LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019073.D
Acq On : 08 Mar 2019 14:54
Operator : JU/SJ
Sample : K1807-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-10

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	386	rBV	3416000	4875681	68.85%	8.385%
2	6.851	631	640	655	rBV	3247277	5261724	74.30%	9.048%
3	7.204	693	700	716	rBV	3538882	5418675	76.51%	9.318%
4	7.669	772	779	788	rBV	776456	1208344	17.06%	2.078%
5	7.987	826	833	843	rVB	2439372	3870198	54.65%	6.655%
6	8.839	970	978	992	rBV	1826503	3073779	43.40%	5.286%
7	10.457	1244	1253	1261	rBV	883752	1508235	21.30%	2.594%
8	12.933	1667	1674	1690	rBV	4032831	6028451	85.12%	10.367%
9	13.786	1813	1819	1828	rBV	223626	364130	5.14%	0.626%
10	14.204	1884	1890	1904	rVB2	105449	275988	3.90%	0.475%
11	14.321	1904	1910	1926	rVB2	1162508	1841633	26.00%	3.167%
12	15.821	2159	2165	2182	rBV	3089644	4646342	65.61%	7.990%
13	17.080	2372	2379	2391	rBV2	1322904	1991970	28.13%	3.426%
14	17.910	2516	2520	2524	rBV3	48139	84068	1.19%	0.145%
15	17.968	2524	2530	2551	rVV	942591	1643845	23.21%	2.827%
16	19.133	2725	2728	2735	rVV5	49754	101444	1.43%	0.174%
17	19.256	2744	2749	2769	rBV	1198047	1985650	28.04%	3.415%
18	19.715	2821	2827	2838	rBV	5910573	7081998	100.00%	12.179%
19	19.992	2870	2874	2877	rBV2	102628	137520	1.94%	0.236%
20	20.027	2877	2880	2886	rVB3	95678	119390	1.69%	0.205%
21	20.974	3037	3041	3051	rBV	594367	749286	10.58%	1.289%
22	21.274	3087	3092	3102	rBV	1713078	2232117	31.52%	3.839%
23	21.409	3113	3115	3121	rVB3	90262	102938	1.45%	0.177%
24	21.845	3186	3189	3195	rVB2	177640	250088	3.53%	0.430%
25	22.303	3263	3267	3274	rVB	237292	333260	4.71%	0.573%
26	22.803	3349	3352	3357	rVB	242953	344062	4.86%	0.592%
27	23.368	3445	3448	3456	rVB	233085	379425	5.36%	0.652%
28	23.515	3468	3473	3485	rVB	1167033	2240243	31.63%	3.852%

Sum of corrected areas: 58150484

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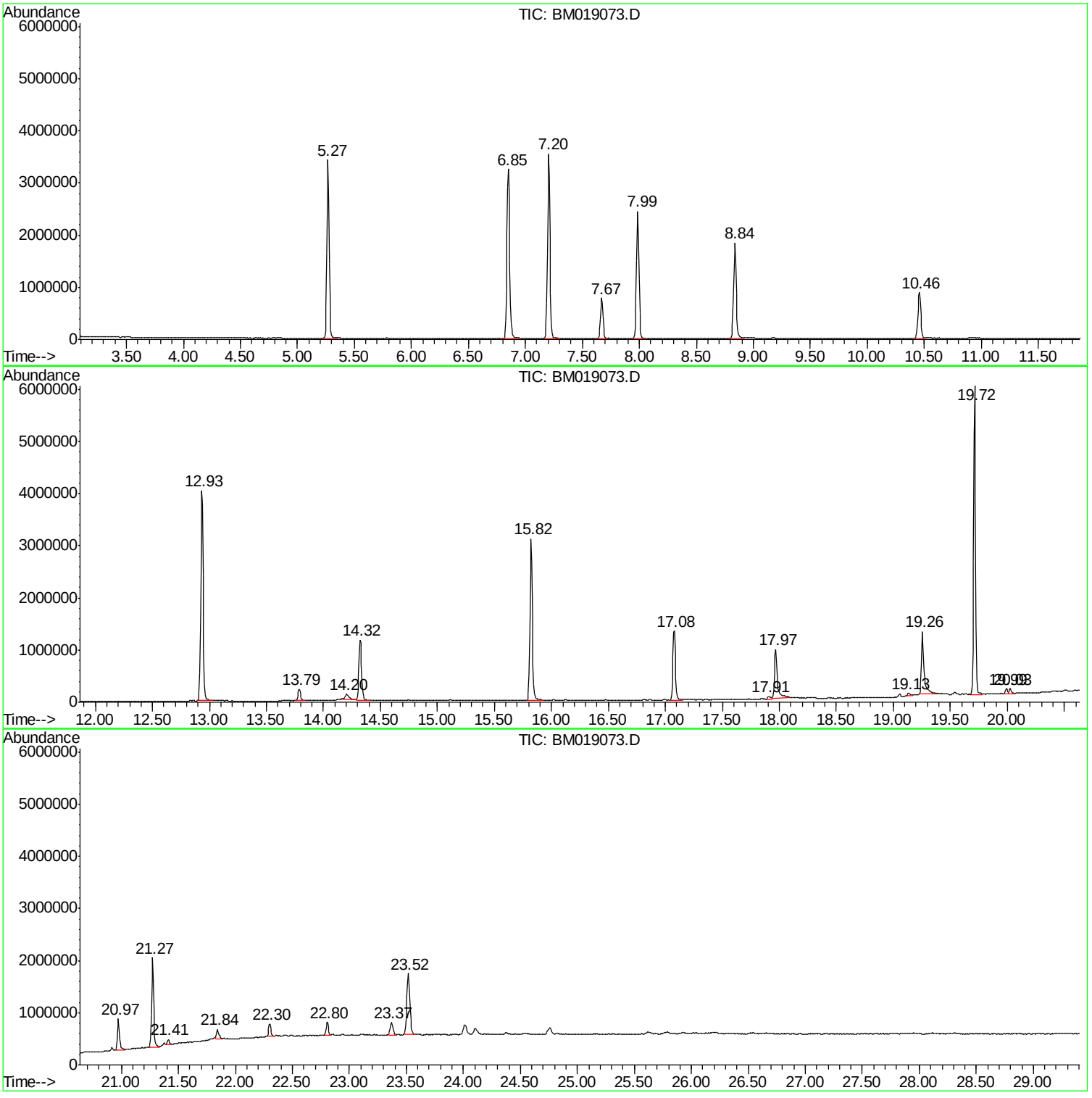
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-10

