LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016204.D
Acq On : 06 Aug 2018 23:00
Operator : SJ/JU
Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

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_M\METHODS\8270-BM072318.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	5.222	324	329	338	rBV2	30329	48623	2.59%	0.291%
2	5.693	404	409	425	rBV	404057	661130	35.24%	3.953%
3	7.334	682	688	708	rBV	411718	695827	37.09%	4.160%
4	7.698	744	750	765	rBV	461256	764015	40.72%	4.568%
5	8.169	825	830	841	rBB	161182	259801	13.85%	1.553%
6	8.493	879	885	895	rBV	425689	695128	37.05%	4.156%
7	9.357	1026	1032	1051	rBV	295259	506152	26.98%	3.026%
8	10.986	1303	1309	1322	rBV	189969	318021	16.95%	1.901%
9	13.422	1717	1723	1735	rVB	747915	1028494	54.82%	6.149%
10	14.798	1952	1957	1965	rBB2	239000	370441	19.74%	2.215%
11	16.286	2205	2210	2218	rVB	492498	683131	36.41%	4.084%
12	17.533	2417	2422	2426	rBV	318335	439321	23.42%	2.626%
13	17.574	2426	2429	2437	rVB	72154	104890	5.59%	0.627%
14	18.380	2561	2566	2573	rBV3	55997	92135	4.91%	0.551%
15	18.457	2575	2579	2585	rVB4	21809	34499	1.84%	0.206%
16	18.521	2585	2590	2595	rBV6	13996	26244	1.40%	0.157%
17	18.604	2595	2604	2606	rBV8	16763	44396	2.37%	0.265%
18	18.957	2660	2664	2670	rVB3	25106	39785	2.12%	0.238%
19	19.433	2742	2745	2747	rBV2	17008	20435	1.09%	0.122%
20	19.568	2762	2768	2774	rVB	262291	350713	18.69%	2.097%
21	19.639	2777	2780	2789	rVB8	26699	40689	2.17%	0.243%
22	19.892	2819	2823	2825	rBV2	40270	54143	2.89%	0.324%
23	19.927	2825	2829	2833	rVV	186014	256171	13.65%	1.532%
24	20.109	2855	2860	2870	rBV	1470471	1876168	100.00%	11.217%
25	20.239	2876	2882	2887	rBV3	375619	840025	44.77%	5.022%
26	20.298	2887	2892	2896	rVV3	372700	817191	43.56%	4.886%
27	20.339	2896	2899	2904	rVV	305698	543073	28.95%	3.247%
28	20.421	2904	2913	2922	rVV6	334005	1253406	66.81%	7.493%
29	20.492	2922	2925	2933	rVV	416973	749398	39.94%	4.480%
30	20.562	2933	2937	2947	rVB	329139	563562	30.04%	3.369%
31	20.709	2959	2962	2965	rBV4	25563	32223	1.72%	0.193%
32	21.498	3093	3096	3099	rBV2	69664	95015	5.06%	0.568%
33	21.533	3099	3102	3107	rVB	218418	237898	12.68%	1.422%
34	21.592	3109	3112	3116	rBV3	37256	59646	3.18%	0.357%

LSC Area Percent Report

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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

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_M\METHODS\8270-BM072318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.662	3118	3124	3128	rBV2	523627	890306	47.45%	5.323%
36	21.768	3139	3142	3148	rVB4	175004	289588	15.44%	1.731%
37	23.303	3399	3403	3408	rBV	118625	223902	11.93%	1.339%
38	23.809	3485	3489	3496	rVB2	105562	183948	9.80%	1.100%
39	24.015	3518	3524	3530	rBV	290028	537162	28.63%	3.211%

