LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080322\
Data File : BM036074.D
Acq On : 03 Aug 2022 12:37
Operator : CG/JU
Sample : PB146663BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB146663BL

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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036074.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	391	398	412	rBV	5483475	7653058	53.85%	10.123%
2	7.039	659	672	686	rBV	4913167	7800717	54.89%	10.319%
3	7.863	805	812	822	rBV	1049145	1585874	11.16%	2.098%
4	9.033	1003	1011	1028	rBV	3142717	5061508	35.61%	6.695%
5	10.669	1279	1289	1303	rBV	1376779	2278562	16.03%	3.014%
6	12.827	1650	1656	1662	rBV	161392	268452	1.89%	0.355%
7	12.892	1662	1667	1680	rVB	419800	702191	4.94%	0.929%
8	13.133	1700	1708	1719	rBV	8005138	11298961	79.50%	14.946%
9	13.315	1730	1739	1753	rBV2	116749	256272	1.80%	0.339%
10	13.433	1753	1759	1766	rVV	129295	203585	1.43%	0.269%
11	13.510	1766	1772	1777	rVV	275482	436297	3.07%	0.577%
12	13.568	1777	1782	1791	rVB	267725	428383	3.01%	0.567%
13	14.504	1934	1941	1949	rBV	1979342	2824315	19.87%	3.736%
14	14.615	1954	1960	1978	rBV4	39374	170721	1.20%	0.226%
15	15.986	2185	2193	2212	rBV	5364708	7722861	54.34%	10.216%
16	17.245	2400	2407	2416	rBV	2232527	3110916	21.89%	4.115%
17	19.868	2847	2853	2863	rBV	11736138	14212350	100.00%	18.800%
18	21.421	3113	3117	3127	rBV	2415486	3051526	21.47%	4.036%
19	22.527	3302	3305	3313	rVB	217174	278830	1.96%	0.369%
20	23.068	3394	3397	3404	rVB	330924	497410	3.50%	0.658%
21	23.691	3499	3503	3510	rVB	473946	778267	5.48%	1.029%
22	23.785	3513	3519	3528	rVB2	1537073	3026324	21.29%	4.003%
23	24.403	3619	3624	3635	rVB	468948	946188	6.66%	1.252%
24	25.232	3761	3765	3775	rVB	460310	1005355	7.07%	1.330%