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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Data File : BM019073.D
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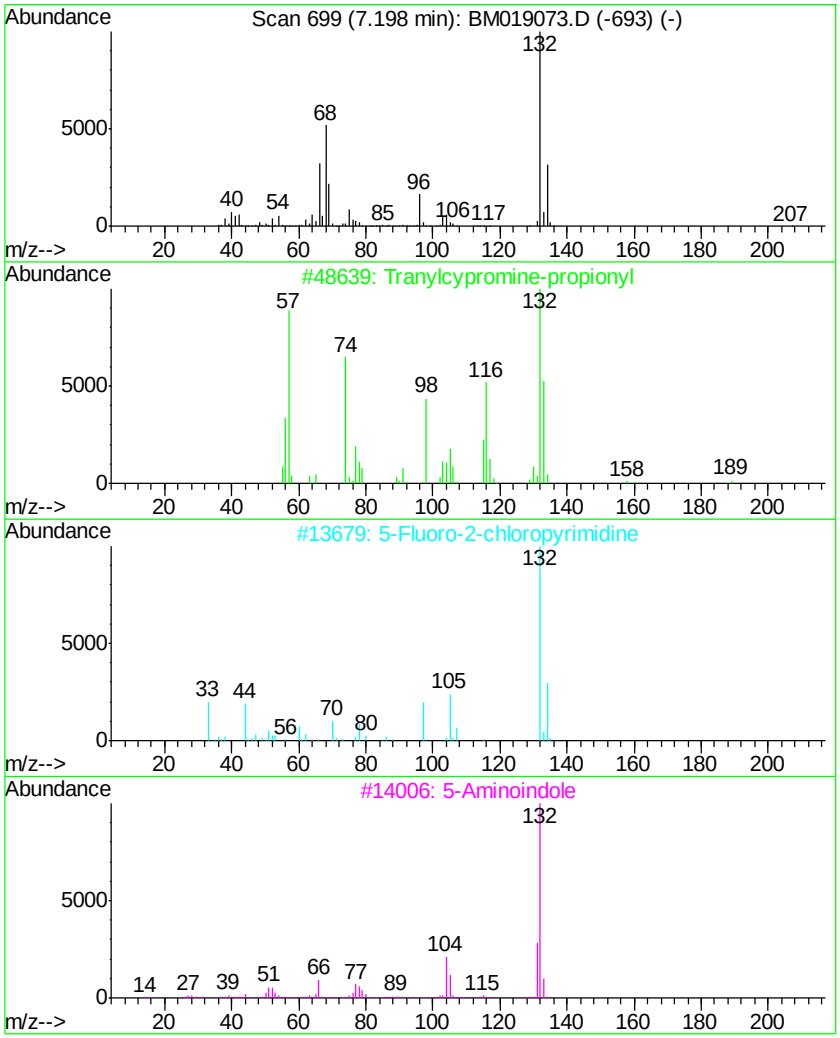
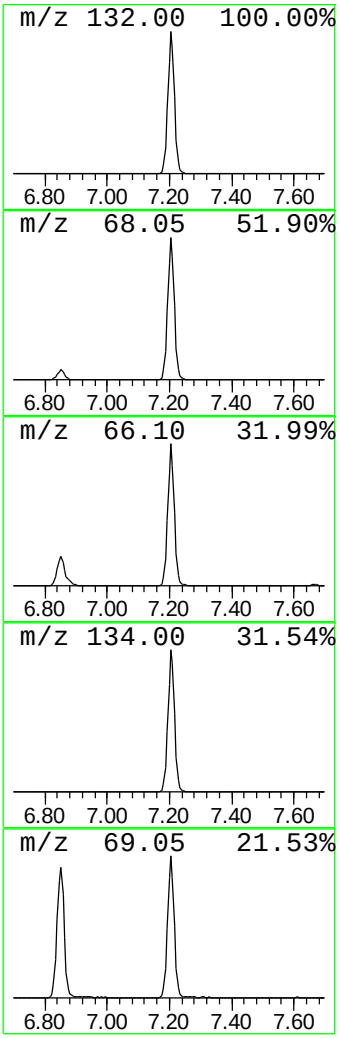
****

Peak Number 1 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	89.69 ng	5418680	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

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Data File : BM019073.D
Acq On : 08 Mar 2019 14:54
Operator : JU/SJ
Sample : K1807-19
Misc :
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Instrument : BNA_M
ClientSampleId : TP-10