Sum of corrected areas: 16726695

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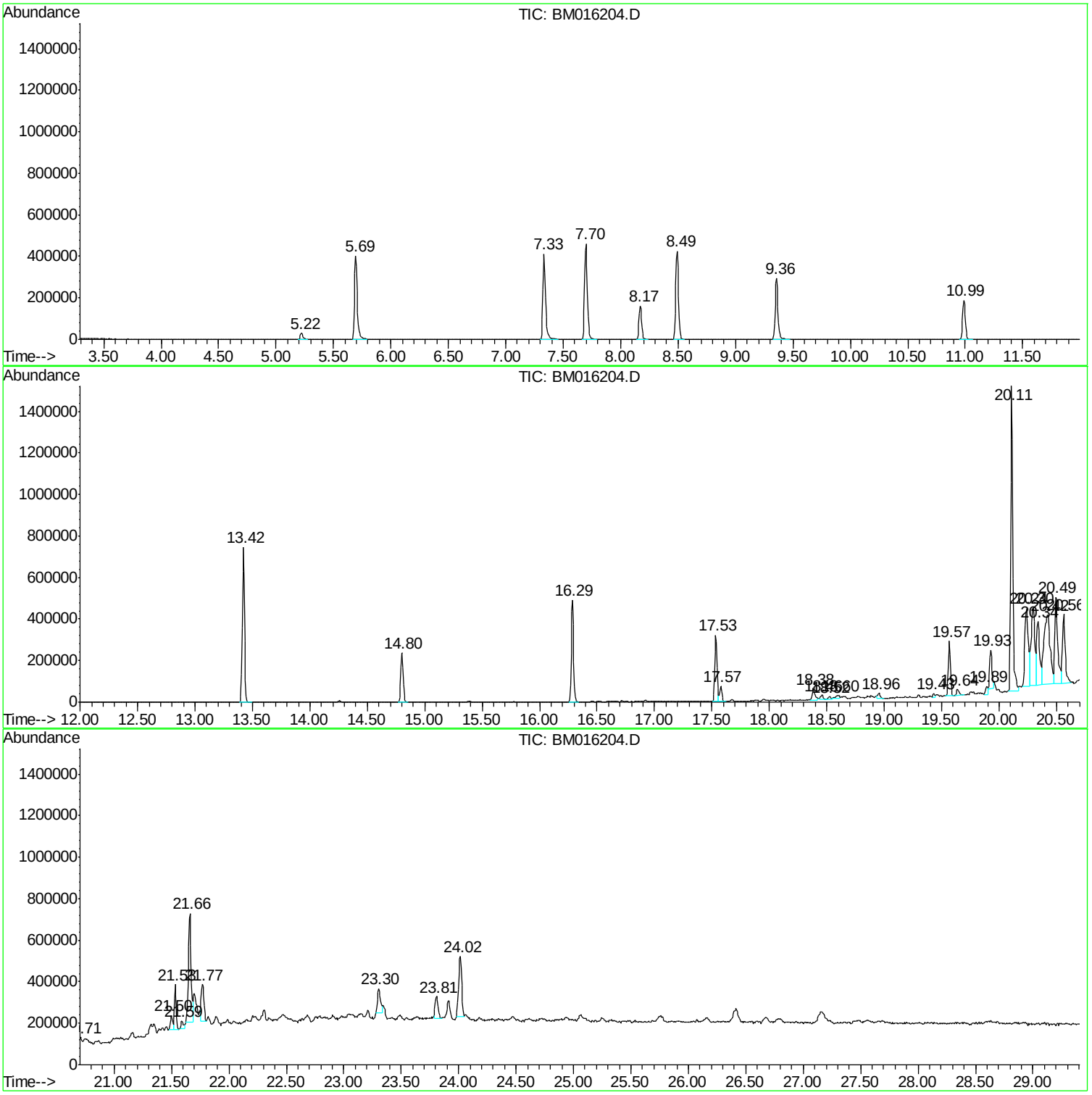
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Operator : SJ/JU
Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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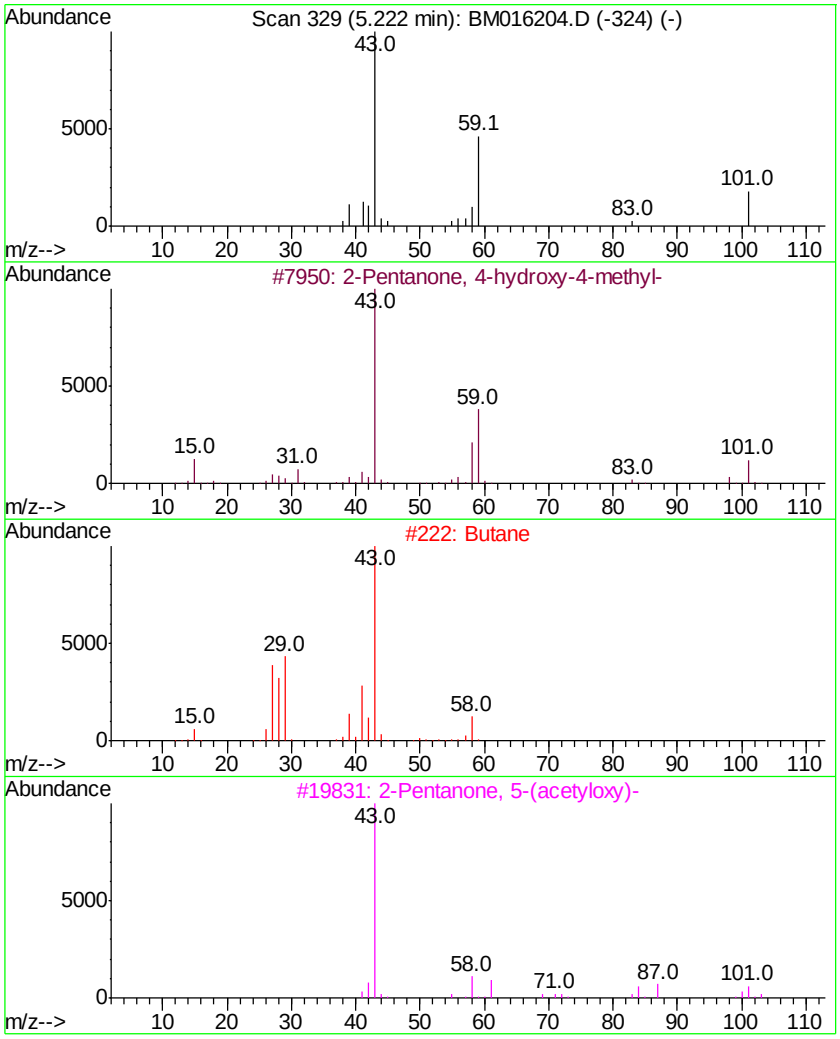
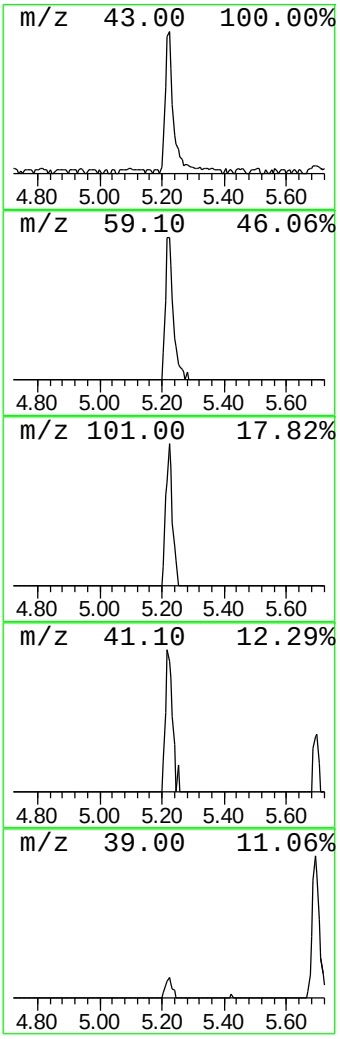
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	3.74 ng	48623	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Butane	58	C4H10	000106-97-8	25
3	2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016204.D
Acq On : 06 Aug 2018 23:00
Operator : SJ/JU
Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

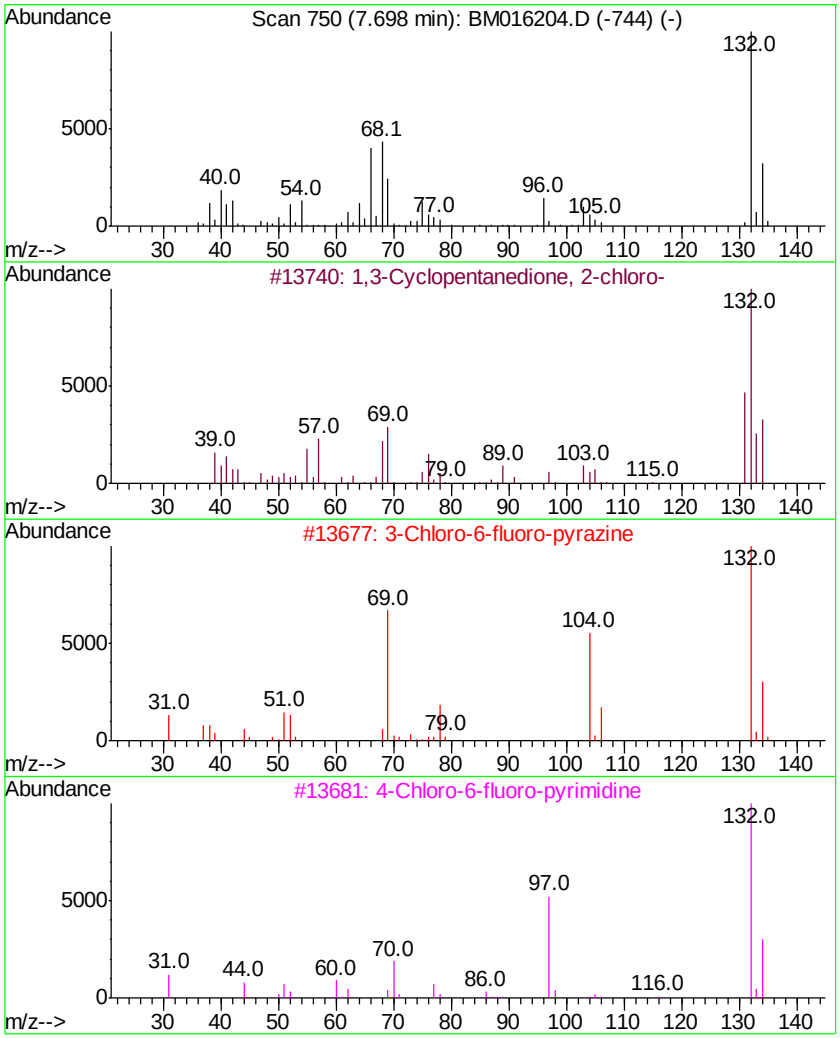
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

