LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019074.D
Acq On : 08 Mar 2019 15:30
Operator : JU/SJ
Sample : K1807-21
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-18

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-BM021119.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	5.269	364	371	385	rBV	3069518	4334156	58.15%	8.599%
2	6.851	632	640	656	rBV	2859036	4697747	63.02%	9.320%
3	7.204	693	700	716	rBV	3063228	4802504	64.43%	9.528%
4	7.669	772	779	786	rBV	650466	986177	13.23%	1.956%
5	7.987	825	833	842	rBV	2237176	3497402	46.92%	6.939%
6	8.839	970	978	991	rBV	1633214	2737053	36.72%	5.430%
7	10.457	1246	1253	1265	rBV	719380	1228885	16.49%	2.438%
8	12.933	1667	1674	1689	rBV	3653256	5481365	73.54%	10.875%
9	13.786	1814	1819	1829	rBV	191382	300868	4.04%	0.597%
10	14.204	1883	1890	1904	rVB2	101116	275114	3.69%	0.546%
11	14.321	1904	1910	1928	rVB2	960800	1555638	20.87%	3.086%
12	15.821	2159	2165	2185	rBV	3130857	4565719	61.25%	9.058%
13	17.080	2373	2379	2394	rBV	1154278	1784547	23.94%	3.540%
14	17.968	2524	2530	2541	rBV	350366	647428	8.69%	1.284%
15	19.256	2744	2749	2762	rBV	325820	609691	8.18%	1.210%
16	19.715	2821	2827	2836	rBV	6024423	7453971	100.00%	14.788%
17	20.974	3037	3041	3047	rBV2	190190	244590	3.28%	0.485%
18	21.274	3087	3092	3101	rBV2	1678942	2244601	30.11%	4.453%
19	21.844	3186	3189	3194	rVB2	112251	133206	1.79%	0.264%
20	22.303	3264	3267	3274	rVB	194866	232891	3.12%	0.462%
21	22.809	3349	3353	3359	rVB	192080	269084	3.61%	0.534%
22	23.521	3467	3474	3488	rVB	1170044	2322606	31.16%	4.608%