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

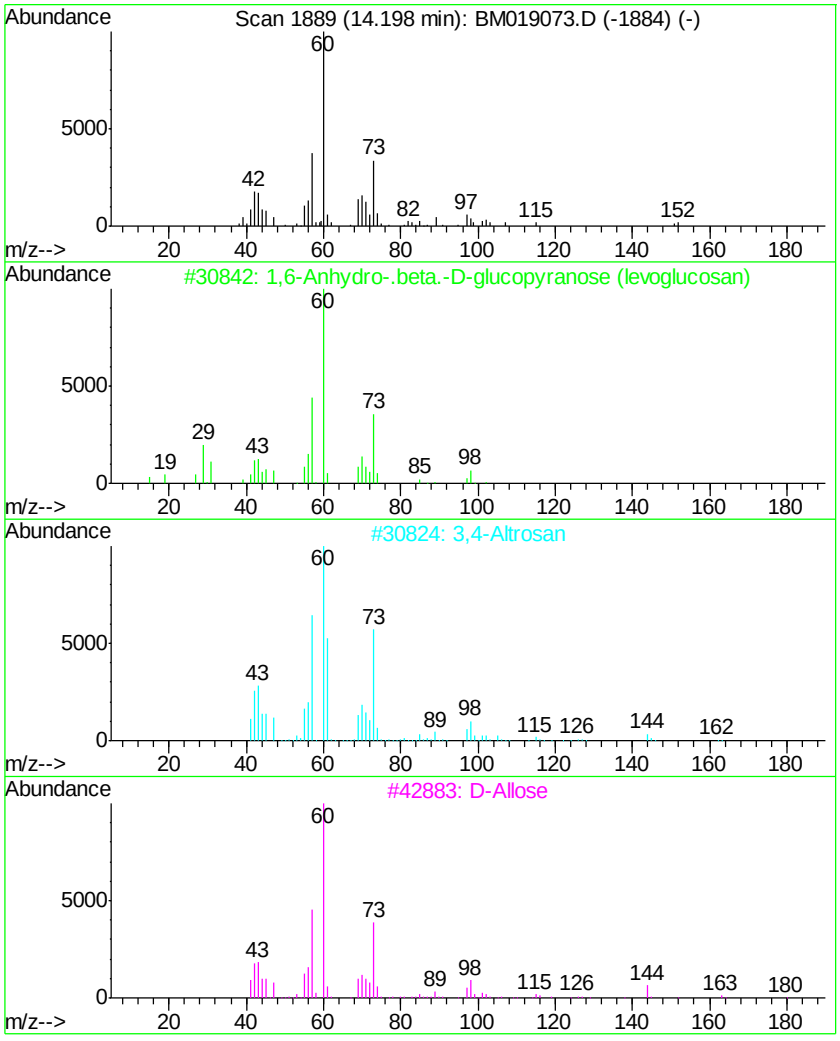
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

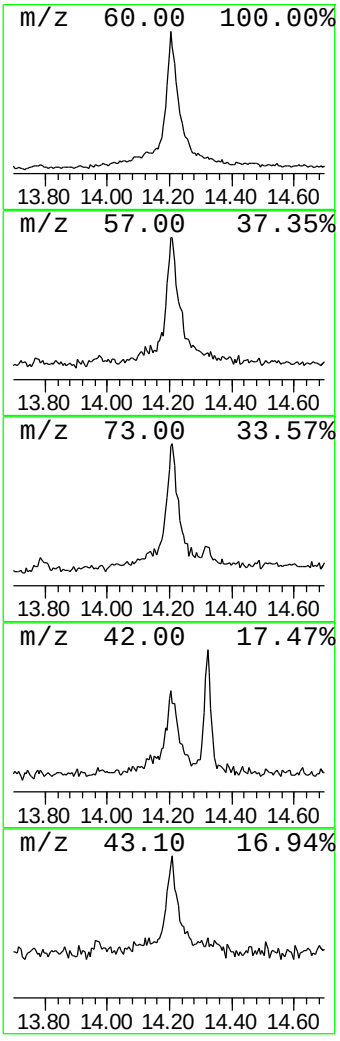
****

Peak Number 3 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	3.00 ng	275988	Acenaphthene-d10	14.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	72
2	3,4-Altrosan	162	C6H10O5	1000129-76-4	53
3	D-Allose	180	C6H12O6	002595-97-3	52
4	Heptanoic acid	130	C7H14O2	000111-14-8	50
5	L-Mannose, 6-deoxy-	164	C6H12O5	003615-41-6	45