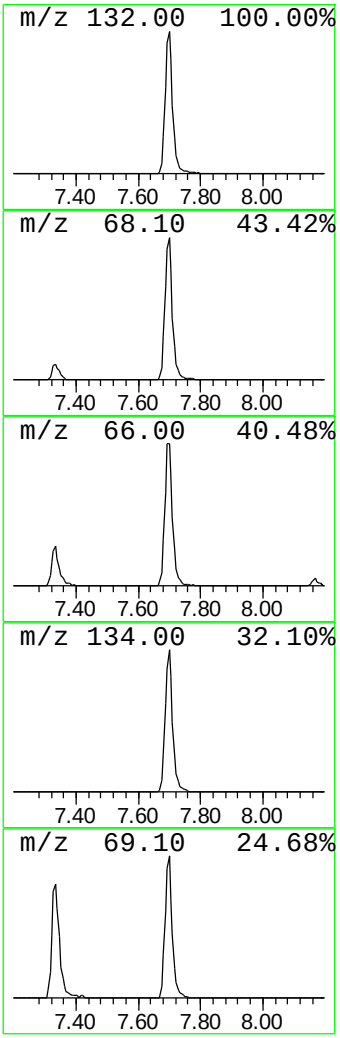
****

Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	58.82 ng	764015	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016204.D
Acq On : 06 Aug 2018 23:00
Operator : SJ/JU
Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

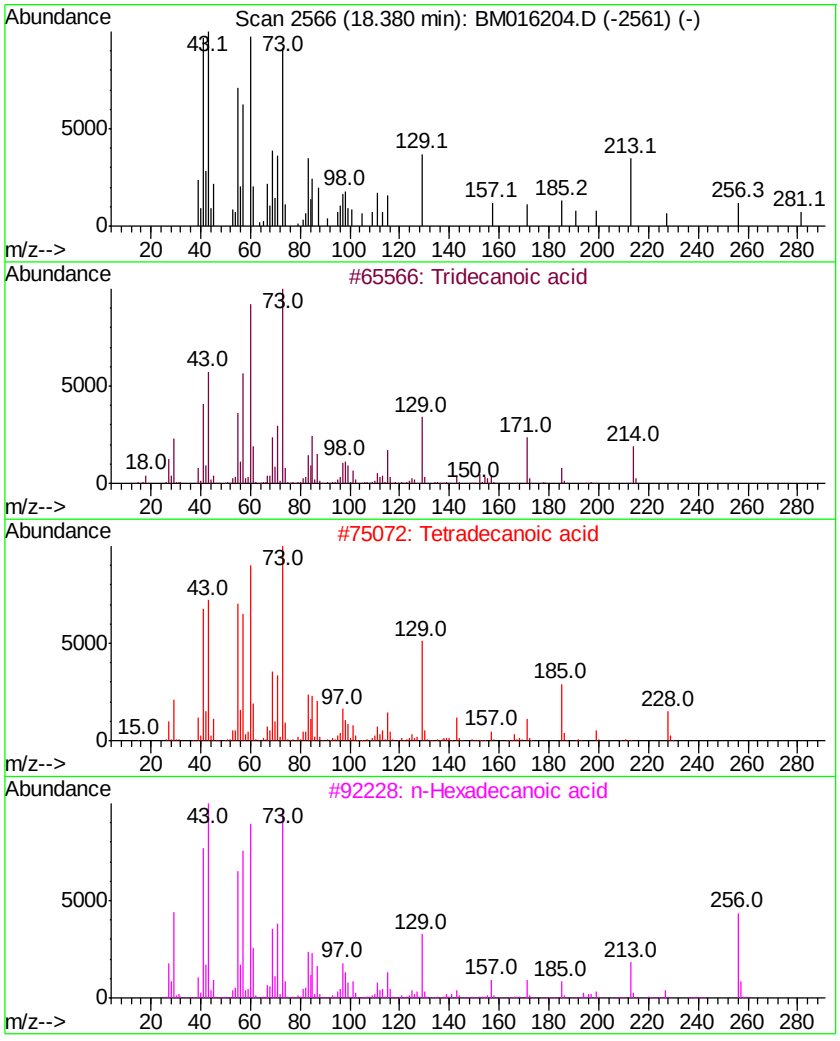
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

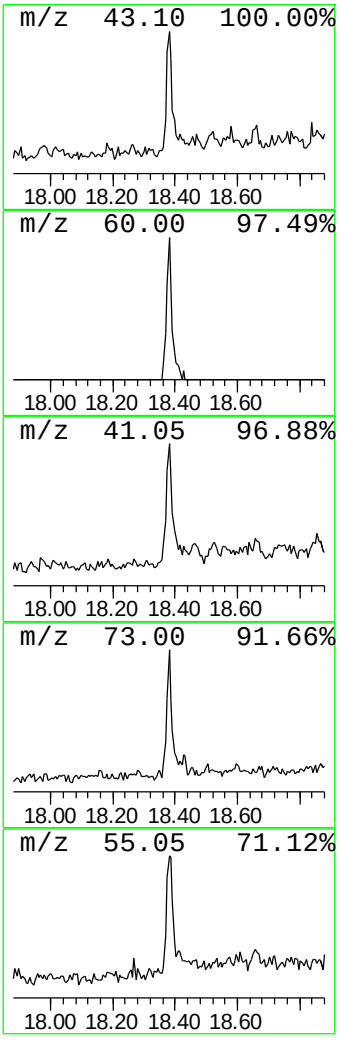
****

Peak Number 4 Tridecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	4.19 ng	92135	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	80
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016204.D
Acq On : 06 Aug 2018 23:00
Operator : SJ/JU
Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

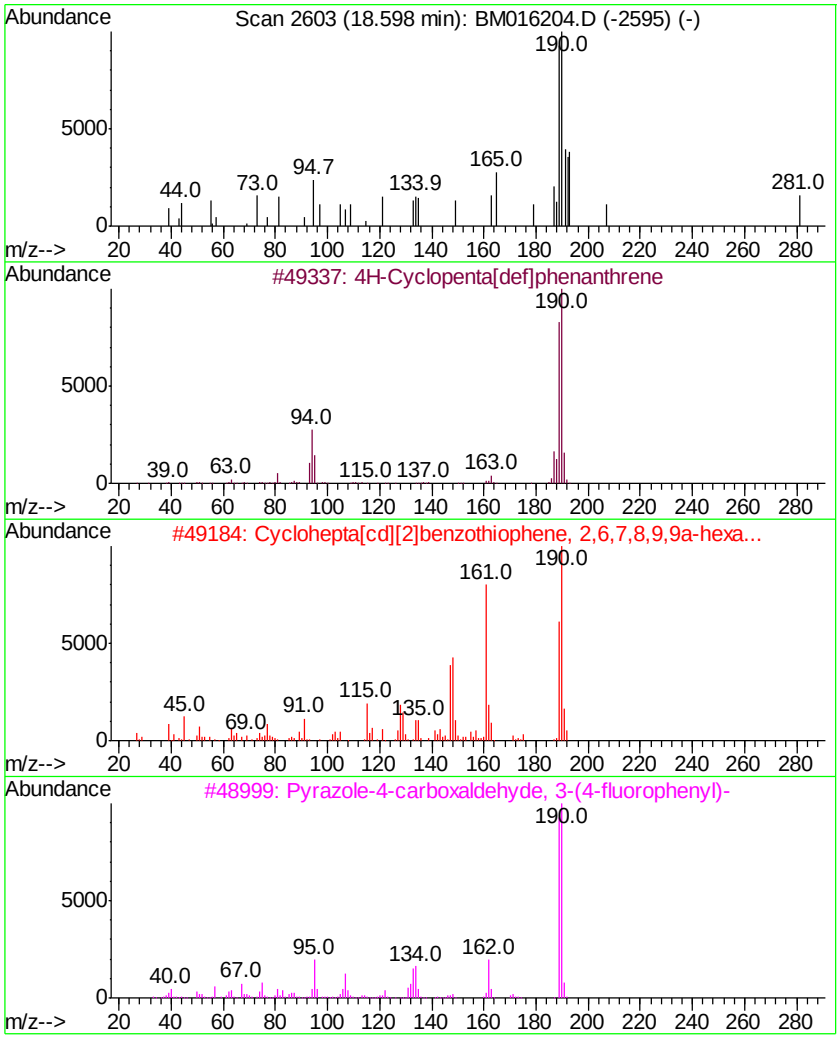
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