Sum of corrected areas: 75598923

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ClientSampleId :
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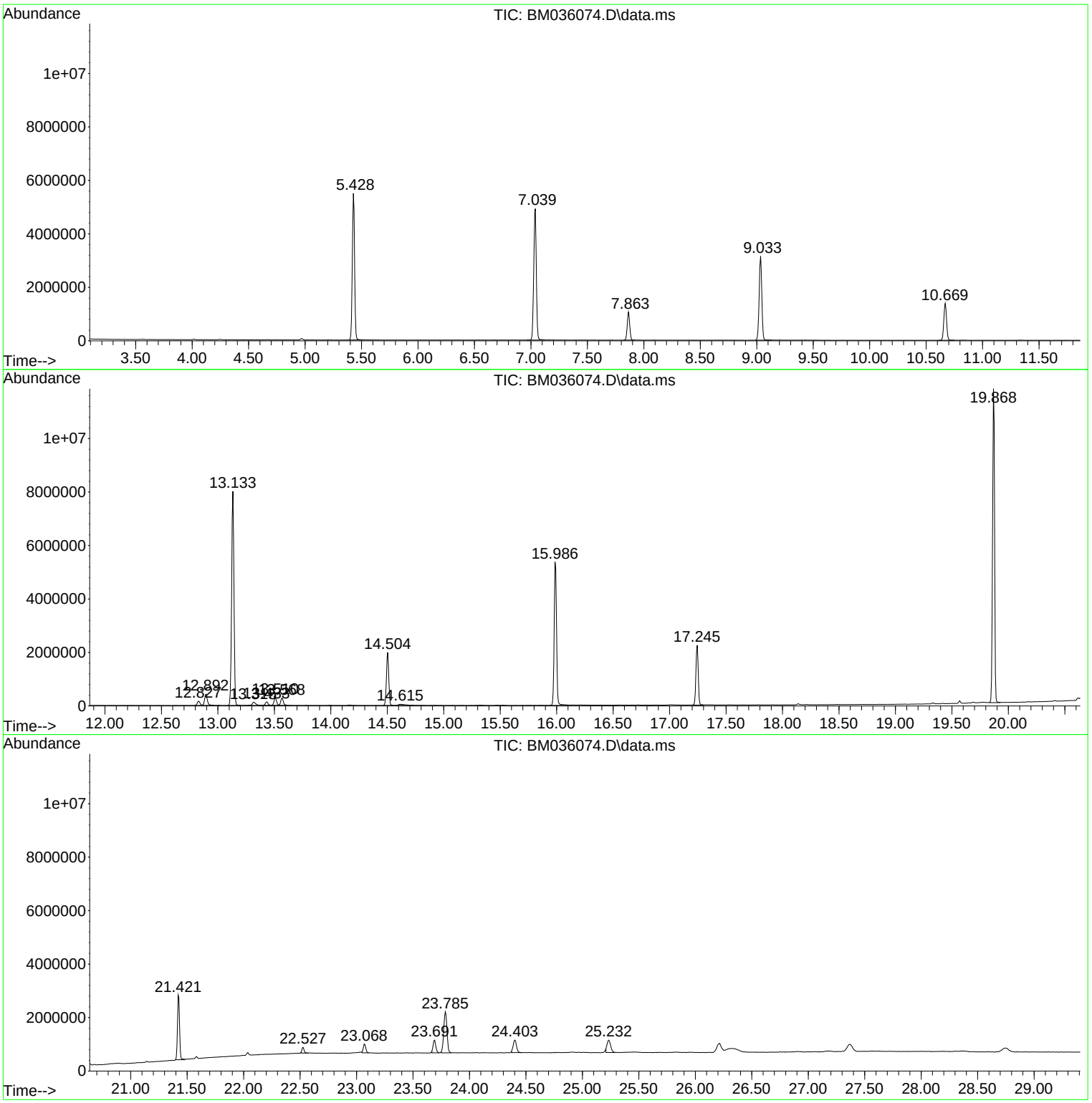
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BM036074.D
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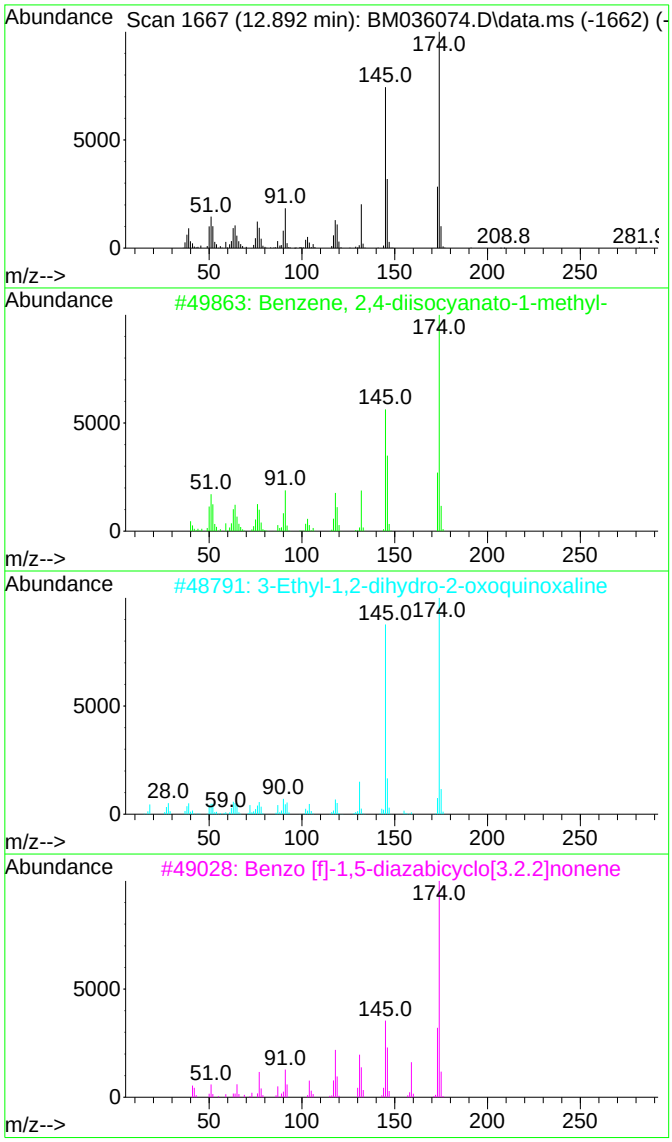
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

