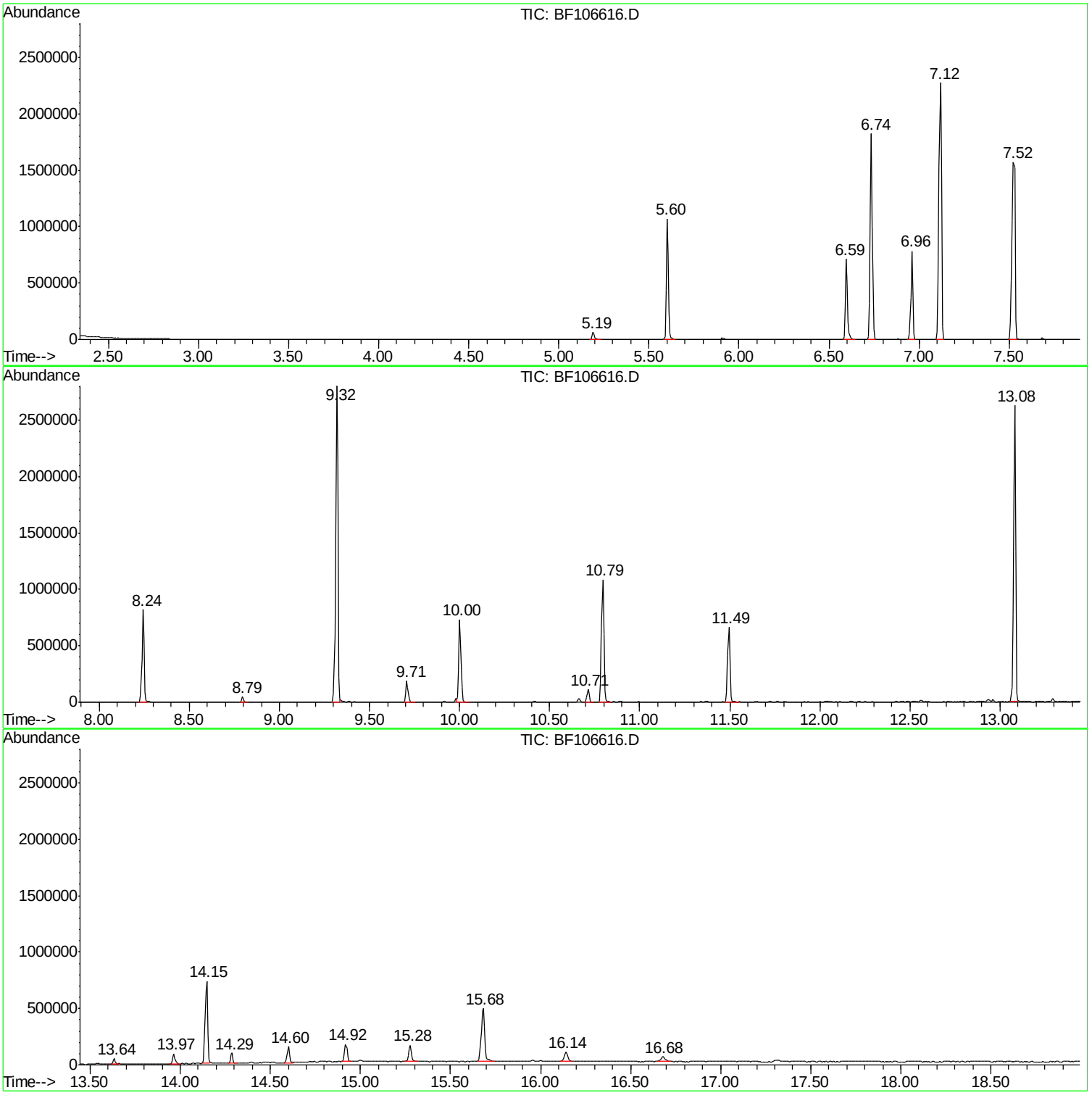
Sum of corrected areas: 18026834

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106616.D
Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106616.D
Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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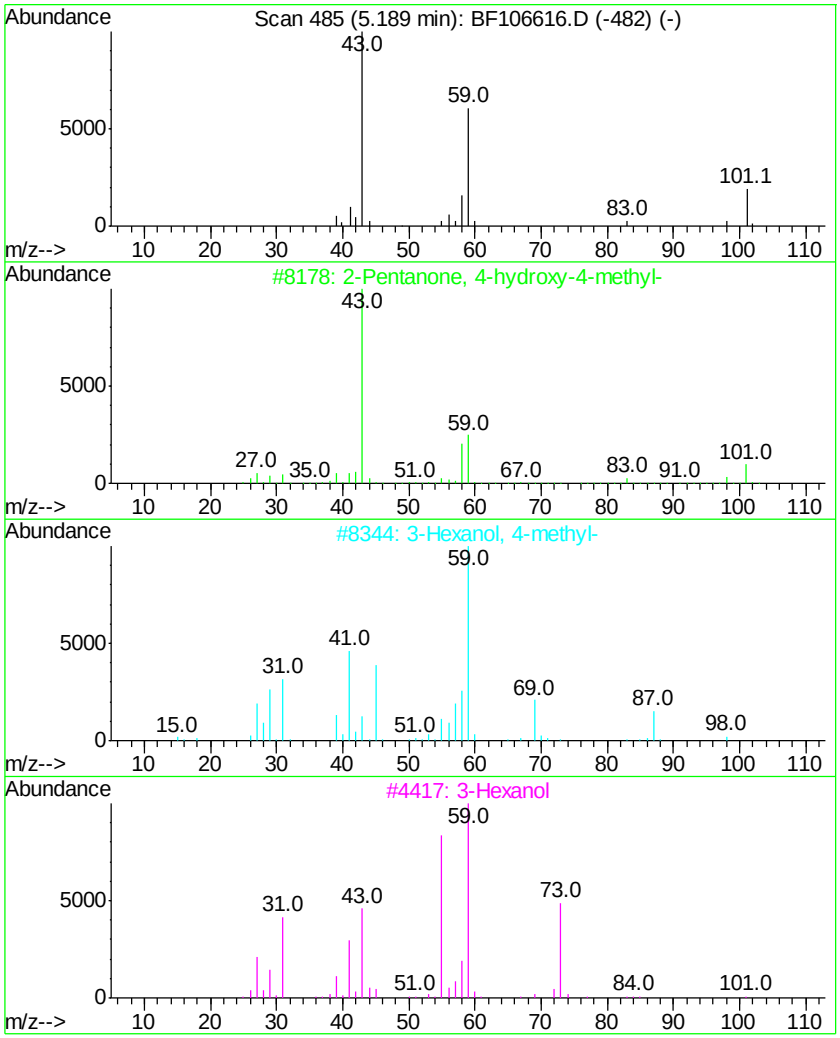
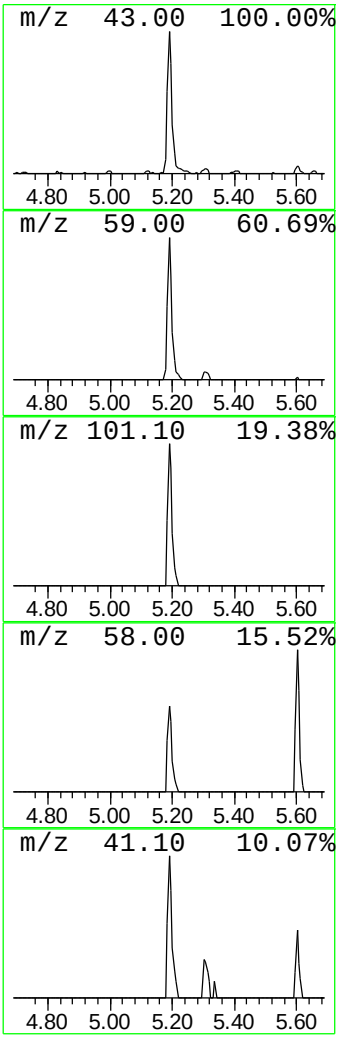