Sum of corrected areas: 50405243

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Instrument :
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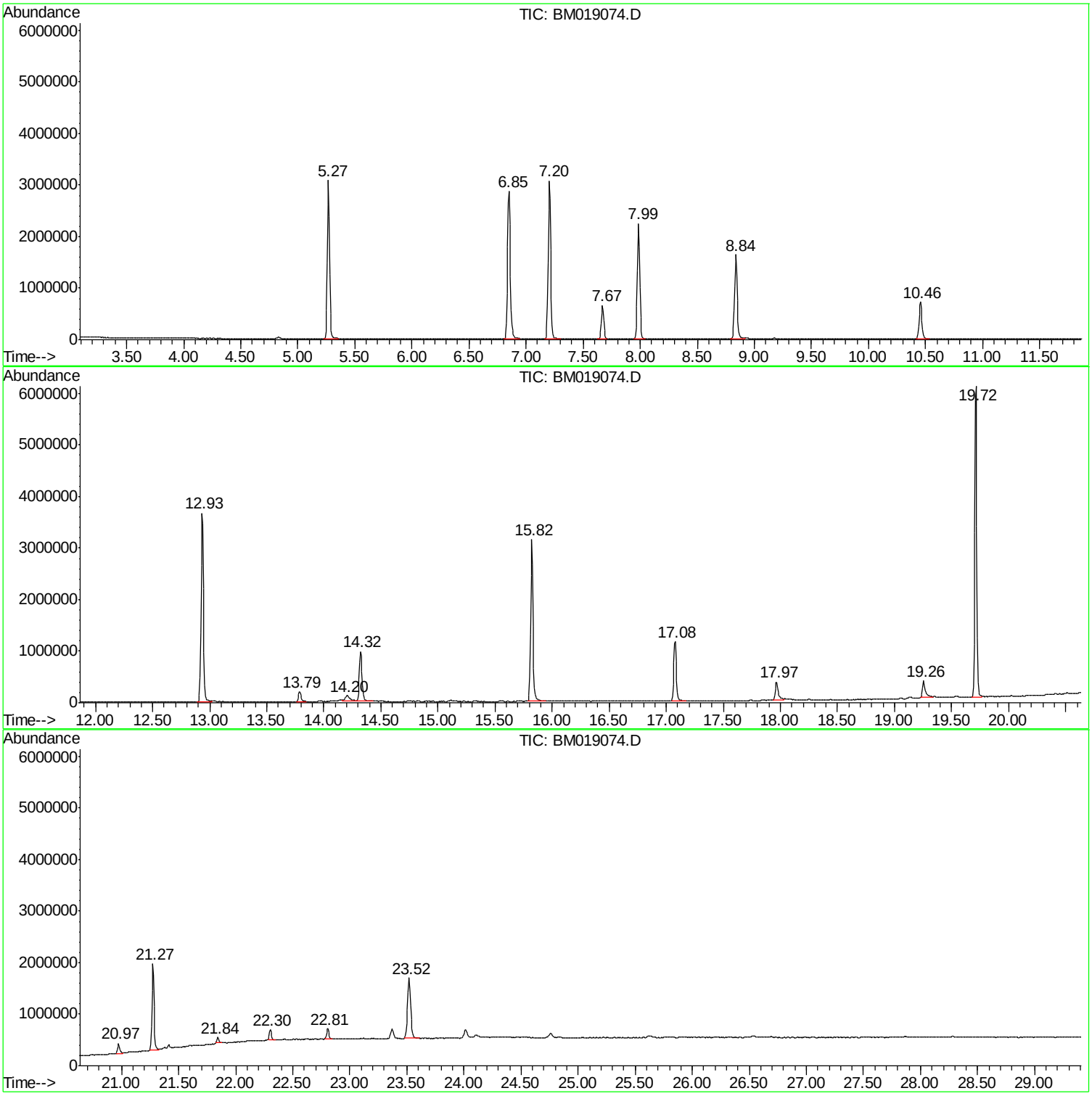
ClientSampleId :
TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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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TIC Library : C:\DATABASE\NIST02.L
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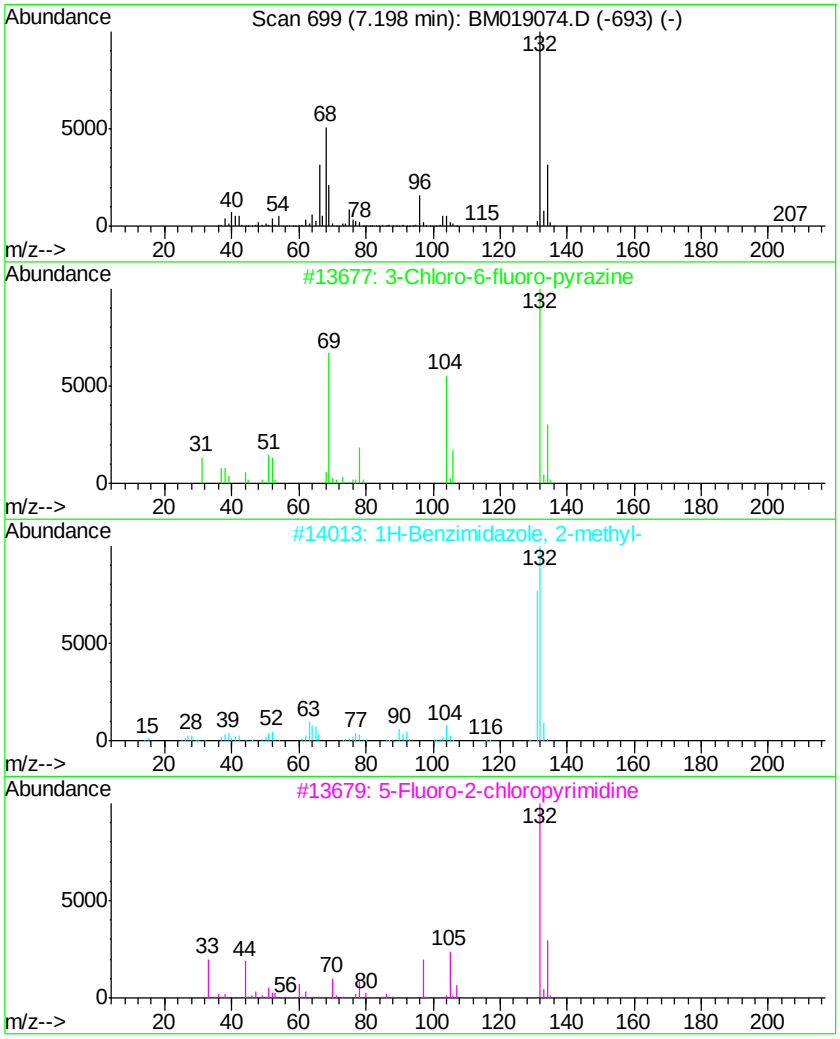
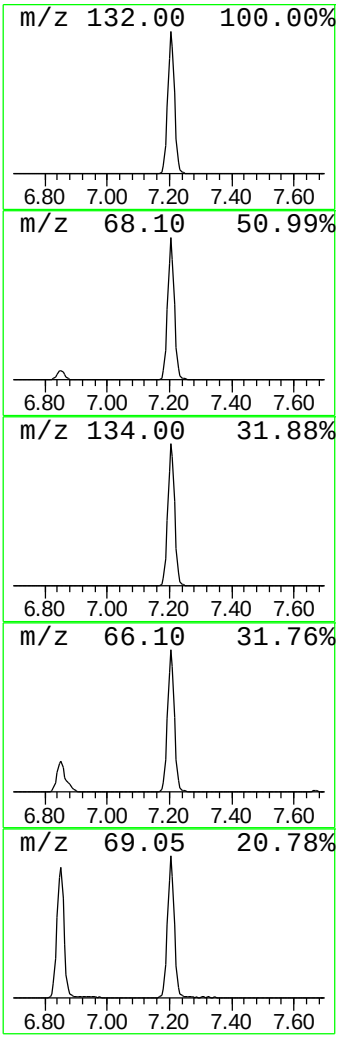
****