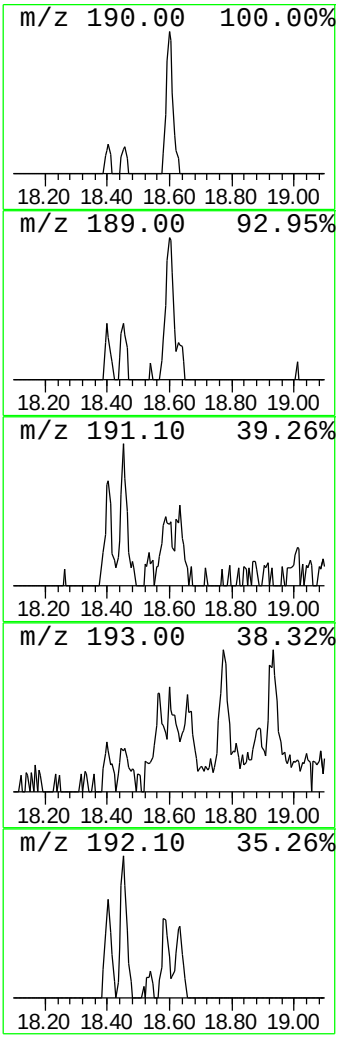
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.60	2.02 ng	44396	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
2	Cyclohepta[cd][2]benzothiophene,...	190	C12H14S	199807-57-3	38
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	37
4	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	37
5	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	28





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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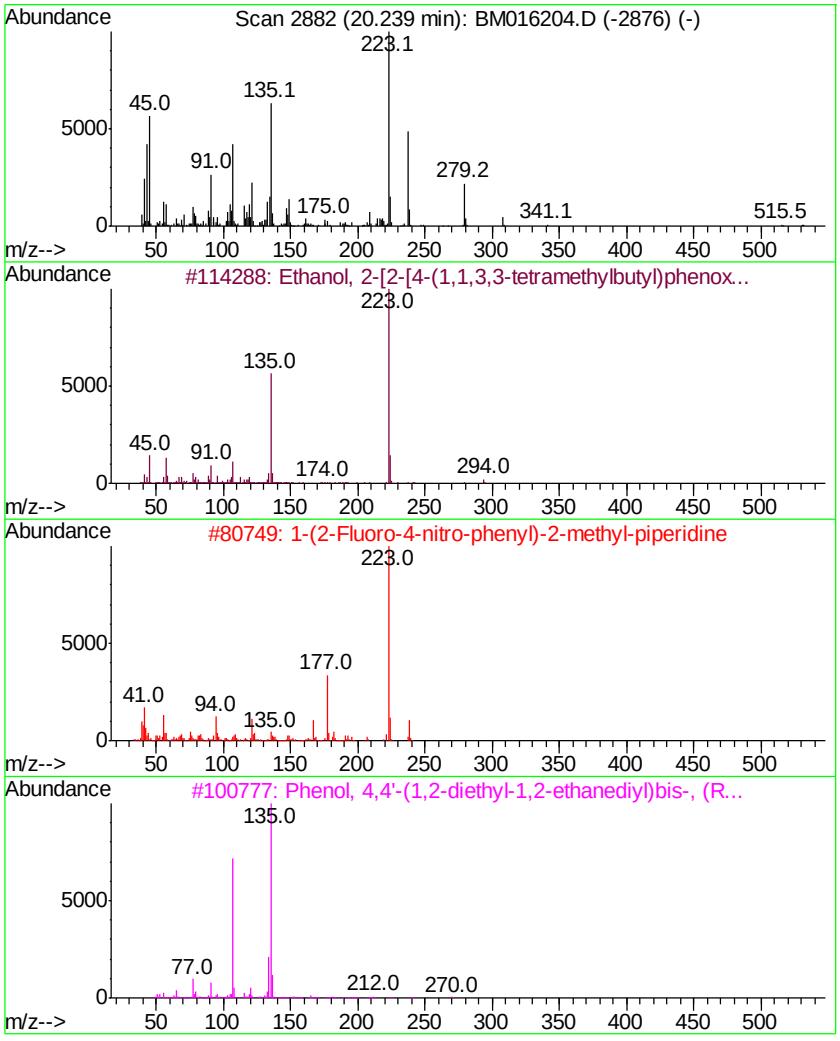
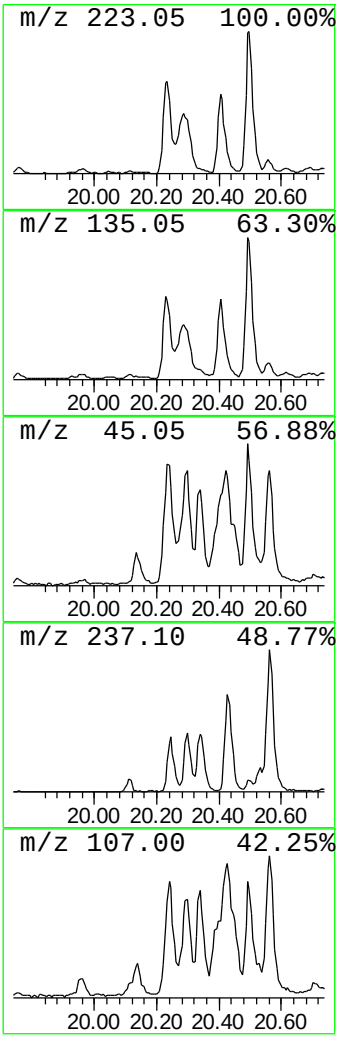
****

Peak Number 6 unknown20.24 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.24	18.87 ng	840025	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	37
2	1-(2-Fluoro-4-nitro-phenyl)-2-me...	238	C12H15FN2O2	1000278-20-9	22
3	Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	14
4	9-Acridinecarboxylic acid	223	C14H9NO2	005336-90-3	14
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	10





