LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019075.D
Acq On : 08 Mar 2019 16:06
Operator : JU/SJ
Sample : K1807-23
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-17

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	387	rBV	3610968	5147638	58.07%	8.730%
2	6.851	632	640	659	rBV	3488009	5572183	62.86%	9.450%
3	7.204	693	700	714	rBV	3734244	5696815	64.27%	9.661%
4	7.669	772	779	786	rBV	715156	1104099	12.46%	1.872%
5	7.987	825	833	841	rBV	2644767	4135866	46.66%	7.014%
6	8.839	970	978	992	rBV	1909248	3265152	36.83%	5.537%
7	10.457	1246	1253	1264	rBV	794606	1369809	15.45%	2.323%
8	12.933	1667	1674	1687	rBV	4322608	6560350	74.01%	11.126%
9	13.786	1814	1819	1830	rBV	270271	423182	4.77%	0.718%
10	14.204	1883	1890	1904	rVB	101796	265591	3.00%	0.450%
11	14.321	1904	1910	1922	rVB2	1077044	1641270	18.52%	2.783%
12	15.821	2158	2165	2187	rBV	3596429	5224476	58.94%	8.860%
13	17.074	2372	2378	2391	rBV2	1241858	1895670	21.39%	3.215%
14	17.968	2524	2530	2551	rBV	388710	756337	8.53%	1.283%
15	19.251	2744	2748	2762	rBV	247778	477672	5.39%	0.810%
16	19.715	2821	2827	2839	rBV	7122333	8864426	100.00%	15.033%
17	20.974	3037	3041	3049	rBV2	278158	375313	4.23%	0.636%
18	21.274	3087	3092	3101	rBV	1844750	2452424	27.67%	4.159%
19	21.409	3113	3115	3120	rVB2	80270	90198	1.02%	0.153%
20	21.839	3186	3188	3196	rVB	137475	168418	1.90%	0.286%
21	22.303	3264	3267	3272	rVB	214995	262005	2.96%	0.444%
22	22.803	3349	3352	3359	rVB	209282	300424	3.39%	0.509%
23	23.368	3445	3448	3455	rVB2	210041	320767	3.62%	0.544%
24	23.521	3468	3474	3483	rVB	1364157	2595993	29.29%	4.403%

Sum of corrected areas: 58966078

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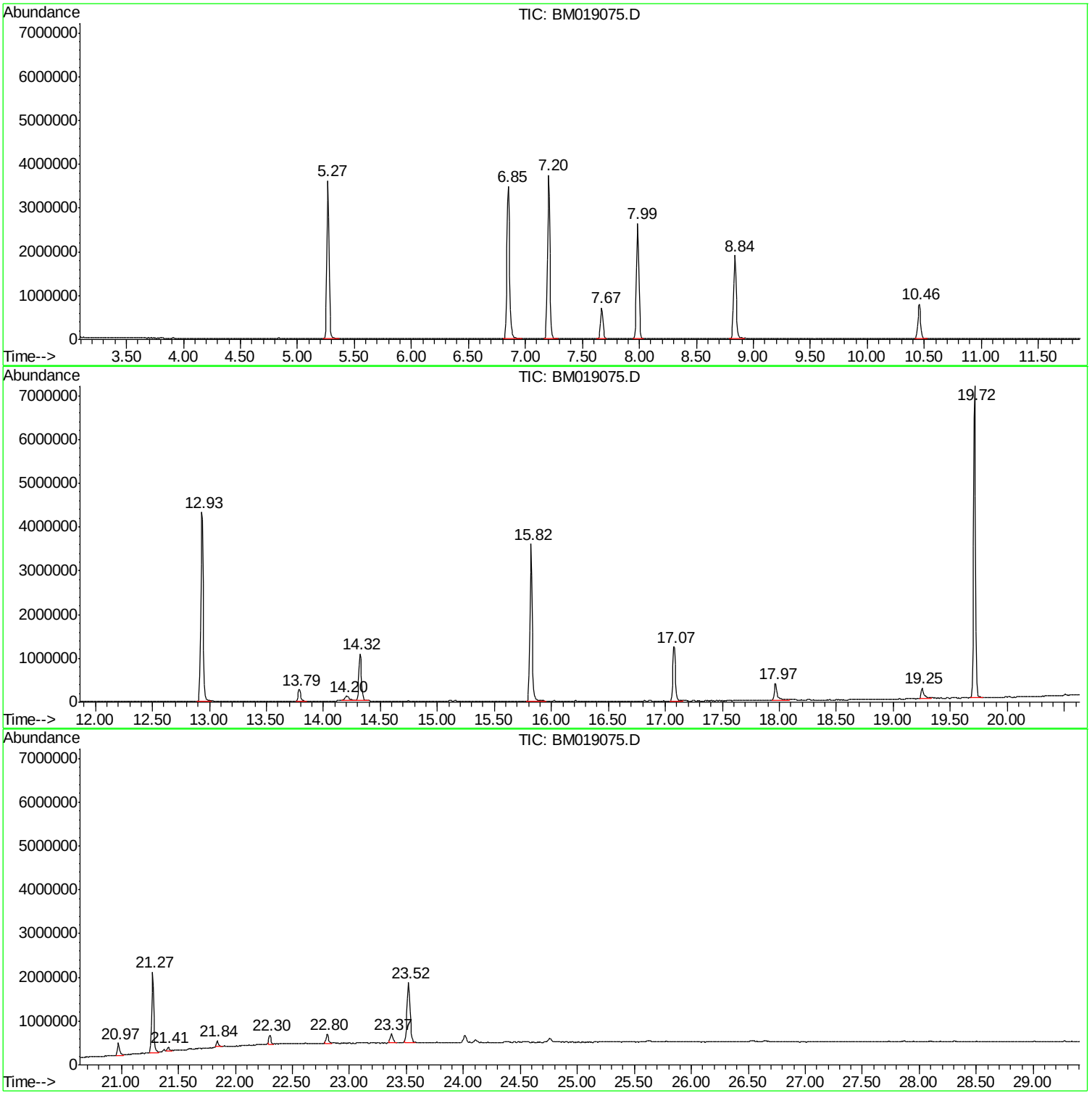
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-17