Peak Number 1 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	97.40 ng	4802500	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11





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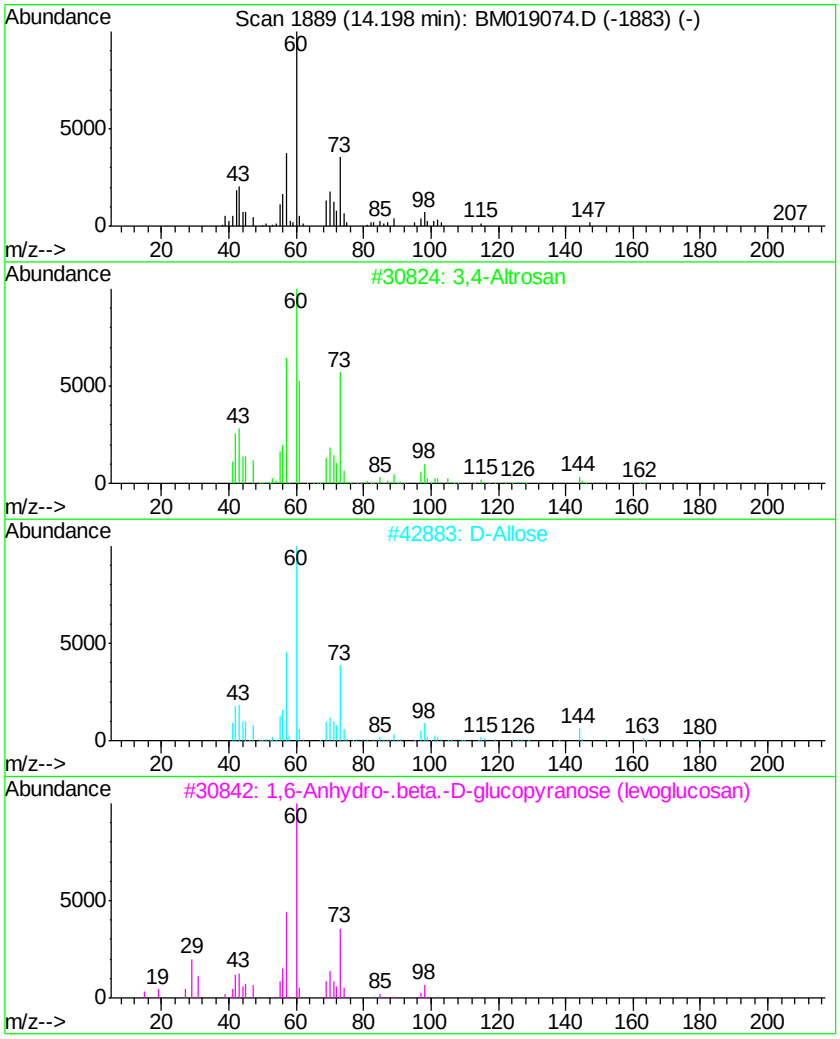
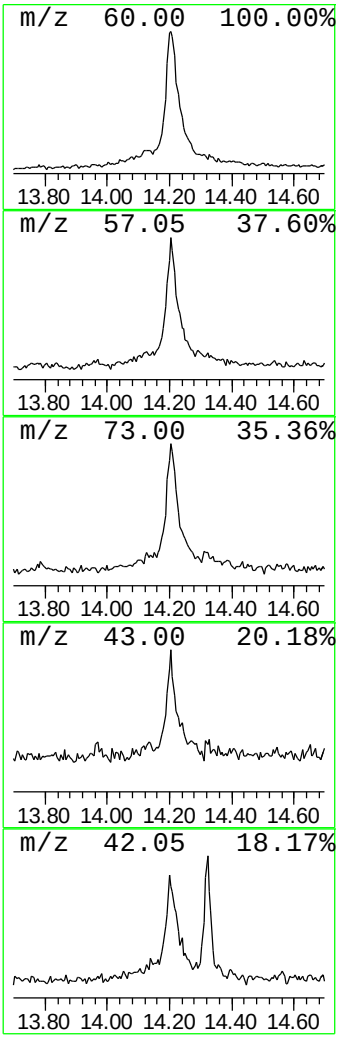
****