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.19 ng	65081	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106616.D
Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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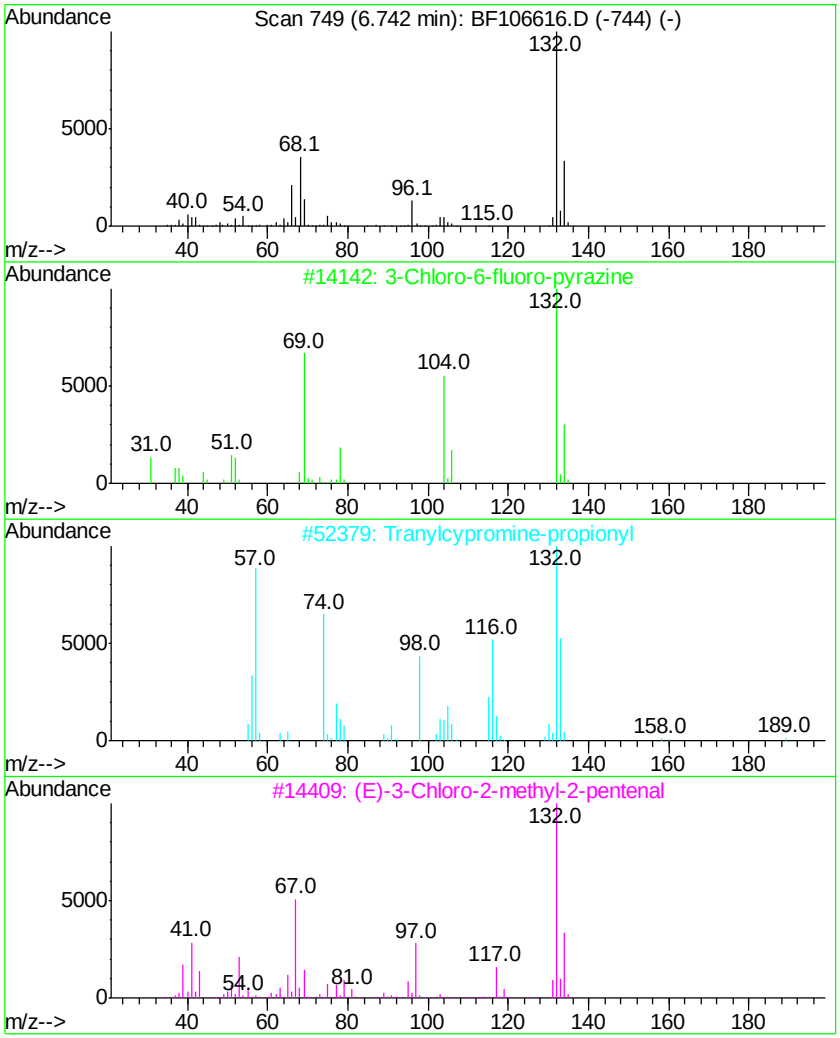
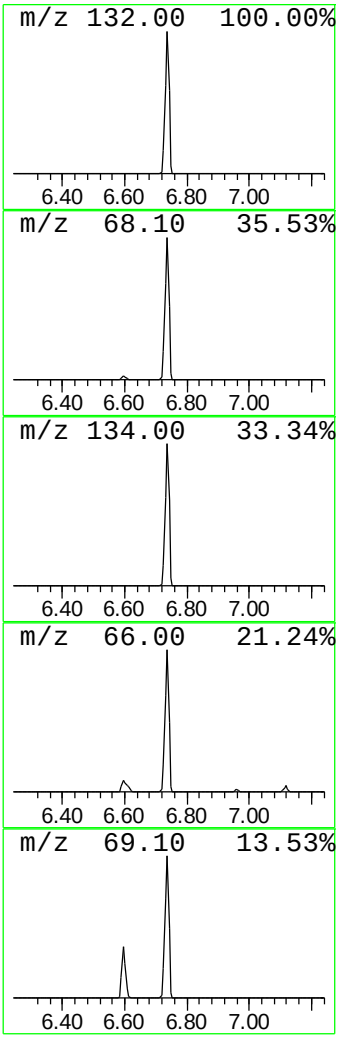
Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	52.94 ng	1571730	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106616.D
Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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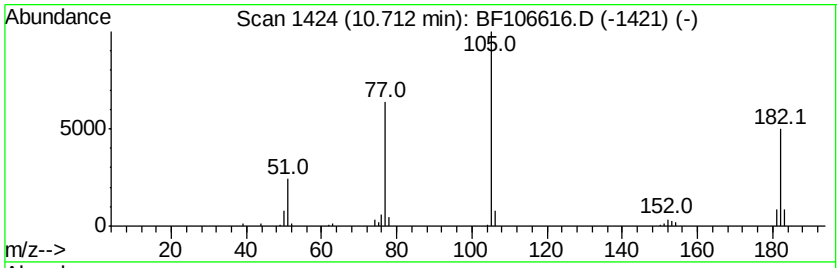
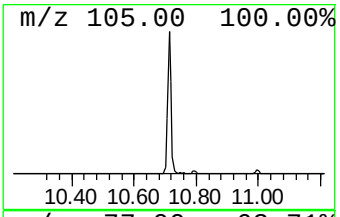
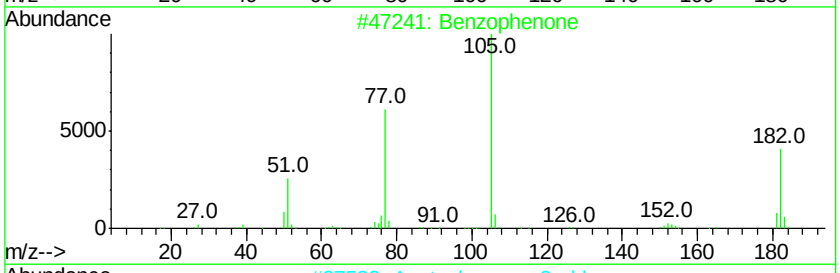
Peak Number 4 Benzophenone Concentration Rank 7