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Misc :
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Instrument : BNA_M
ClientSampleId : TP-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
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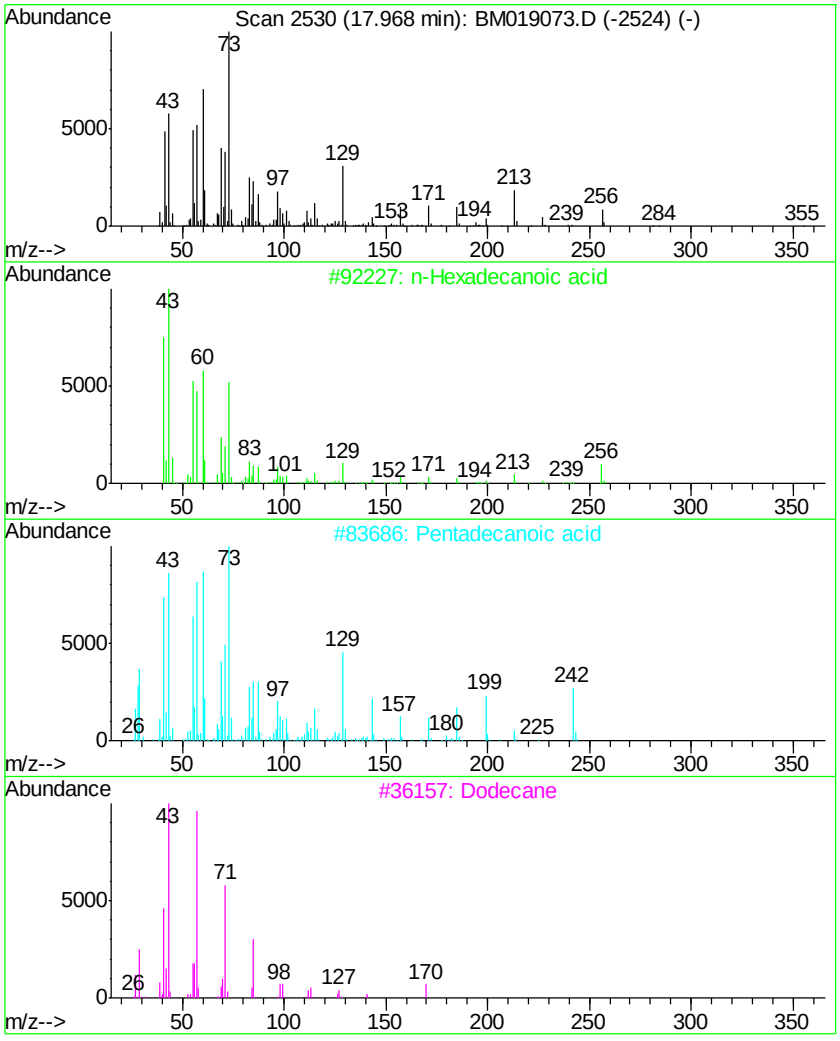
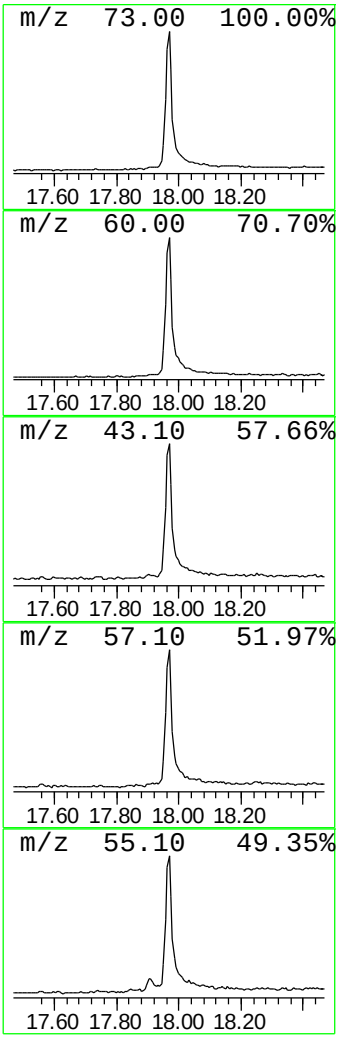
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	16.50 ng	1643850	Phenanthrene-d10	17.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Dodecane	170	C12H26	000112-40-3	25
4	Tridecane	184	C13H28	000629-50-5	22
5	Eicosane	282	C20H42	000112-95-8	18





Library Search Compound Report

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Operator : JU/SJ
Sample : K1807-19
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-10

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

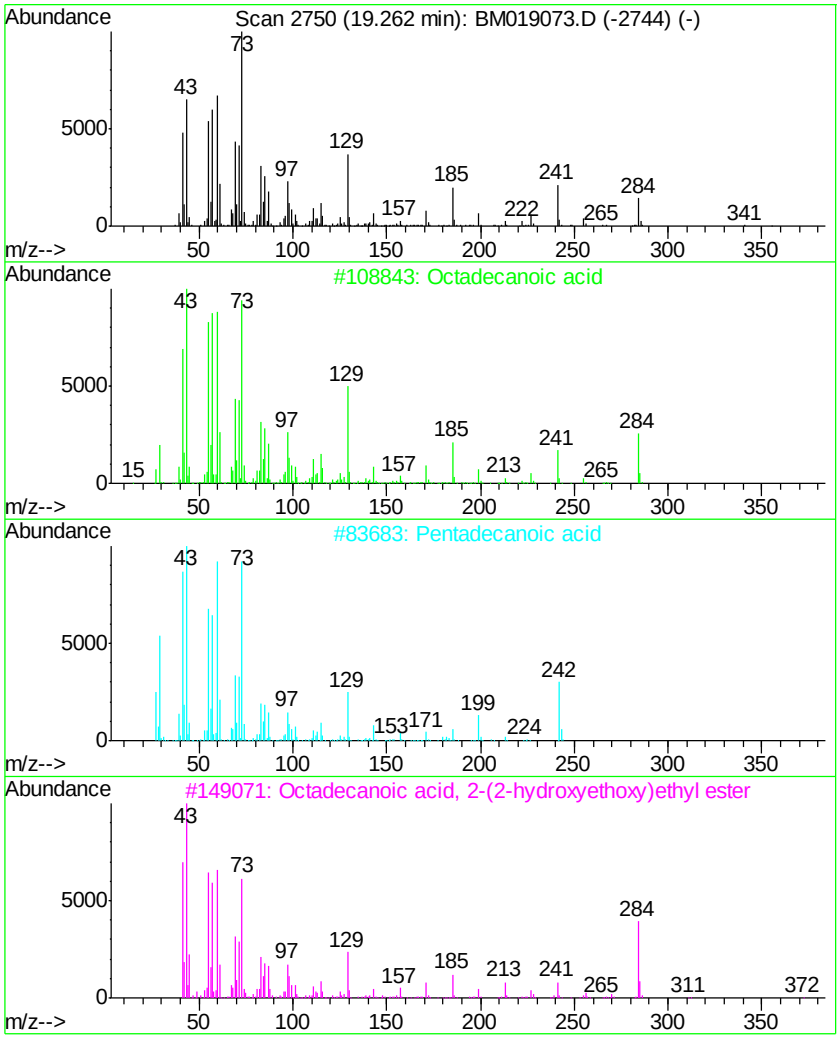
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