Peak Number 3 3,4-Altrosan Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	3.54 ng	275114	Acenaphthene-d10	14.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Altrosan	162	C6H10O5	1000129-76-4	72
2	D-Allose	180	C6H12O6	002595-97-3	64
3	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	64
4	Pentanoic acid	102	C5H10O2	000109-52-4	50
5	1,6-Anhydro-.beta.-d-talopyranose	162	C6H10O5	1000133-05-8	50





Library Search Compound Report

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Data File : BM019074.D
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Operator : JU/SJ
Sample : K1807-21
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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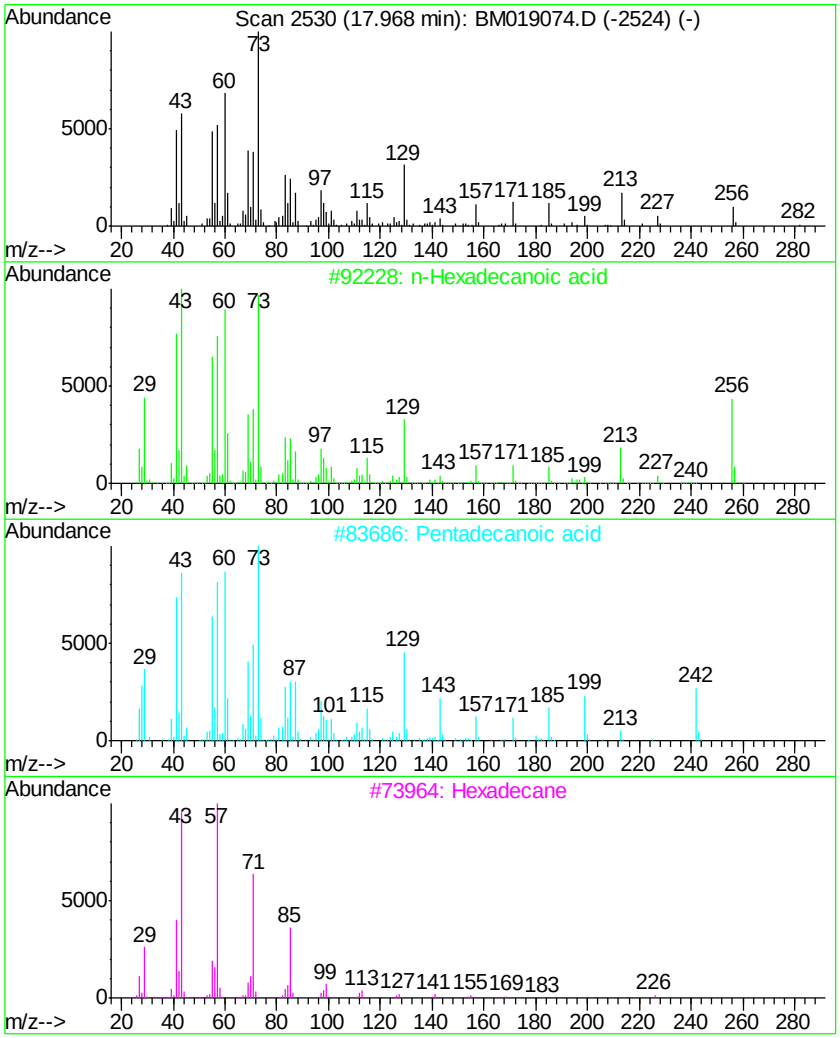
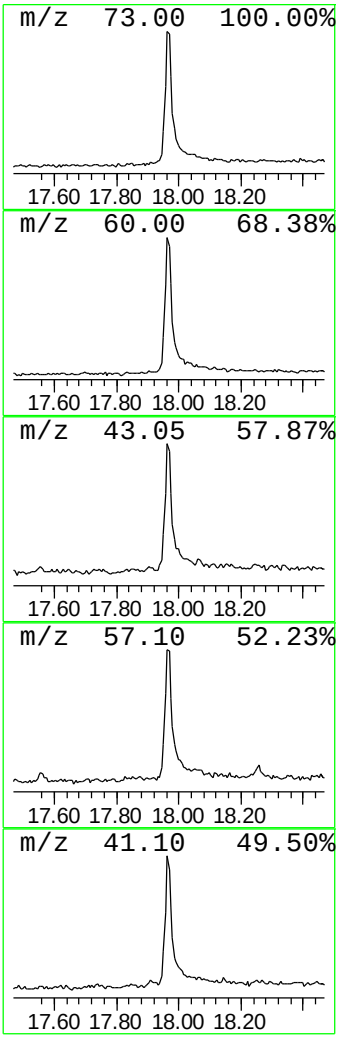
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	7.26 ng	647428	Phenanthrene-d10	17.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Hexadecane	226	C16H34	000544-76-3	18
4	Tetradecane	198	C14H30	000629-59-4	18
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	18