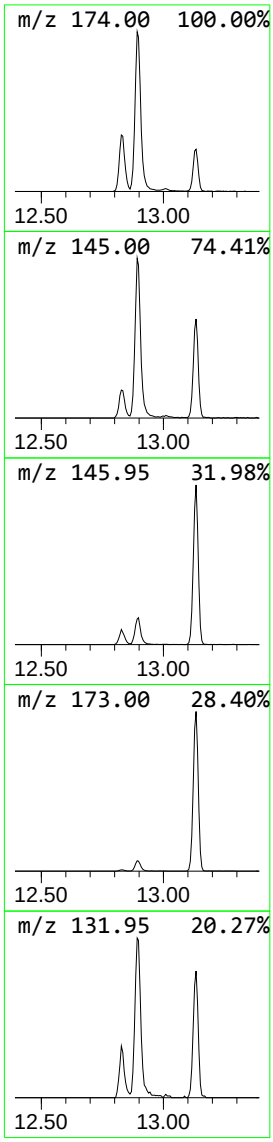
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 2,4-diisocyanato-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.892	4.97 ng	702191	Acenaphthene-d10	14.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	98
2	3-Ethyl-1,2-dihydro-2-oxoquinoxa...	174	C10H10N2O	013297-35-3	59
3	Benzo [f]-1,5-diazabicyclo[3.2.2...	174	C11H14N2	007092-76-4	59
4	2H-1-Benzopyran-2-one, 4,6-dimet...	174	C11H10O2	014002-89-2	50
5	Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	47





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Operator : CG/JU
Sample : PB146663BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB146663BL

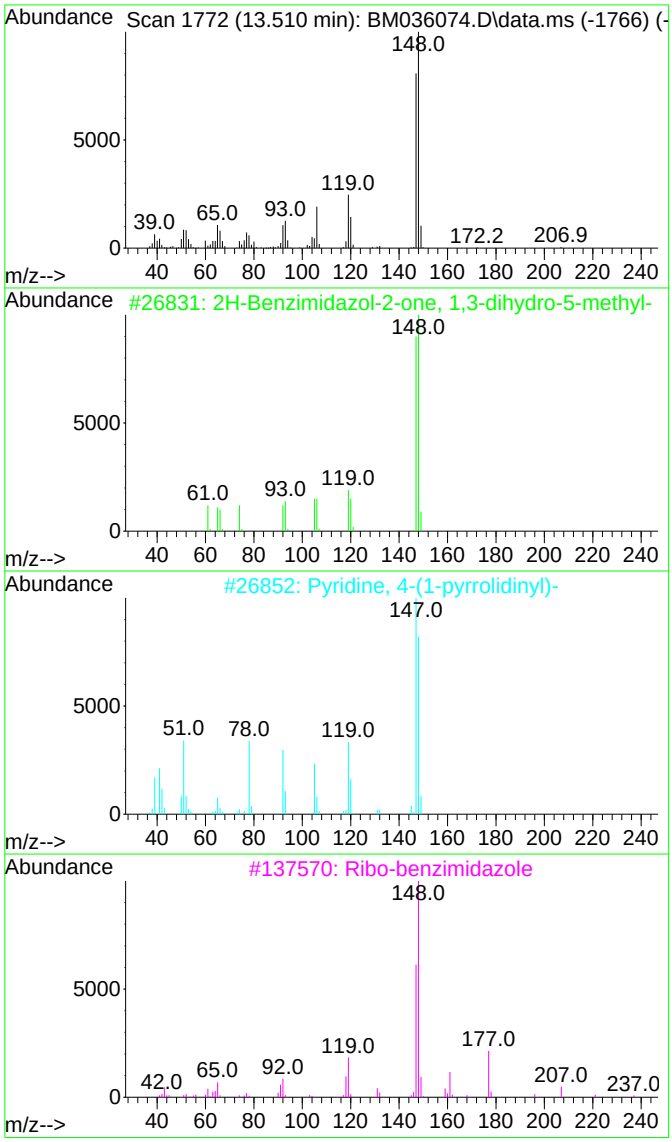
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