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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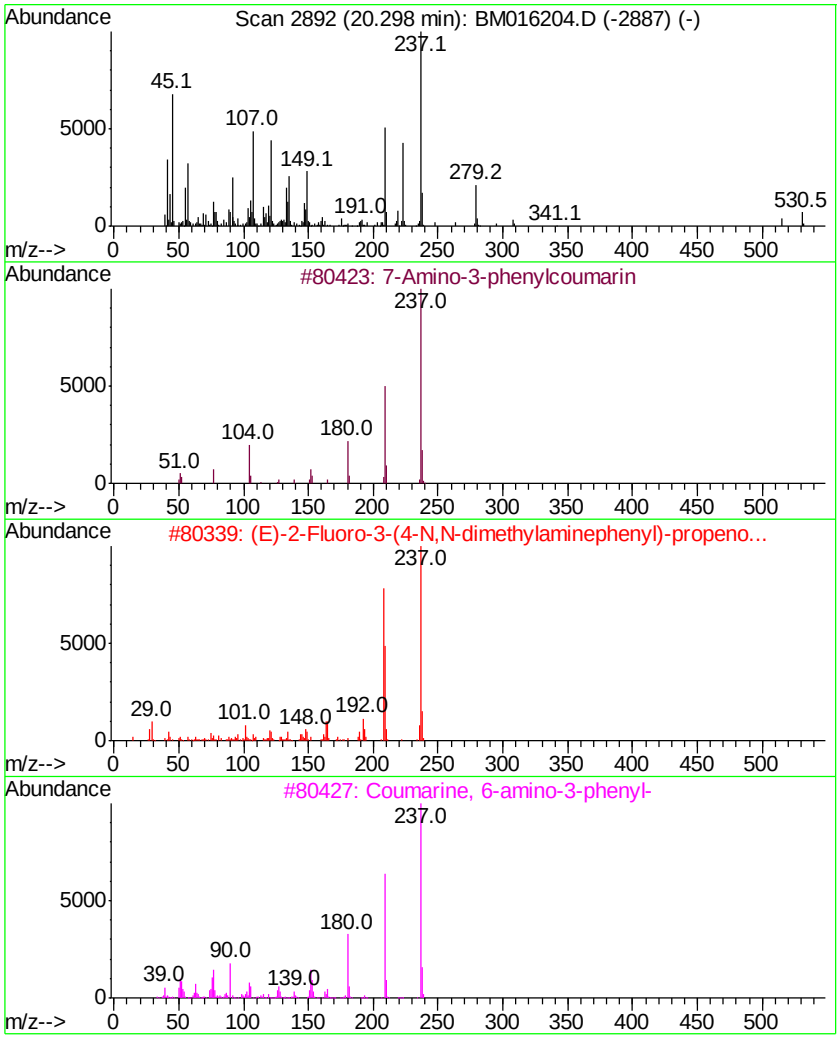
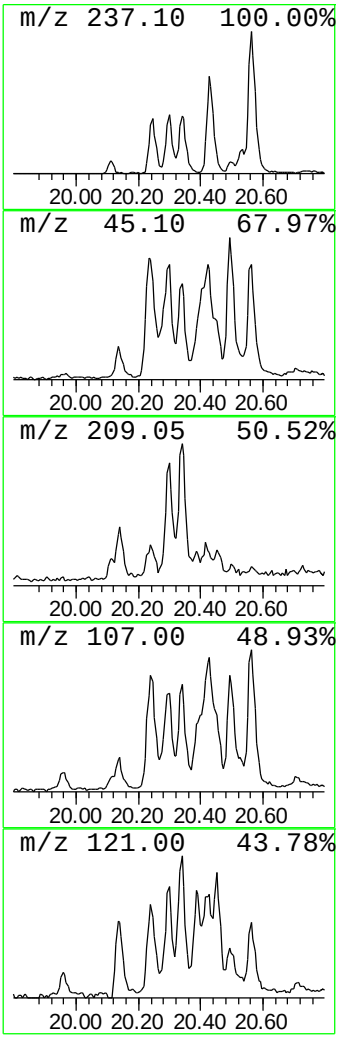
Peak Number 7 unknown20.30 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.30	18.36 ng	817191	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Amino-3-phenylcoumarin	237	C15H11NO2	004108-61-6	45
2	(E)-2-Fluoro-3-(4-N,N-dimethylam...	237	C13H16FNO2	110915-65-6	43
3	Coumarine, 6-amino-3-phenyl-	237	C15H11NO2	021408-16-2	38
4	7-Methyl-3-phenyl-benzo[1,4]oxaz...	237	C15H11NO2	062103-88-2	38
5	Pyrazolo[1,5-a]pyrimidine, 5,6-d...	279	C18H21N3	1000273-96-0	27





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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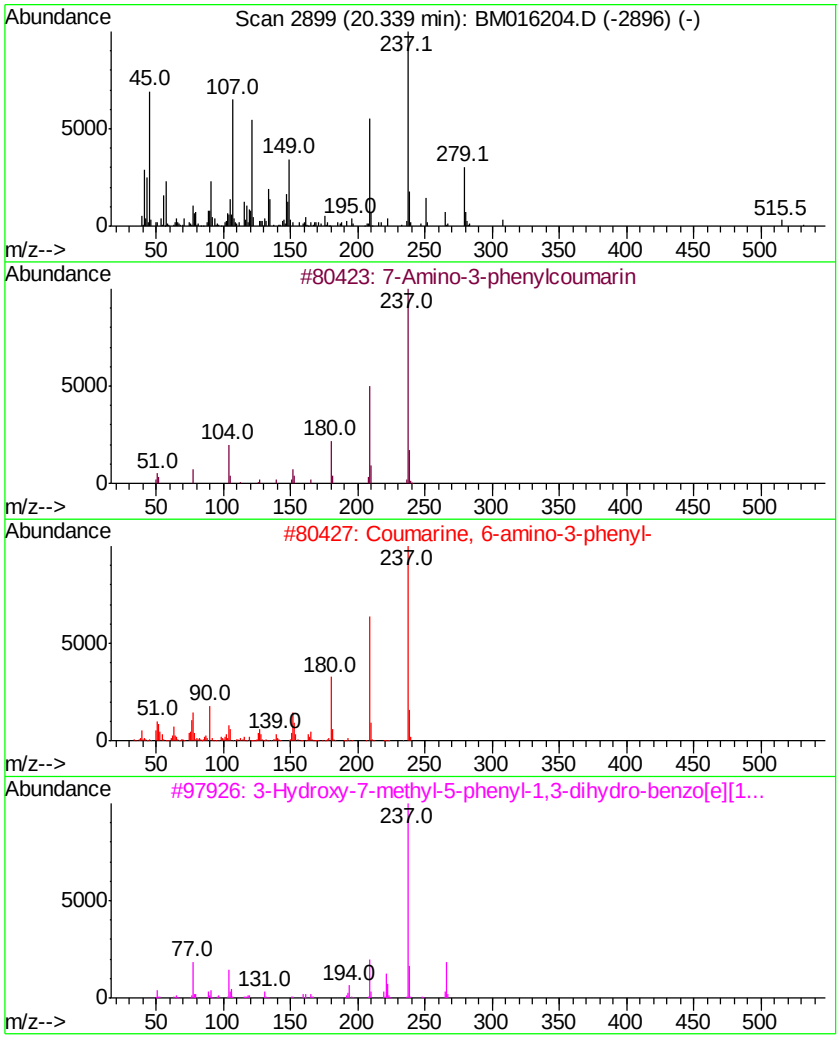
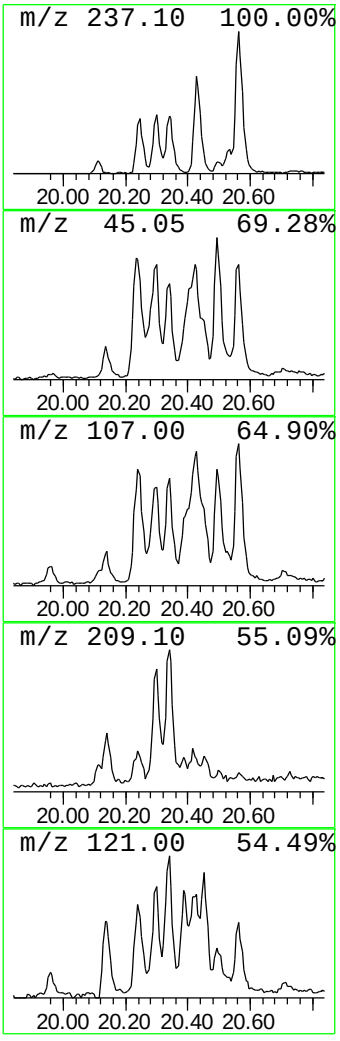
Peak Number 8 unknown20.34 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.34	12.20 ng	543073	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Amino-3-phenylcoumarin	237	C15H11NO2	004108-61-6	45
2	Coumarine, 6-amino-3-phenyl-	237	C15H11NO2	021408-16-2	35
3	3-Hydroxy-7-methyl-5-phenyl-1,3-...	266	C16H14N2O2	040762-10-5	35
4	(E)-2-Fluoro-3-(4-N,N-dimethylam...	237	C13H16FNO2	110915-65-6	35
5	Pyrazolo[1,5-a]pyrimidine, 5,6-d...	279	C18H21N3	1000273-96-0	30