Library Search Compound Report

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Instrument :
BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
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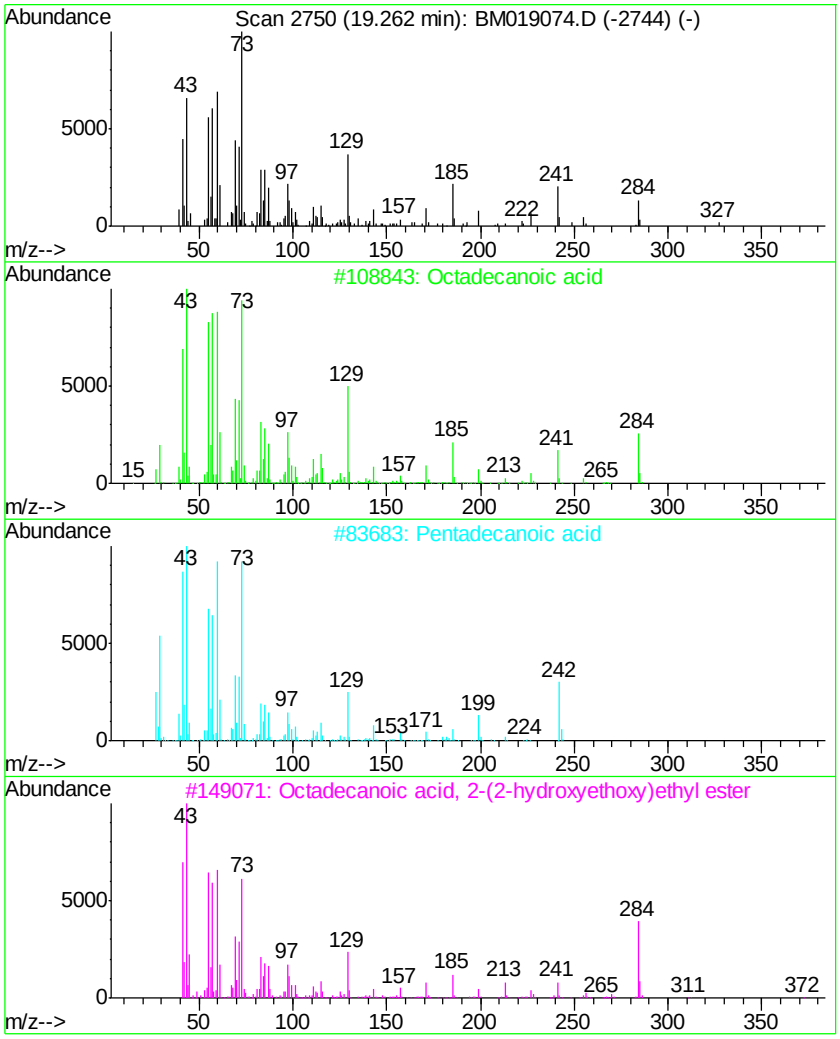
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

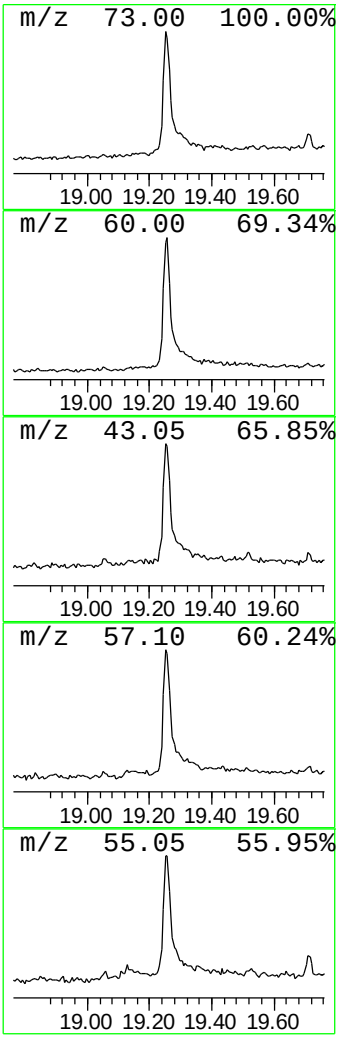
****

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	5.43 ng	609691	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	41