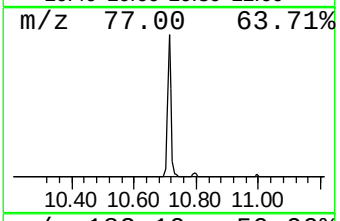
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.71	2.86 ng	90269	Acenaphthene-d10	10.00

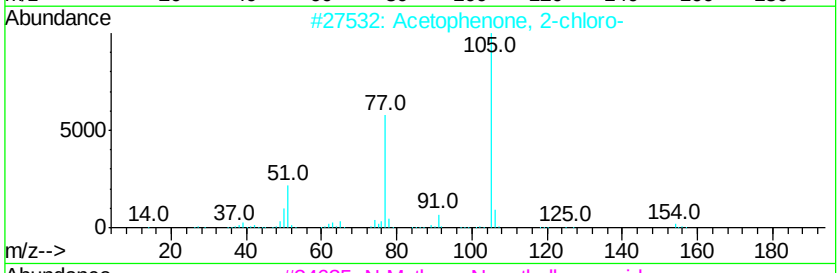
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
5	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47

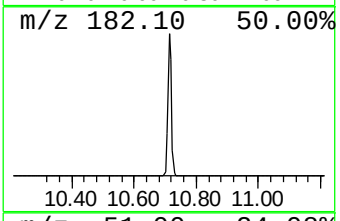


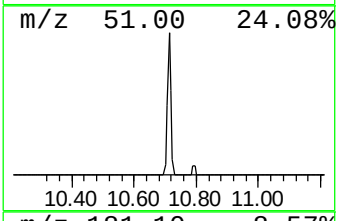


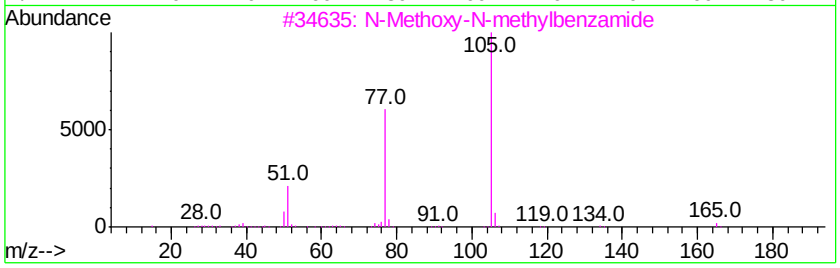


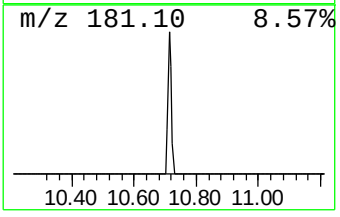












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106616.D
Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