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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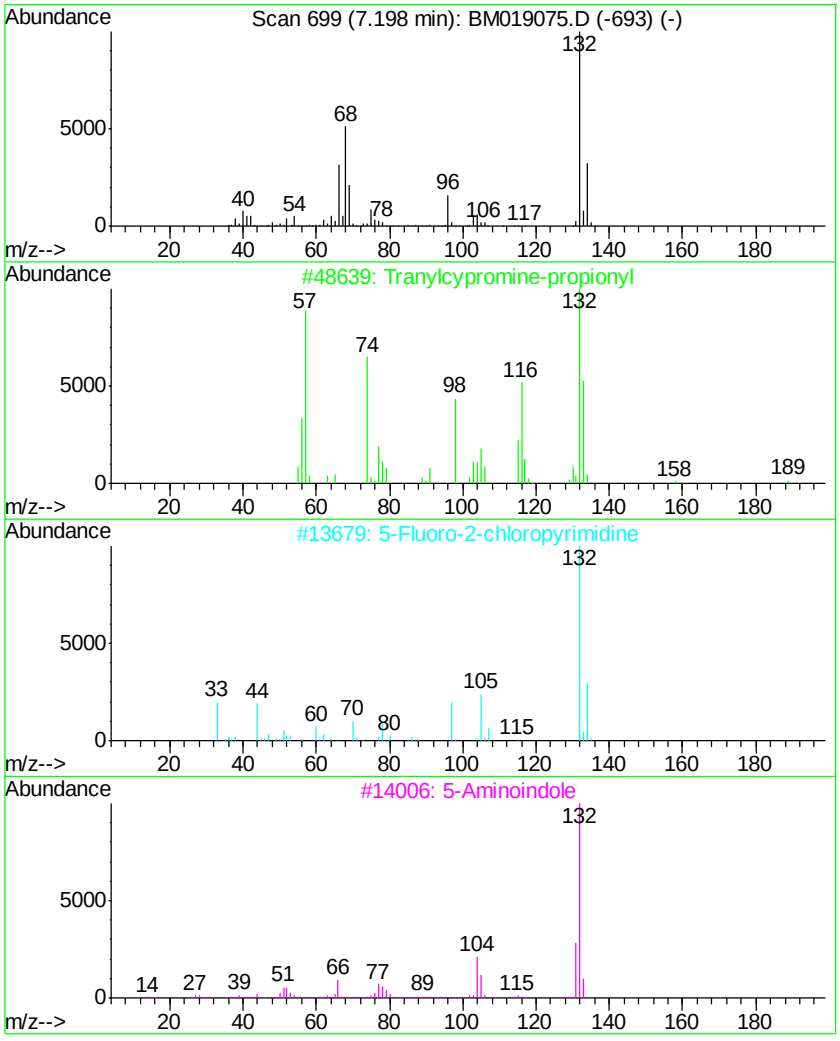
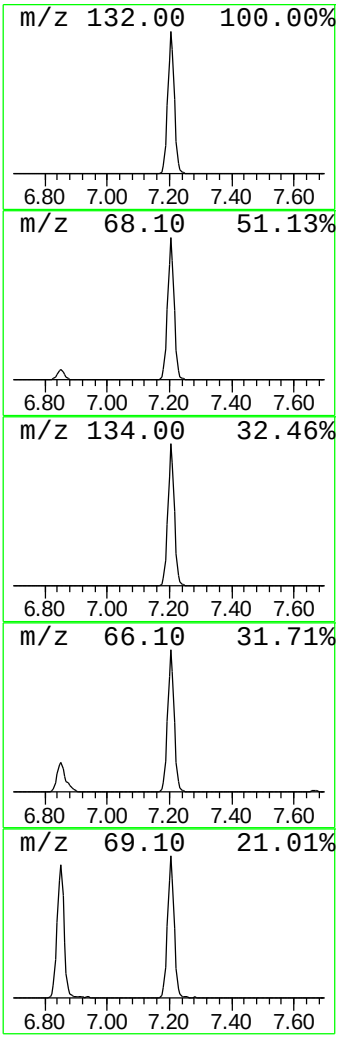
****