Library Search Compound Report

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ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
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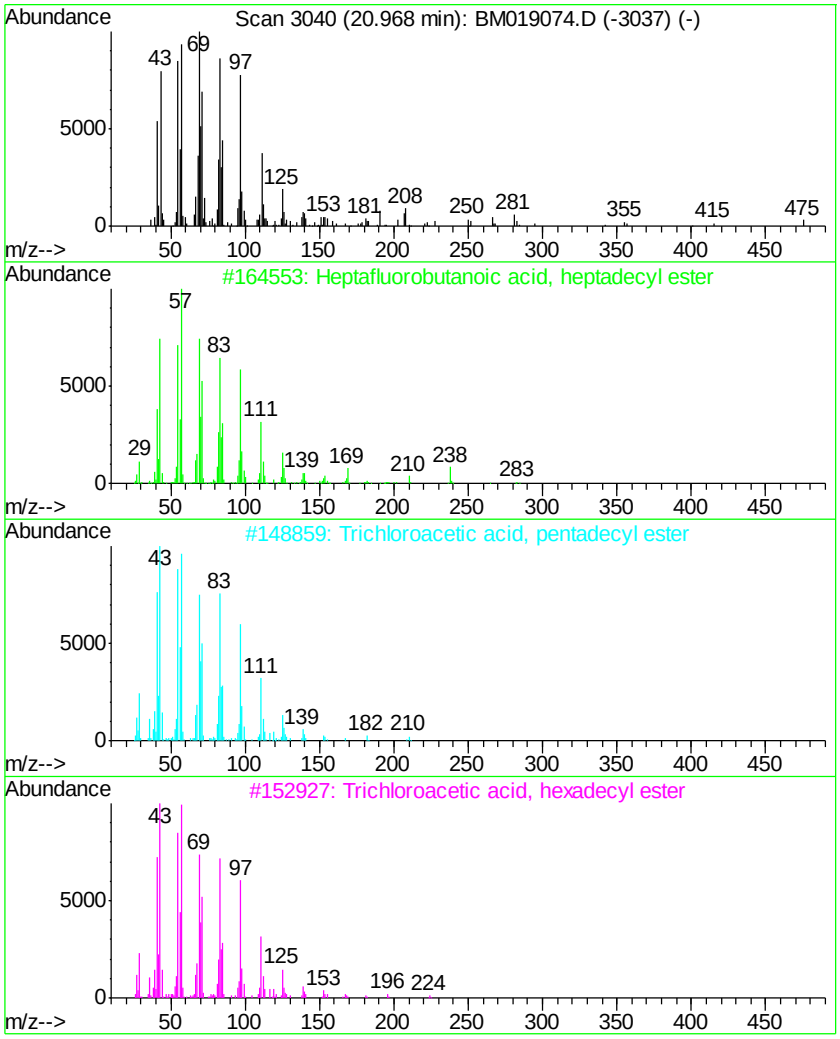
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

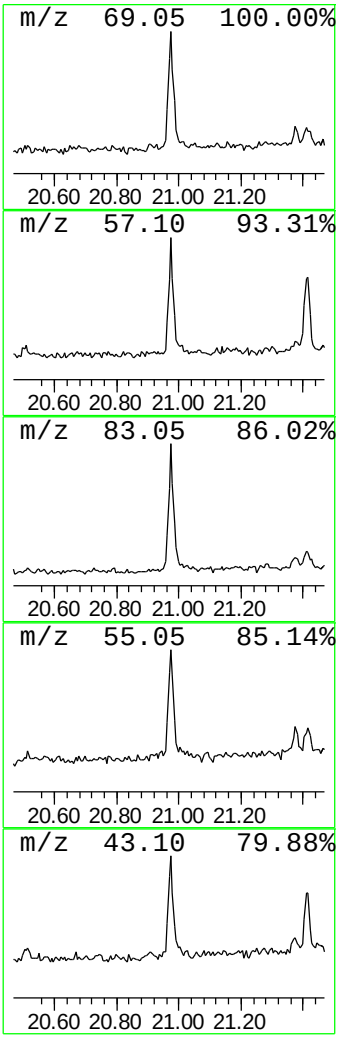
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptafluorobutanoic acid, h... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	2.18 ng	244590	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





Library Search Compound Report

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BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