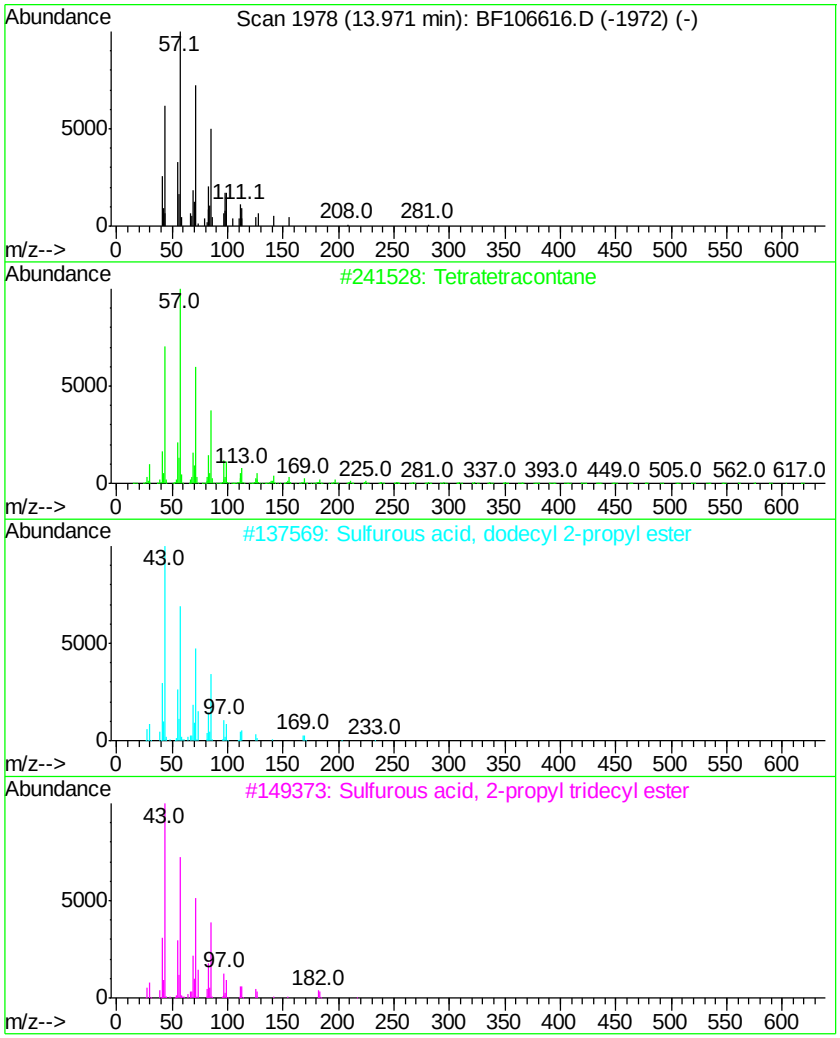
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

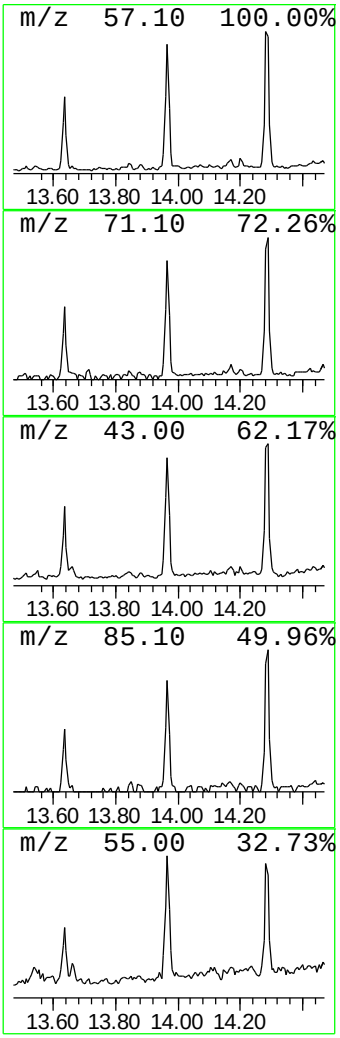
****

Peak Number 5 Tetratetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.52 ng	85482	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	90
3	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	90
4	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	90
5	Octacosane	394	C28H58	000630-02-4	87