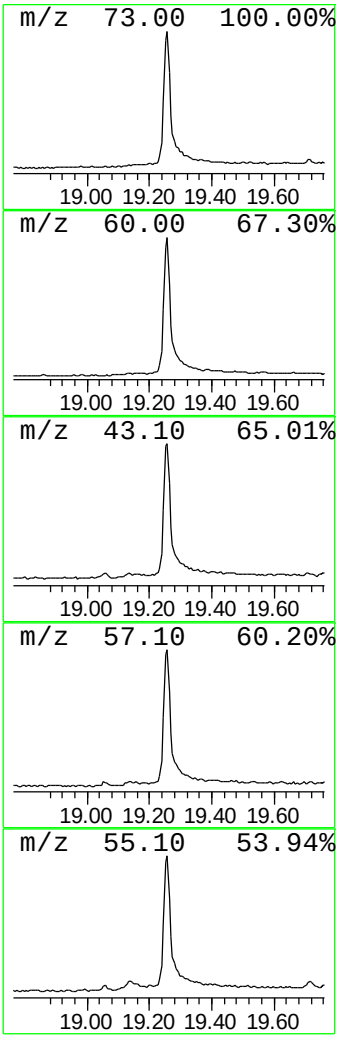
****

Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.26	17.79 ng	1985650	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	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64





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Operator : JU/SJ
Sample : K1807-19
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Instrument : BNA_M
ClientSampleId : TP-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
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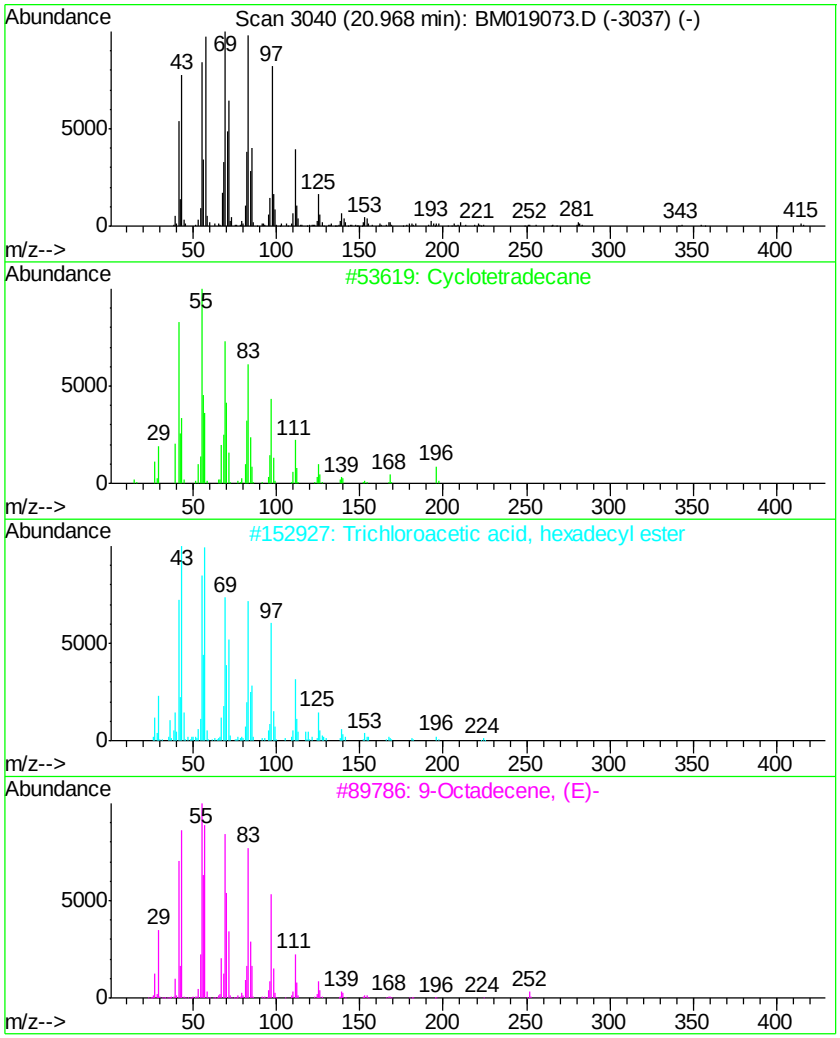
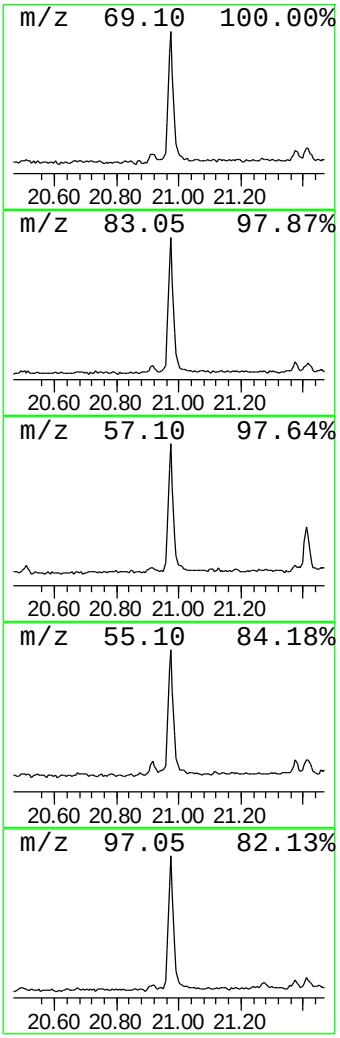
Peak Number 6 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	6.71 ng	749286	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91