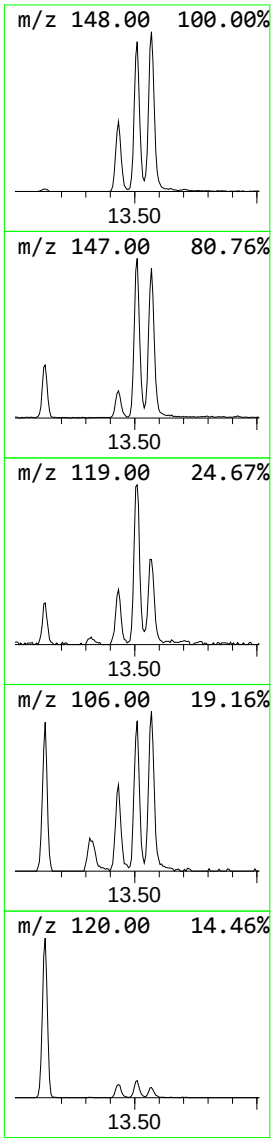
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2H-Benzimidazol-2-one, 1,3-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.510	3.09 ng	436297	Acenaphthene-d10	14.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Benzimidazol-2-one, 1,3-dihyd...	148	C8H8N2O	005400-75-9	91
2	Pyridine, 4-(1-pyrrolidinyl)-	148	C9H12N2	002456-81-7	72
3	Ribo-benzimidazole	252	C12H16N2O4	1000128-23-5	64
4	Pyrrole-2-carbonitrile, 5-formyl...	148	C8H8N2O	026187-38-2	64
5	Arabo-benzimidazole	250	C12H14N2O4	055175-30-9	64





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Data File : BM036074.D
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Operator : CG/JU
Sample : PB146663BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB146663BL

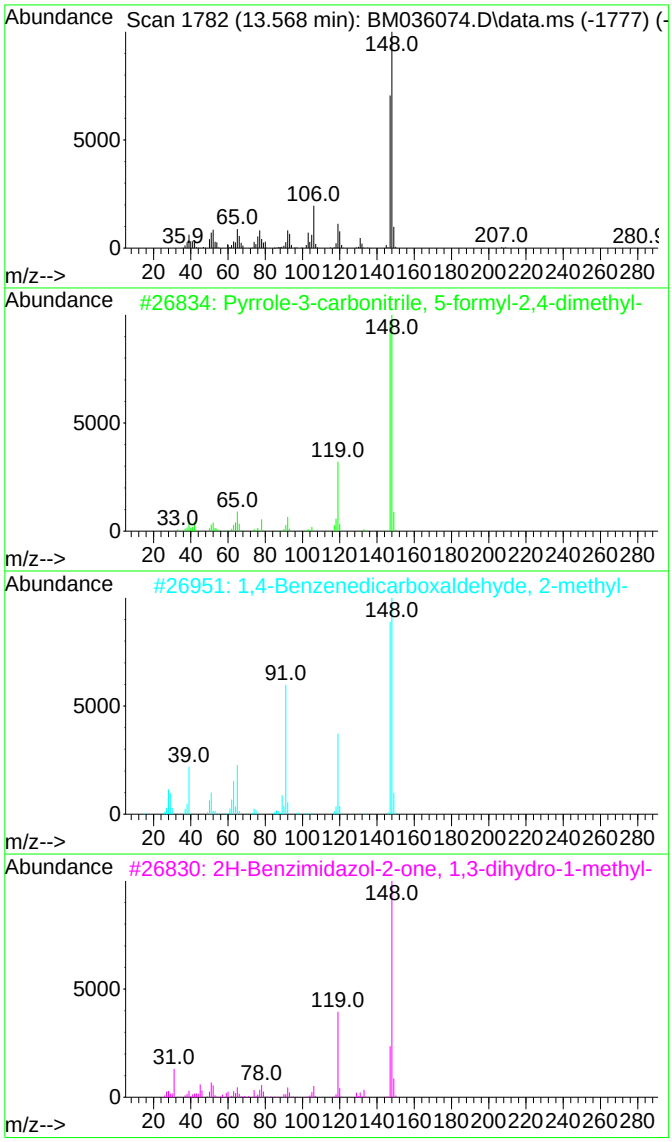
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