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Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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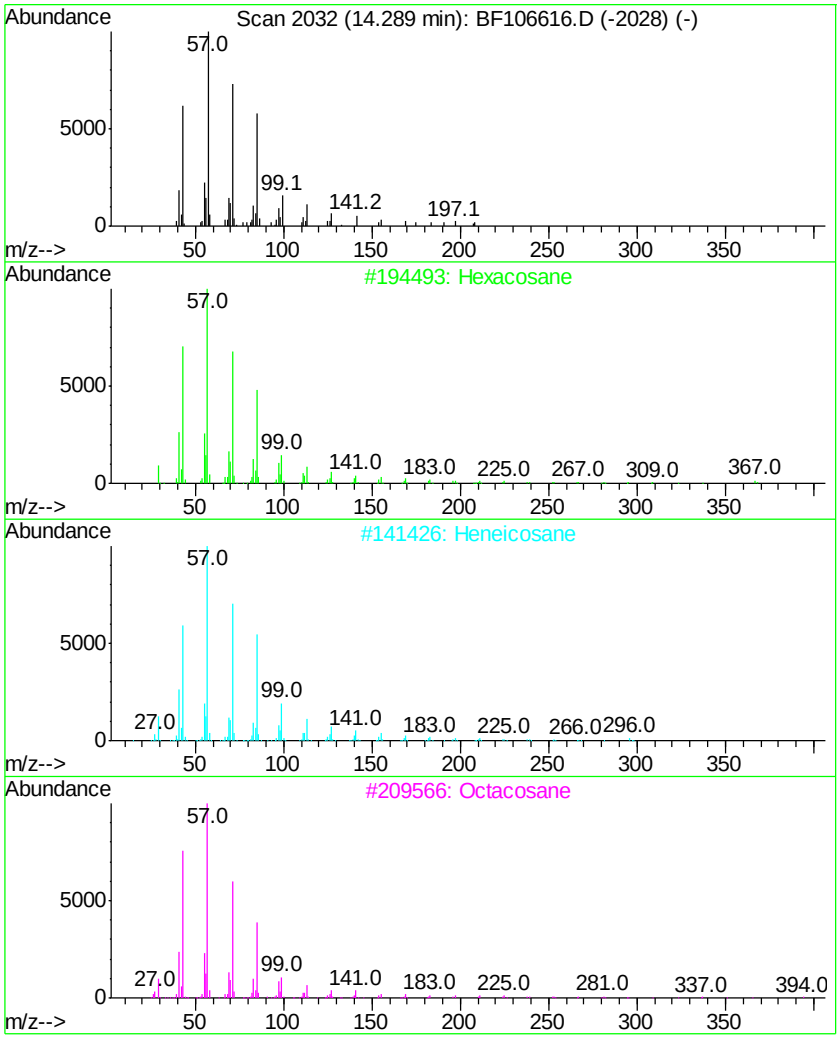
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