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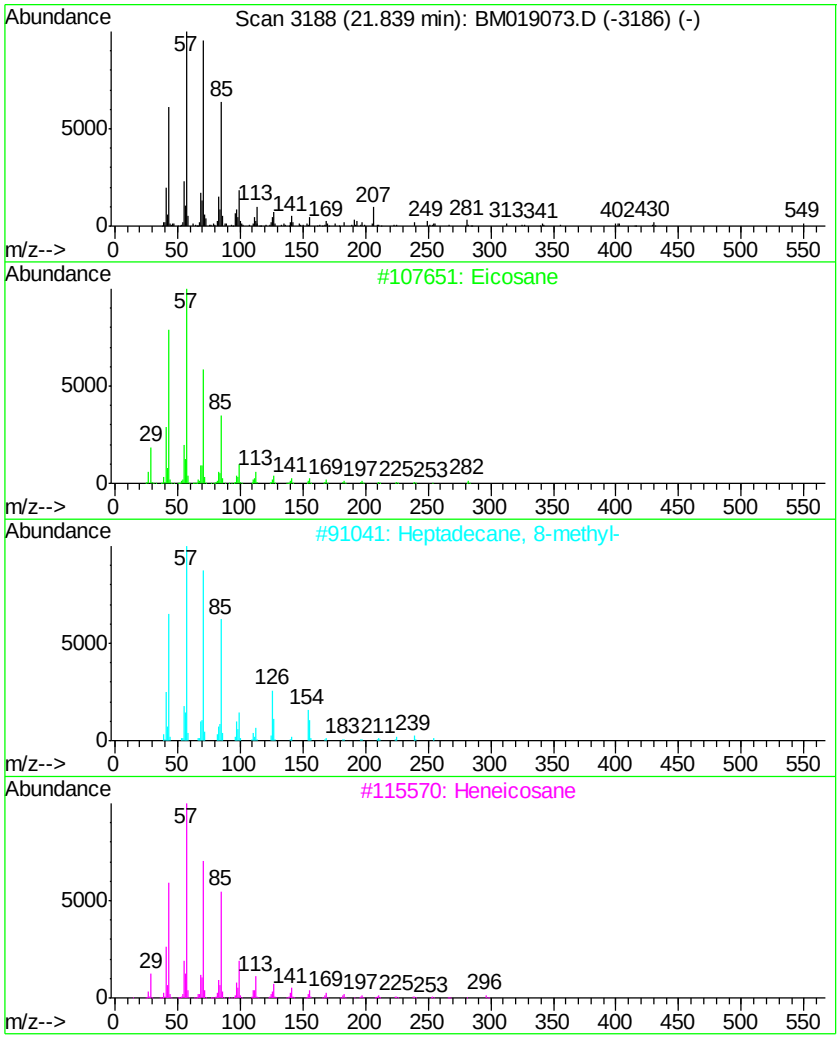
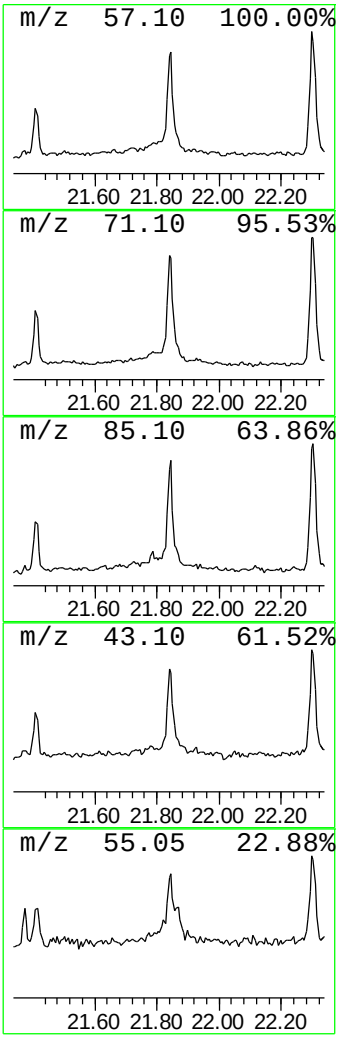
****

Peak Number 7 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.84	2.24 ng	250088	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	91
3	Heneicosane	296	C21H44	000629-94-7	87
4	10-Methylnonadecane	282	C20H42	056862-62-5	83
5	Octacosane	394	C28H58	000630-02-4	83





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

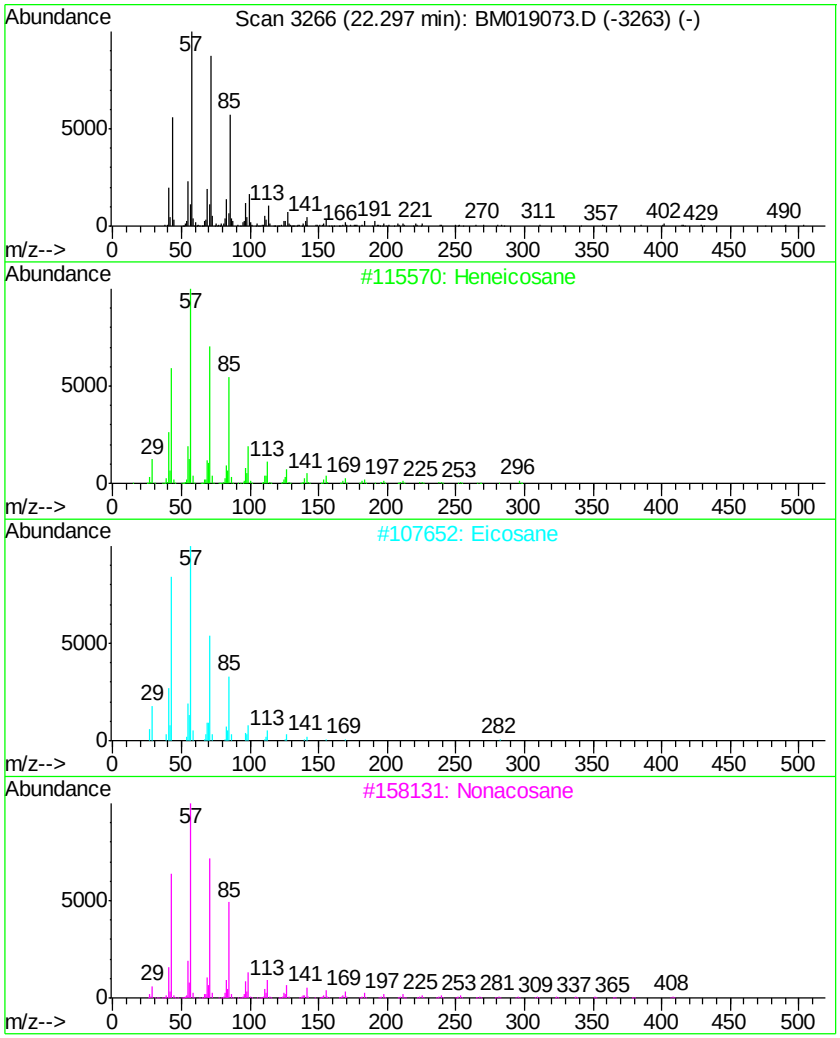
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