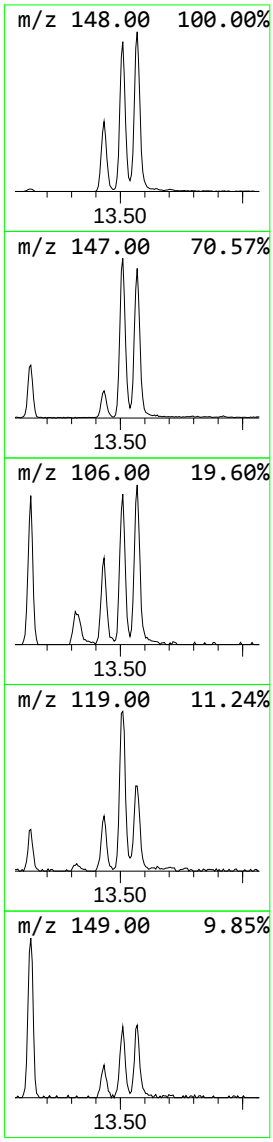
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pyrrole-3-carbonitrile, 5-f... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.568	3.03 ng	428383	Acenaphthene-d10	14.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrole-3-carbonitrile, 5-formyl...	148	C8H8N2O	032487-71-1	72
2	1,4-Benzenedicarboxaldehyde, 2-m...	148	C9H8O2	027587-17-3	59
3	2H-Benzimidazol-2-one, 1,3-dihyd...	148	C8H8N2O	001849-01-0	53
4	Benzaldehyde, 2,4,6-trimethyl-	148	C10H12O	000487-68-3	53
5	7-Hydroxy-1-indanone	148	C9H8O2	006968-35-0	52





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Data File : BM036074.D
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Operator : CG/JU
Sample : PB146663BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB146663BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
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TIC Library : C:\Database\NIST20.L
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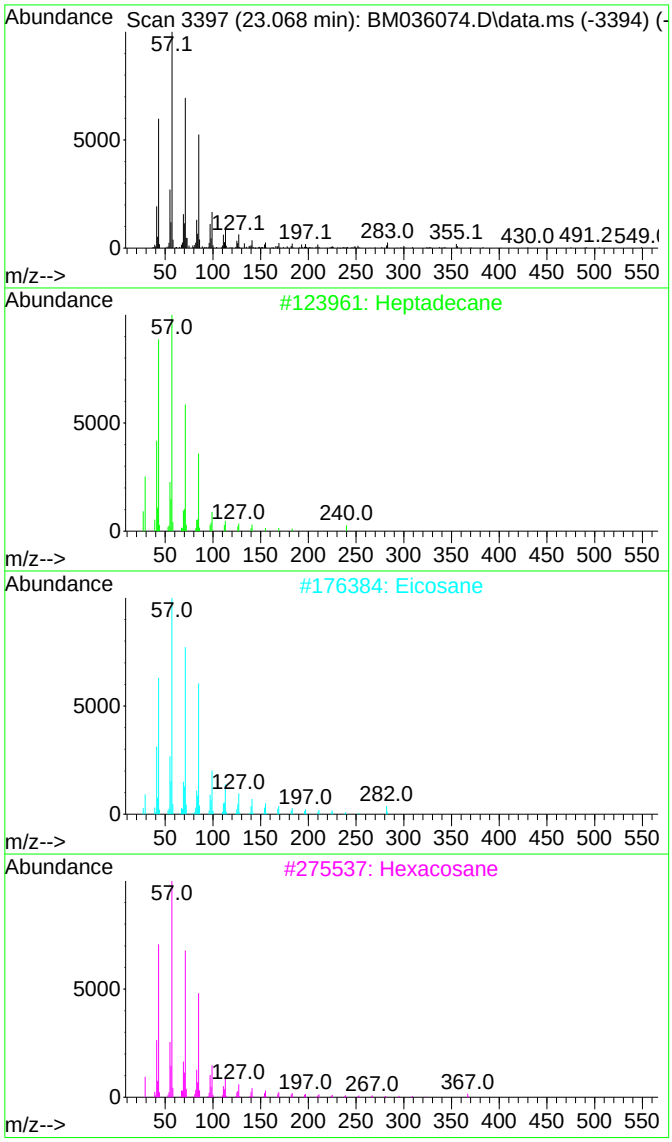
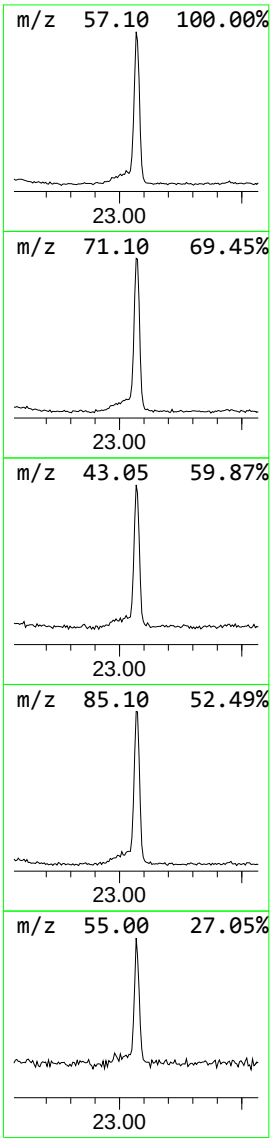
****