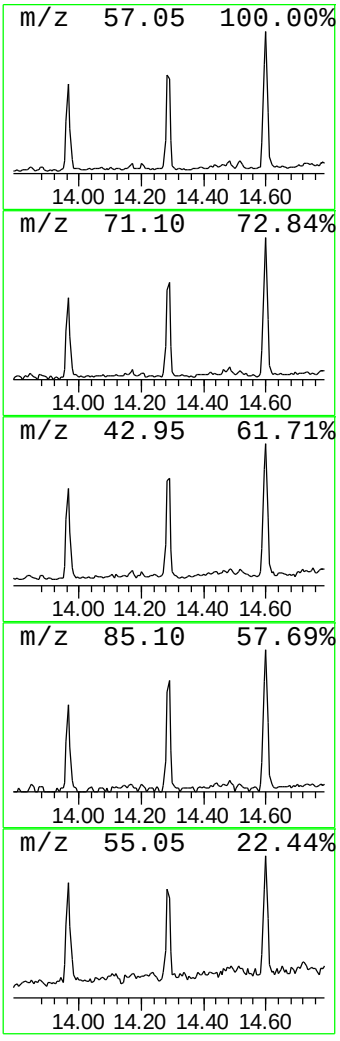
****

Peak Number 6 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.72 ng	92175	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Octadecane	254	C18H38	000593-45-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061918\
Data File : BF106616.D
Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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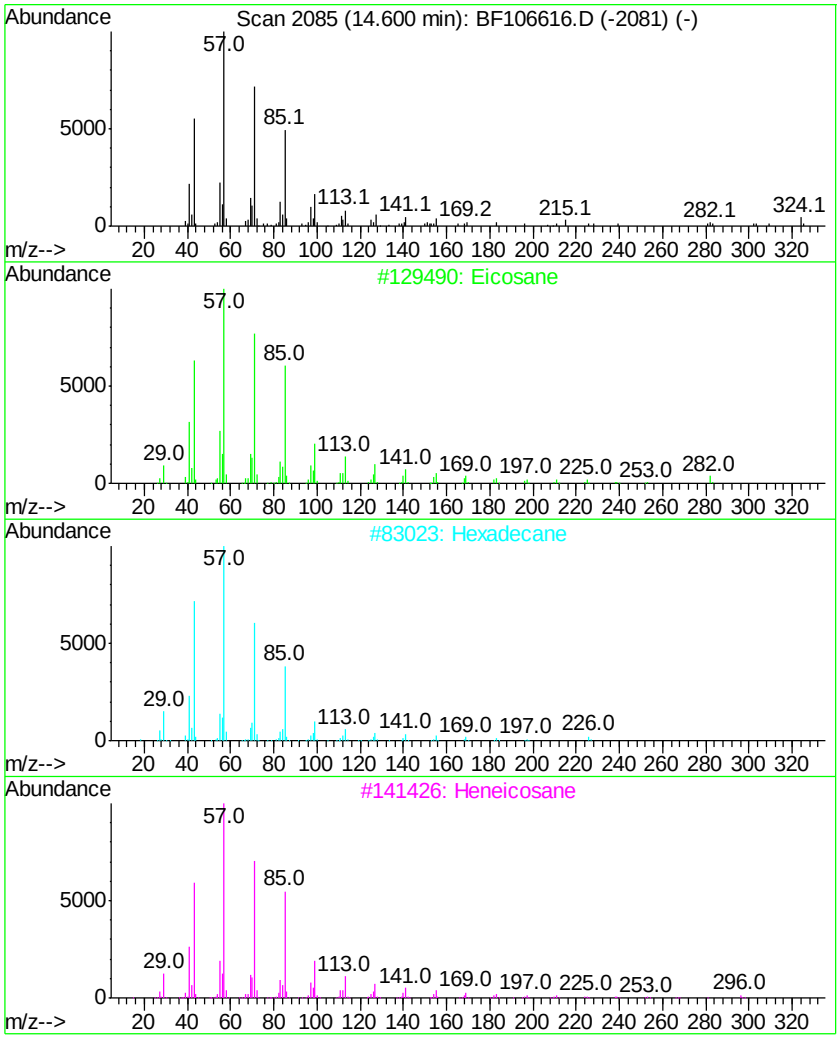
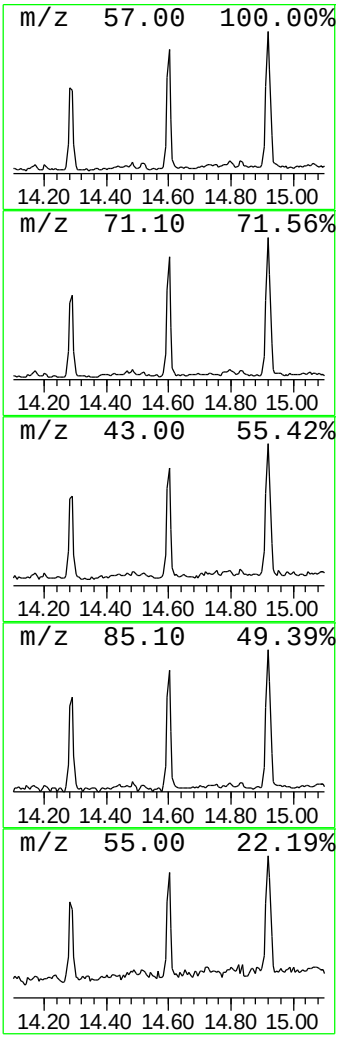
Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	3.73 ng	126483	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexadecane	226	C16H34	000544-76-3	93
3	Heneicosane	296	C21H44	000629-94-7	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Docosane	310	C22H46	000629-97-0	83