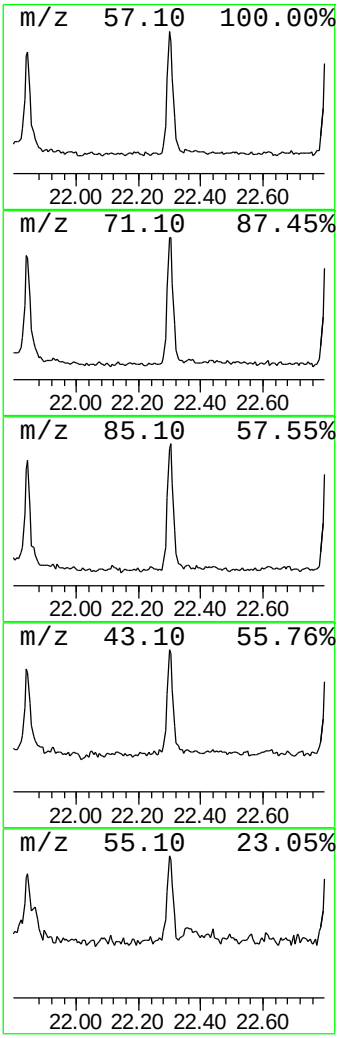
****

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.30	2.99 ng	333260	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Eicosane	282	C20H42	000112-95-8	89
3	Nonacosane	408	C29H60	000630-03-5	86
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Hexadecane	226	C16H34	000544-76-3	83





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : TP-10

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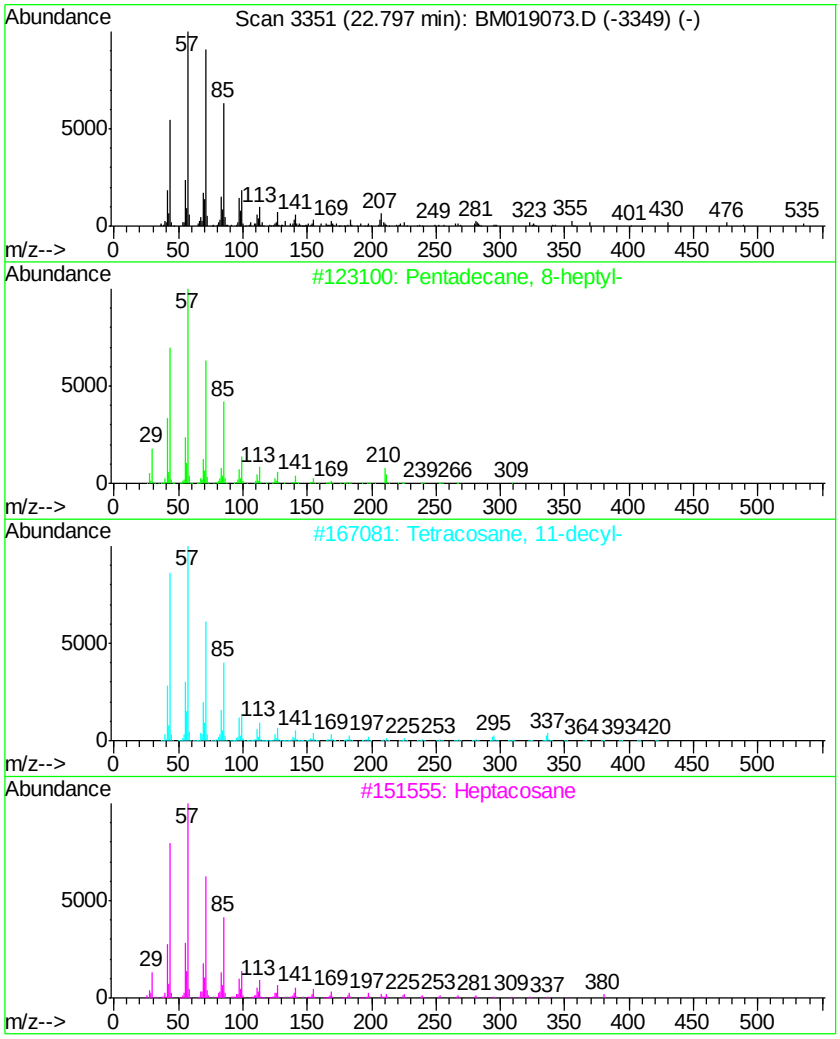
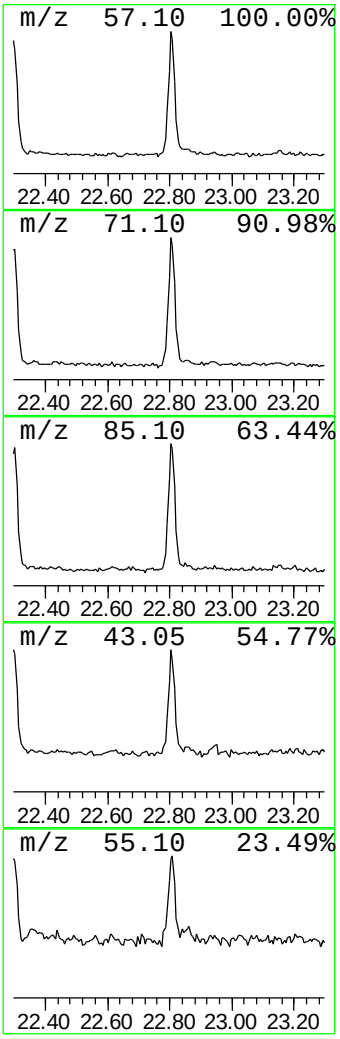
****