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Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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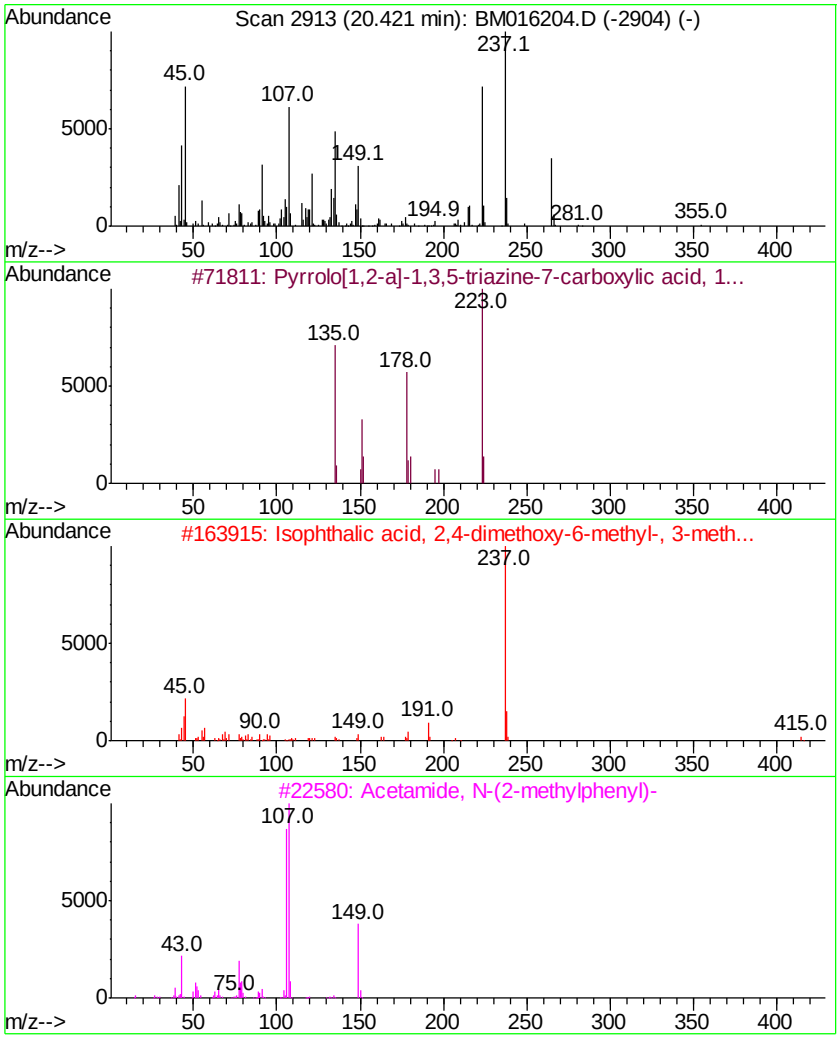
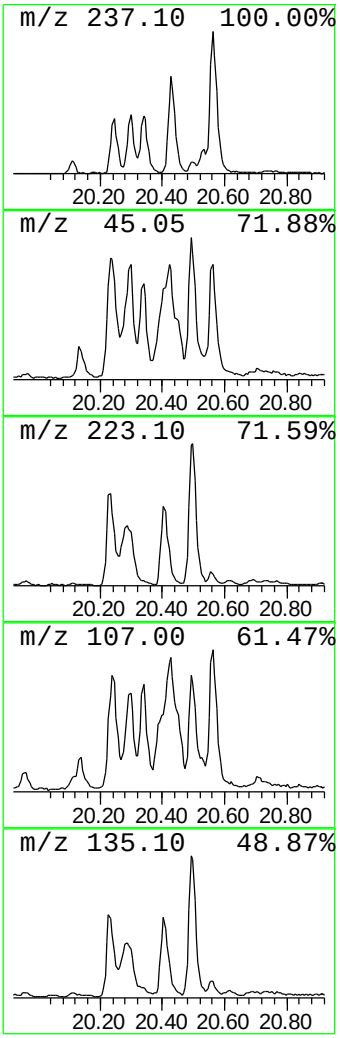
Peak Number 9 unknown20.42 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.42	28.16 ng	1253410	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	30
2	Isophthalic acid, 2,4-dimethoxy-...	446	C23H26O9	019314-77-3	25
3	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	15
4	2,4-Diphenylthiazole	237	C15H11NS	001826-14-8	14
5	9,10-Anthracenedione, 1-amino-2-...	237	C15H11NO2	000082-28-0	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016204.D
Acq On : 06 Aug 2018 23:00
Operator : SJ/JU
Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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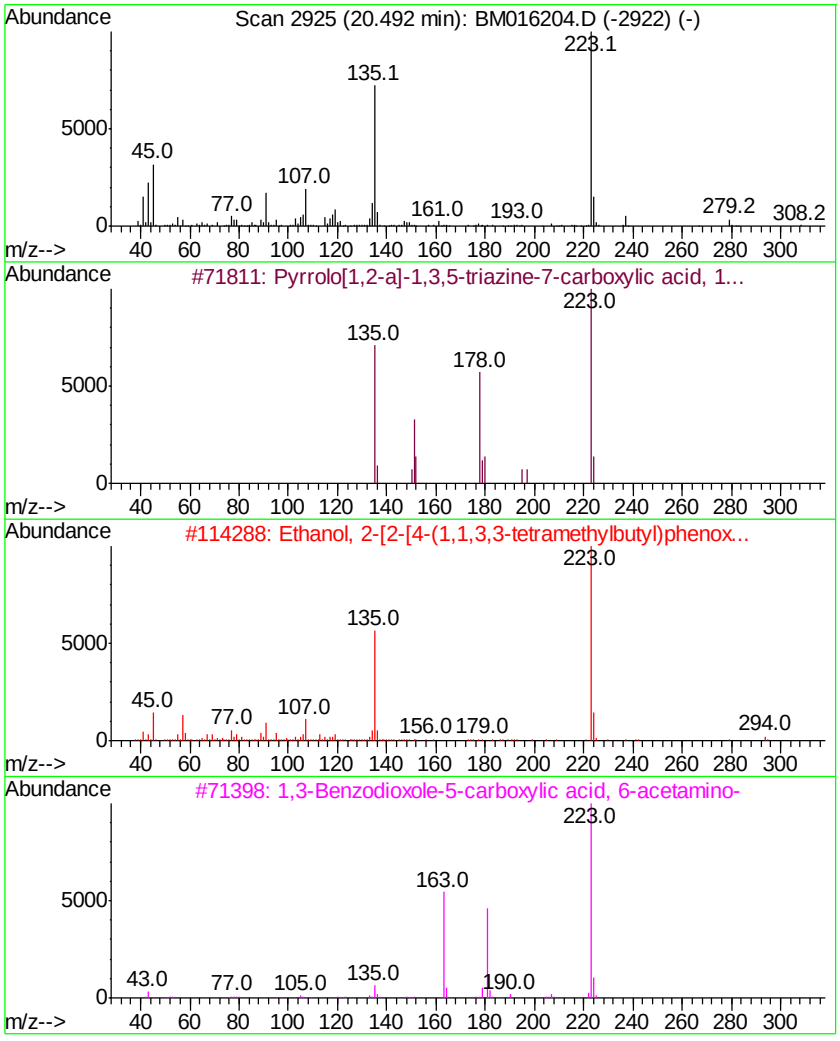
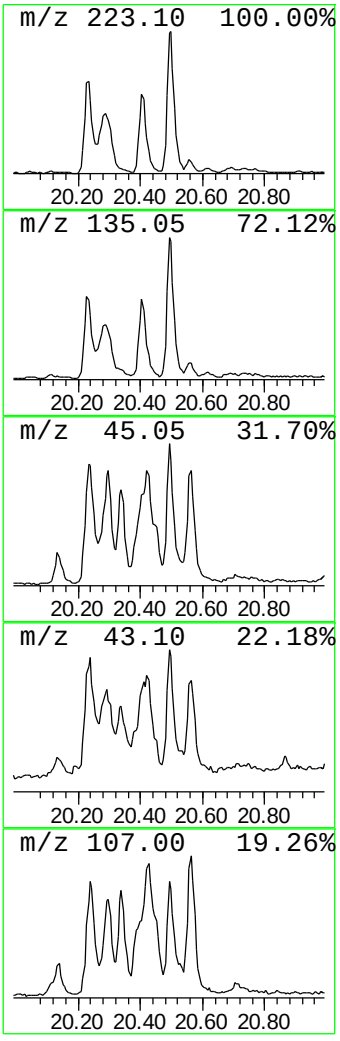
Peak Number 10 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.49	16.83 ng	749398	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	83
3	1,3-Benzodioxole-5-carboxylic ac...	223	C10H9NO5	099185-29-2	38
4	Tetrazole, 1-(4-ethylphenyl)-5-(...	410	C25H26N6	125038-06-4	35
5	4(1H)-Quinazolinone, 2,3-dihydro...	238	C15H14N2O	017761-74-9	32