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Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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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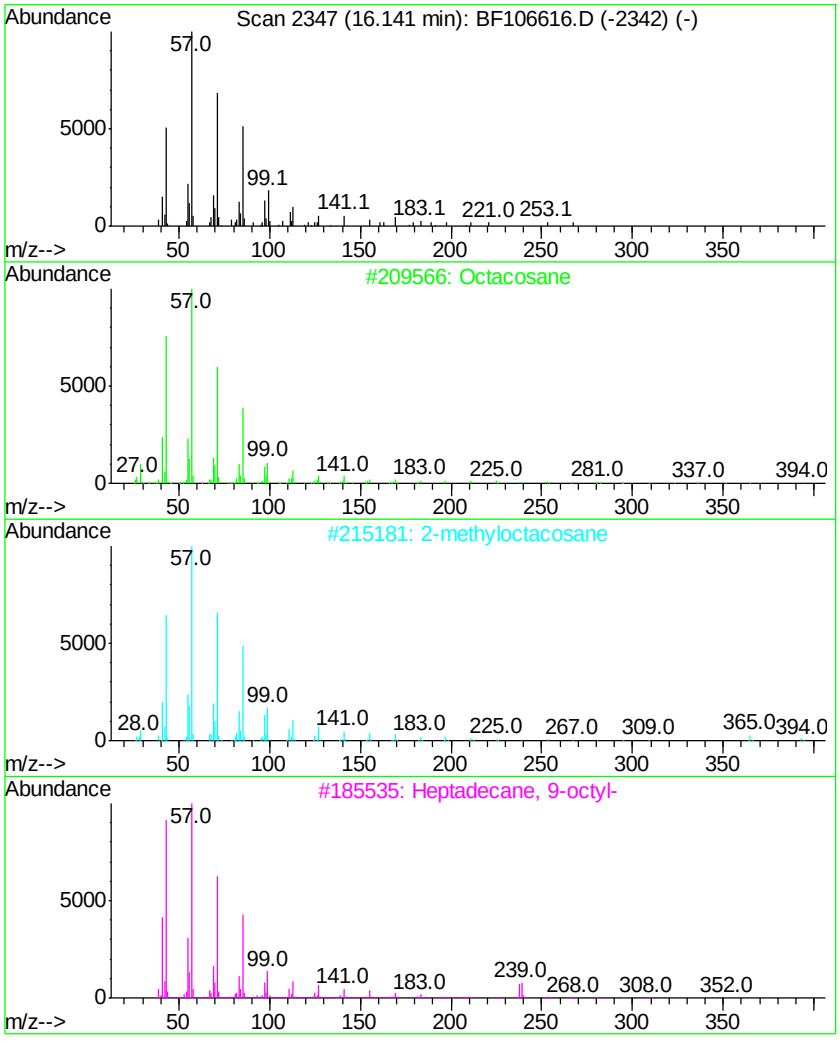
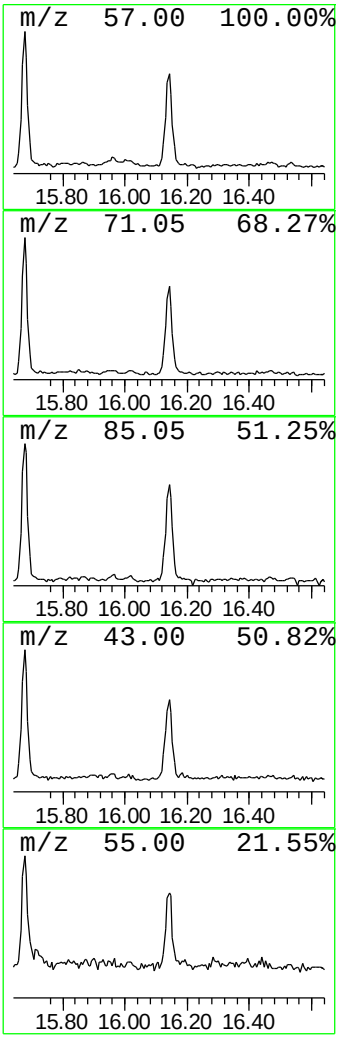
Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	3.75 ng	120794	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061918\
Data File : BF106616.D
Acq On : 20 Jun 2018 7:11
Operator : JU/SJ
Sample : J3548-06
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061318-DBRI-E-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	2.2	ng	65081	1	6.96	593807	20.0
unknown6.74	6.74	52.9	ng	1571730	1	6.96	593807	20.0
Benzophenone	10.71	2.9	ng	90269	3	10.00	631082	20.0
Tetratetracontane	13.97	2.5	ng	85482	5	14.15	678099	20.0
Hexacosane	14.29	2.7	ng	92175	5	14.15	678099	20.0
Eicosane	14.60	3.7	ng	126483	5	14.15	678099	20.0
Octacosane	16.14	3.8	ng	120794	6	15.68	643774	20.0