Peak Number 9 Pentadecane, 8-heptyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.80	3.07 ng	344062	Perylene-d12	23.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91
3	Heptacosane	380	C27H56	000593-49-7	90
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5	10-Methylnonadecane	282	C20H42	056862-62-5	90





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-10

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

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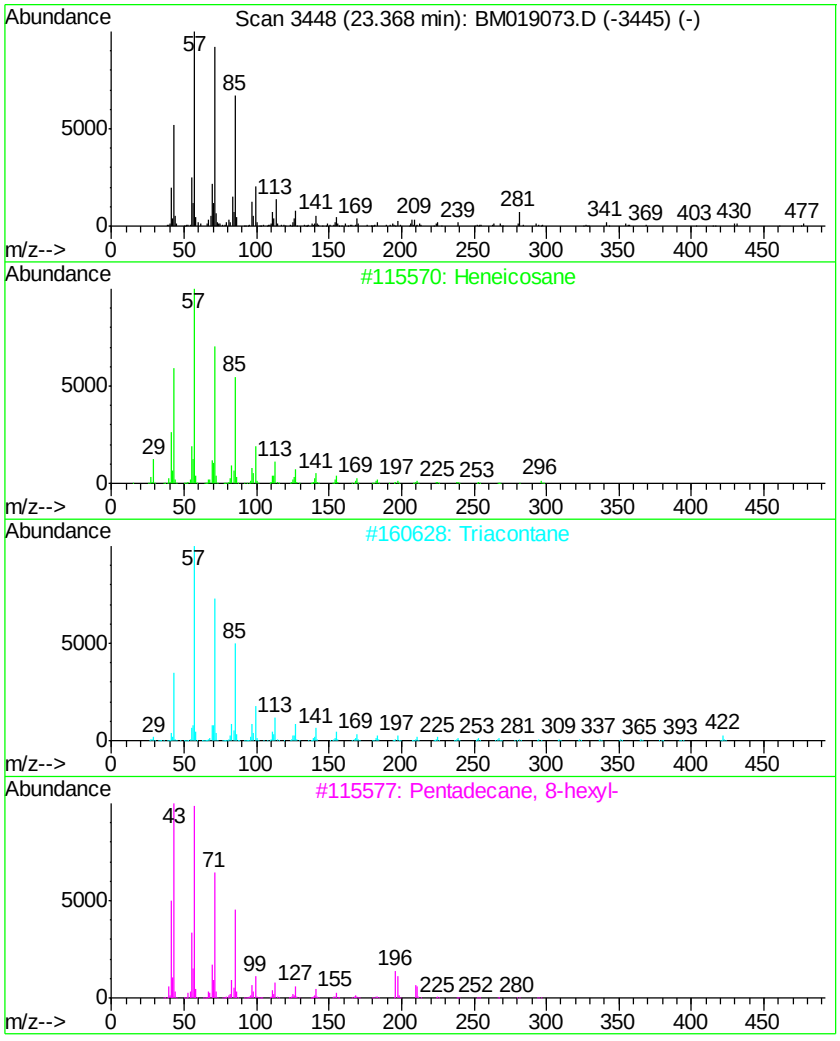
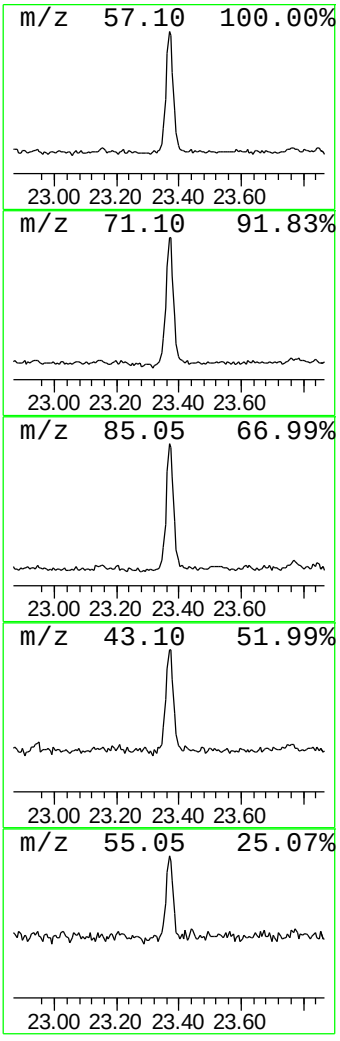
Peak Number 10 unknown23.37 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.37	3.39 ng	379425	Perylene-d12	23.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Triacontane	422	C30H62	000638-68-6	87
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	87
4	Heptadecane	240	C17H36	000629-78-7	80
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019073.D
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.20	7.20	89.7	ng	5418680	1	7.67	1208340	20.0
1,6-Anhydro-.beta...	14.20	3.0	ng	275988	3	14.32	1841630	20.0
n-Hexadecanoic acid	17.97	16.5	ng	1643850	4	17.07	1991970	20.0
Octadecanoic acid	19.26	17.8	ng	1985650	5	21.27	2232120	20.0
Cyclotetradecane	20.97	6.7	ng	749286	5	21.27	2232120	20.0
Eicosane	21.84	2.2	ng	250088	5	21.27	2232120	20.0
Heneicosane	22.30	3.0	ng	333260	5	21.27	2232120	20.0
Pentadecane, 8-he...	22.80	3.1	ng	344062	6	23.52	2240240	20.0
unknown23.37	23.37	3.4	ng	379425	6	23.52	2240240	20.0