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
Data File : BM016204.D
Acq On : 06 Aug 2018 23:00
Operator : SJ/JU
Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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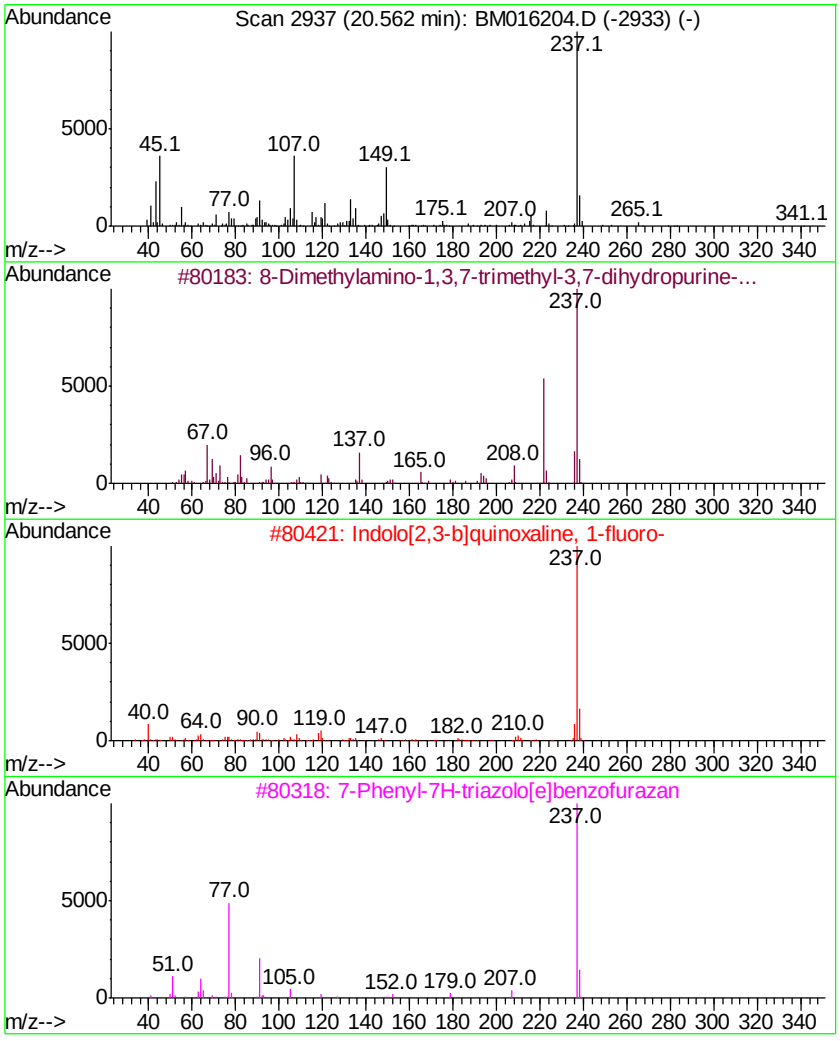
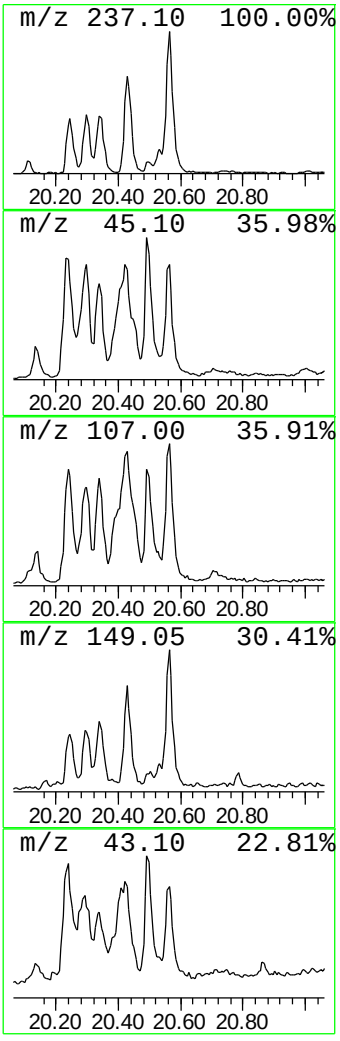
Peak Number 11 unknown20.56 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.56	12.66 ng	563562	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Dimethylamino-1,3,7-trimethyl-...	237	C10H15N5O2	078146-62-0	38
2	Indolo[2,3-b]quinoxaline, 1-fluoro-	237	C14H8FN3	296244-71-8	35
3	7-Phenyl-7H-triazolo[e]benzofurazan	237	C12H7N5O	035142-93-9	35
4	Pyrido[2,3-d]pyrimidin-5(8H)-one...	237	C14H11N3O	161465-98-1	32
5	2-Amino-10-oxo-10H-9-oxa-1-aza-a...	237	C13H7N3O2	061424-81-5	32