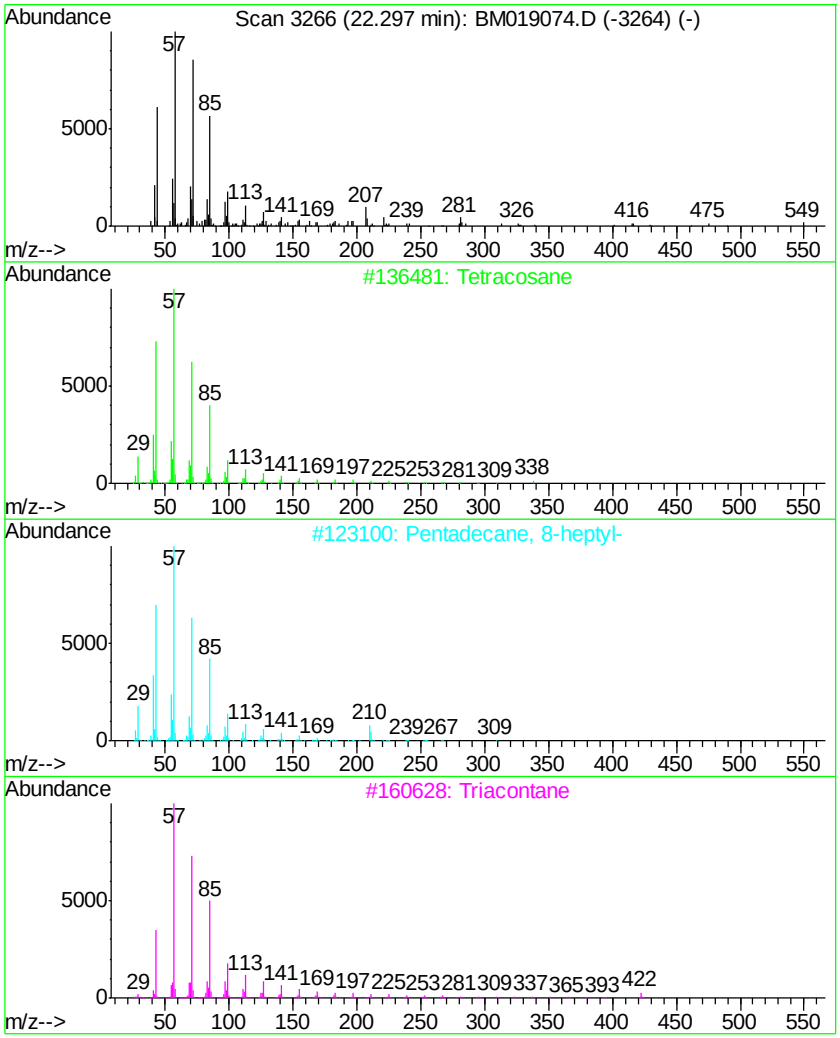
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

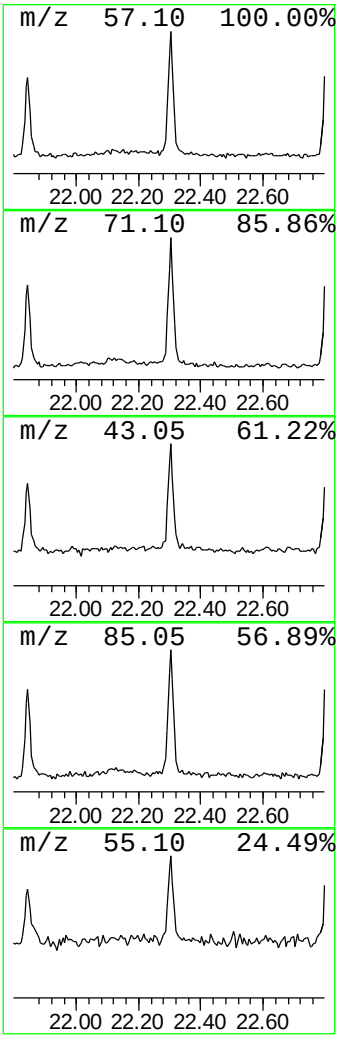
****

Peak Number 7 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.30	2.08 ng	232891	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5	Hexadecane	226	C16H34	000544-76-3	83