Peak Number 4 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.068	3.29 ng	497410	Perylene-d12	23.785

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Eicosane	282	C20H42	000112-95-8	93
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87





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Operator : CG/JU
Sample : PB146663BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PB146663BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
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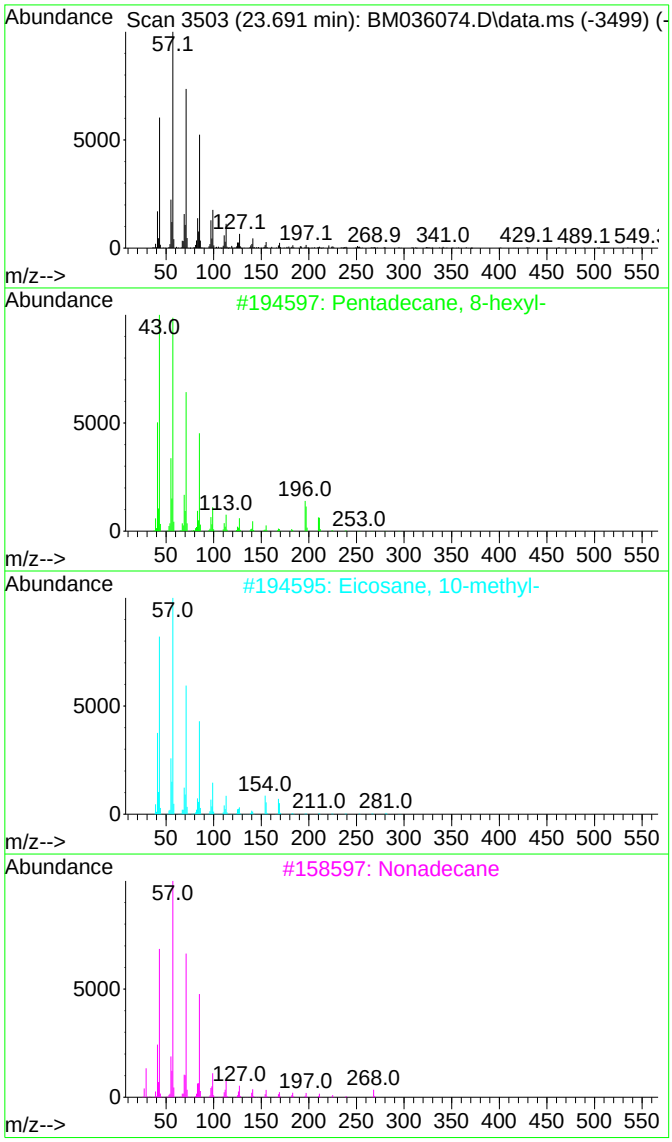
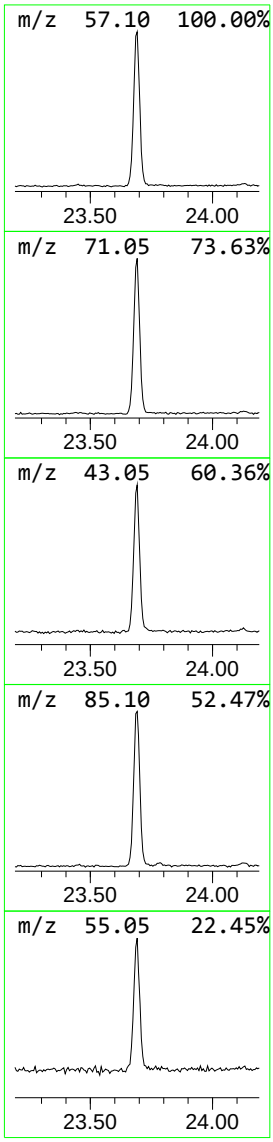
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecane, 8-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.691	5.14 ng	778267	Perylene-d12	23.785