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Acq On : 06 Aug 2018 23:00
Operator : SJ/JU
Sample : J4318-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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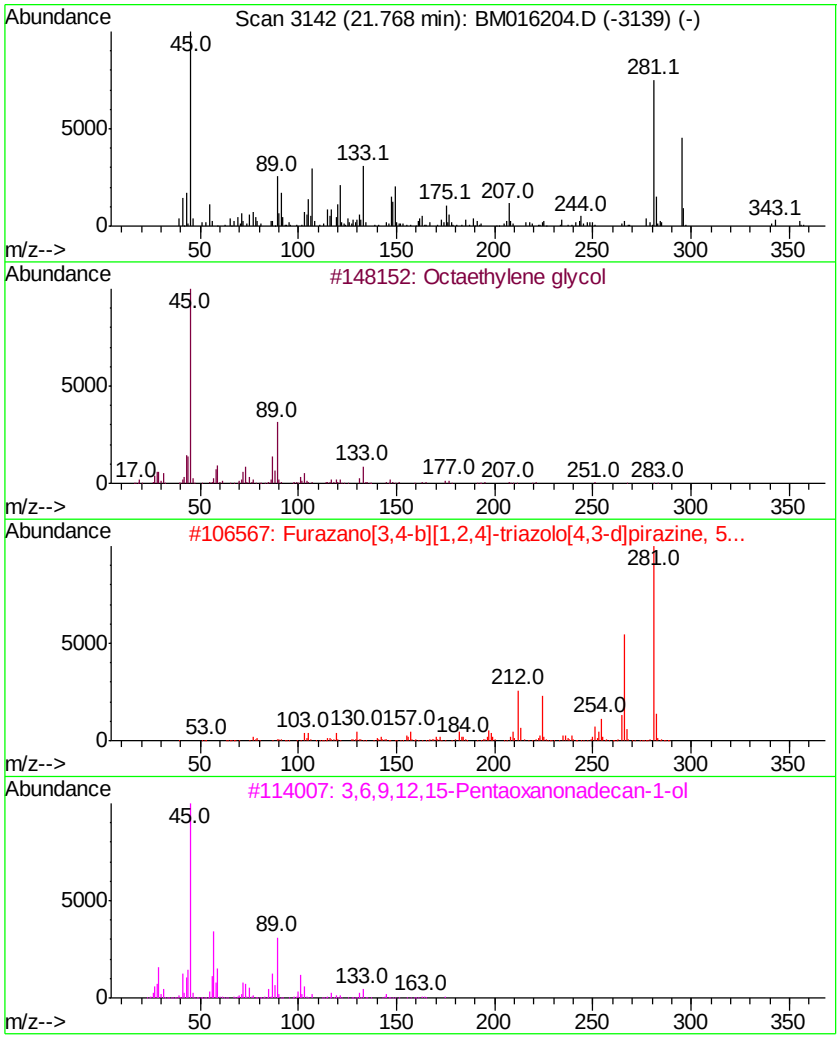
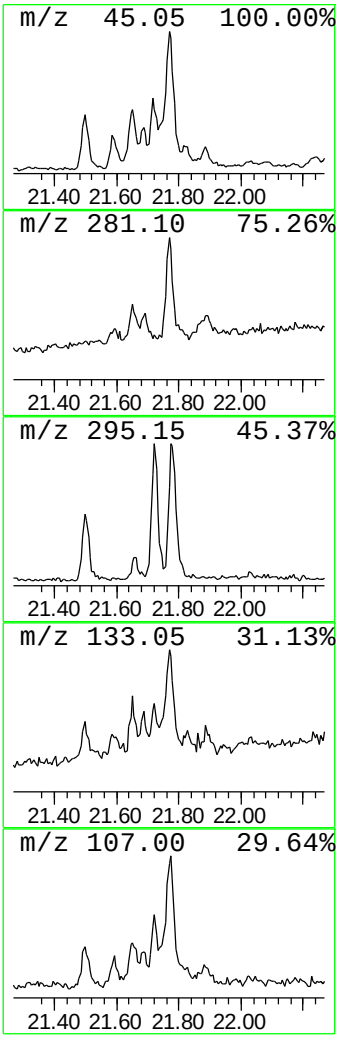
Peak Number 12 unknown21.77 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.77	6.51 ng	289588	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octaethylene glycol	370	C16H34O9	1000289-34-2	30
2	Furazano[3,4-b][1,2,4]-triazolo[...	281	C13H11N7O	311783-53-6	27
3	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	27
4	Benzoic acid, 4-methyl-2-trimeth...	296	C14H24O3Si2	1000153-59-3	22
5	5-(p-Aminophenyl)-4-(p-tolyl)-2-...	281	C16H15N3S	094460-46-5	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080618\
Data File : BM016204.D
Acq On : 06 Aug 2018 23:00
Operator : SJ/JU
Sample : J4318-03
Misc :
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Instrument : BNA_M
ClientSampleId : BEEBEE-SITE-DEMO-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.22	3.7	ng	48623	1	8.17	259801	20.0
unknown7.70	7.70	58.8	ng	764015	1	8.17	259801	20.0
Tridecanoic acid	18.38	4.2	ng	92135	4	17.53	439321	20.0
4H-Cyclopenta[def...	18.60	2.0	ng	44396	4	17.53	439321	20.0
unknown20.24	20.24	18.9	ng	840025	5	21.66	890306	20.0
unknown20.30	20.30	18.4	ng	817191	5	21.66	890306	20.0
unknown20.34	20.34	12.2	ng	543073	5	21.66	890306	20.0
unknown20.42	20.42	28.2	ng	1253410	5	21.66	890306	20.0
Pyrrolo[1,2-a]-1,...	20.49	16.8	ng	749398	5	21.66	890306	20.0
unknown20.56	20.56	12.7	ng	563562	5	21.66	890306	20.0
unknown21.77	21.77	6.5	ng	289588	5	21.66	890306	20.0