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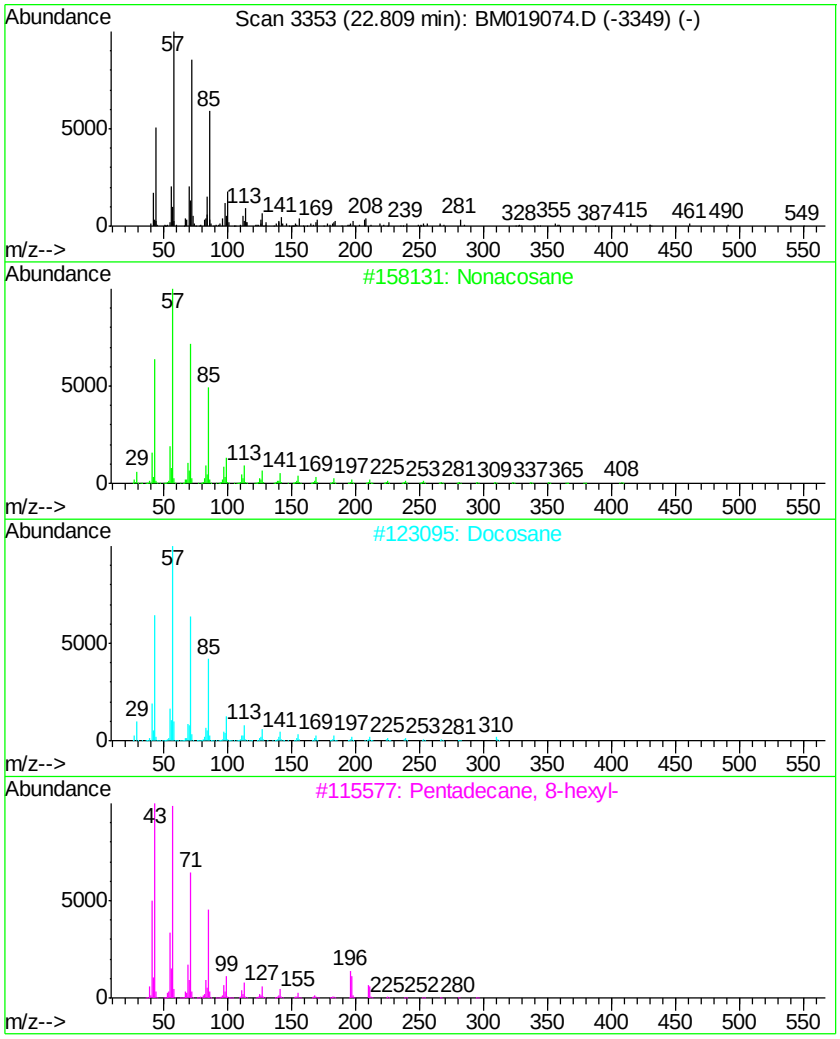
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

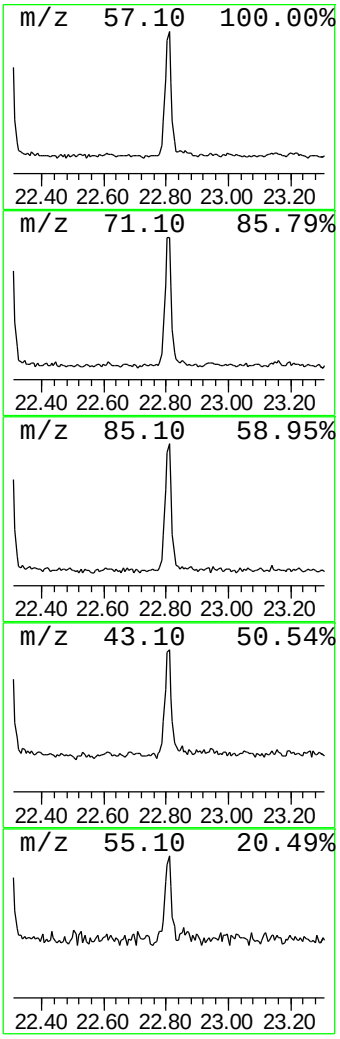
****

Peak Number 8 Nonacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.81	2.32 ng	269084	Perylene-d12	23.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane	408	C29H60	000630-03-5	87
2	Docosane	310	C22H46	000629-97-0	87
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
4	Benzeneacetic acid, 2-tetradecyl...	332	C22H36O2	1000282-02-4	86
5	Tetracosane	338	C24H50	000646-31-1	86





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown7.20	7.20	97.4	ng	4802500	1	7.67	986177	20.0
3,4-Altrosan	14.20	3.5	ng	275114	3	14.32	1555640	20.0
n-Hexadecanoic acid	17.97	7.3	ng	647428	4	17.08	1784550	20.0
Octadecanoic acid	19.26	5.4	ng	609691	5	21.27	2244600	20.0
Heptafluorobutano...	20.97	2.2	ng	244590	5	21.27	2244600	20.0
Tetracosane	22.30	2.1	ng	232891	5	21.27	2244600	20.0
Nonacosane	22.81	2.3	ng	269084	6	23.52	2322610	20.0