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
3	Nonadecane	268	C19H40	000629-92-5	93
4	Heptadecane	240	C17H36	000629-78-7	93
5	Hexacosane	366	C26H54	000630-01-3	91





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BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
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TIC Library : C:\Database\NIST20.L
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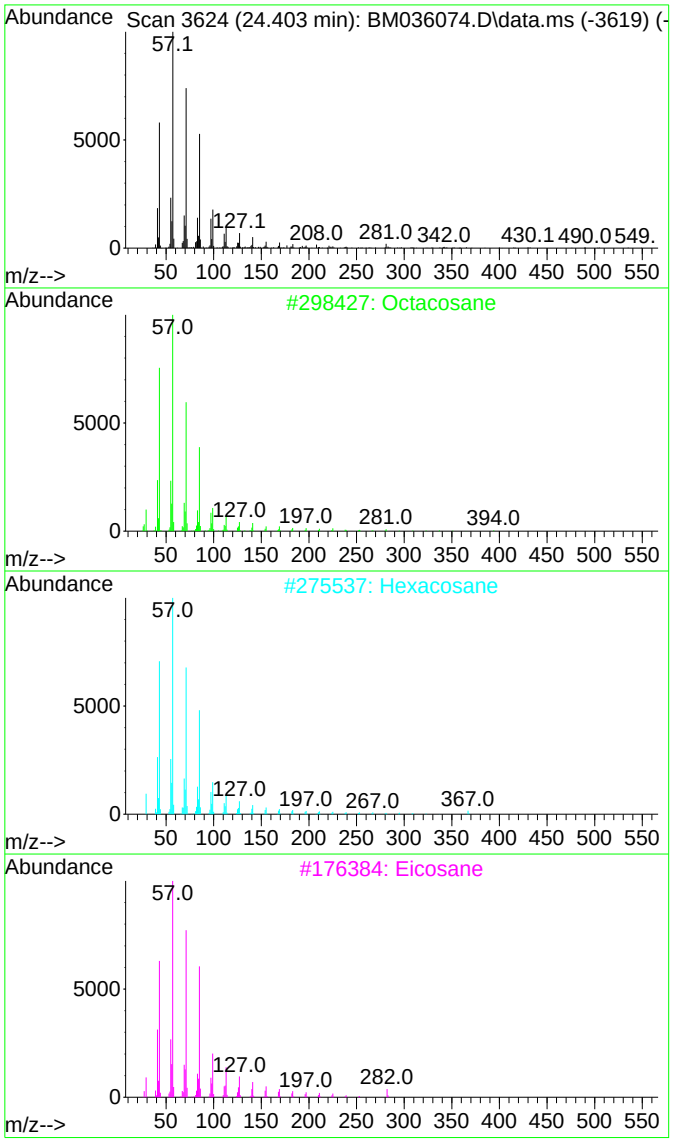
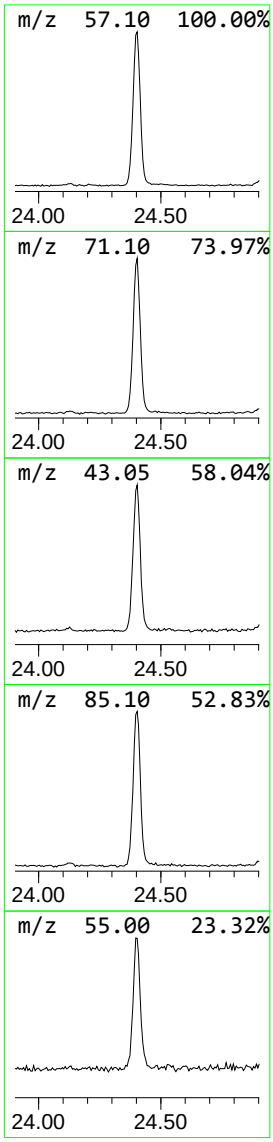
****

Peak Number 6 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.403	6.25 ng	946188	Perylene-d12	23.785

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hentriacontane	437	C31H64	000630-04-6	91





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ClientSampleId :
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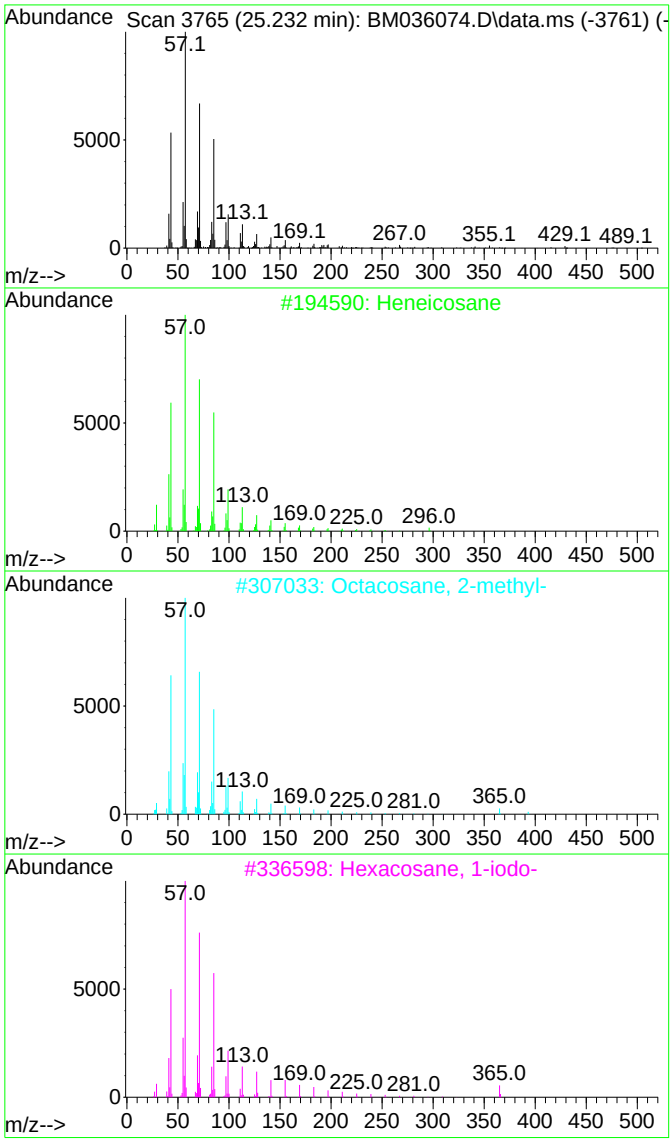
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

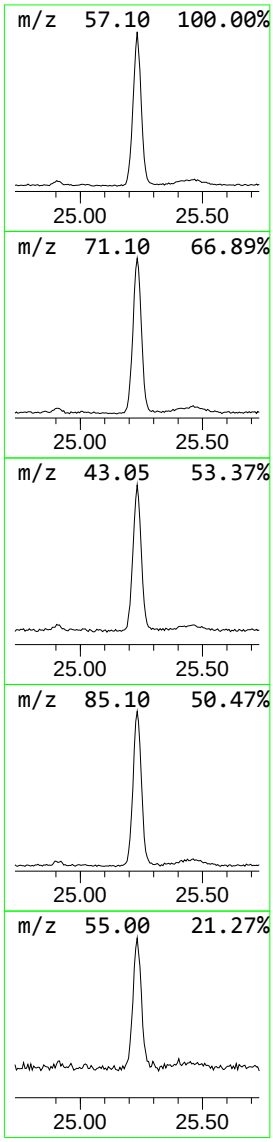
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.232	6.64 ng	1005360	Perylene-d12	23.785

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzene, 2,4-di...	12.892	5.0	ng	702191	3	14.504	2824320	20.0
2H-Benzimidazol...	13.510	3.1	ng	436297	3	14.504	2824320	20.0
Pyrrole-3-carbo...	13.568	3.0	ng	428383	3	14.504	2824320	20.0
Heptadecane	23.068	3.3	ng	497410	6	23.785	3026320	20.0
Pentadecane, 8-...	23.691	5.1	ng	778267	6	23.785	3026320	20.0
Octacosane	24.403	6.3	ng	946188	6	23.785	3026320	20.0
Heneicosane	25.232	6.6	ng	1005360	6	23.785	3026320	20.0