Peak Number 1 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	103.19 ng	5696820	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	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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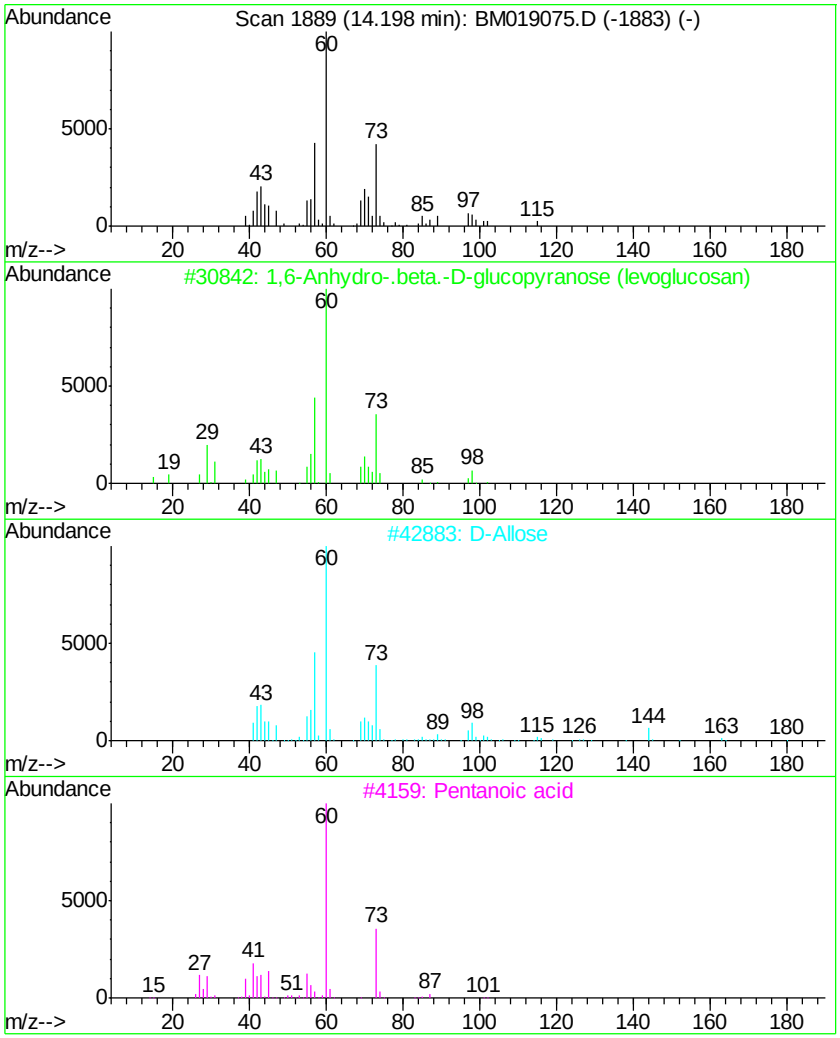
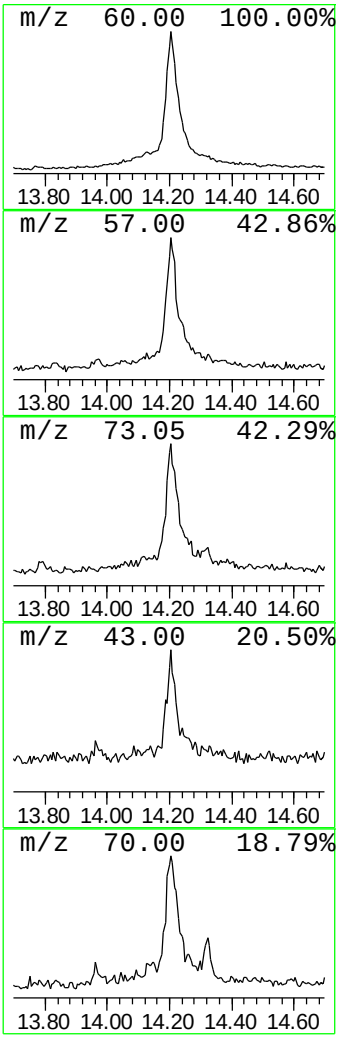
Peak Number 3 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	3.24 ng	265591	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	80
2	D-Allose	180	C6H12O6	002595-97-3	80
3	Pentanoic acid	102	C5H10O2	000109-52-4	50
4	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	47
5	Hexanoic acid	116	C6H12O2	000142-62-1	40





Library Search Compound Report

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Data File : BM019075.D
Acq On : 08 Mar 2019 16:06
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Misc :
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Instrument : BNA_M
ClientSampleId : TP-17

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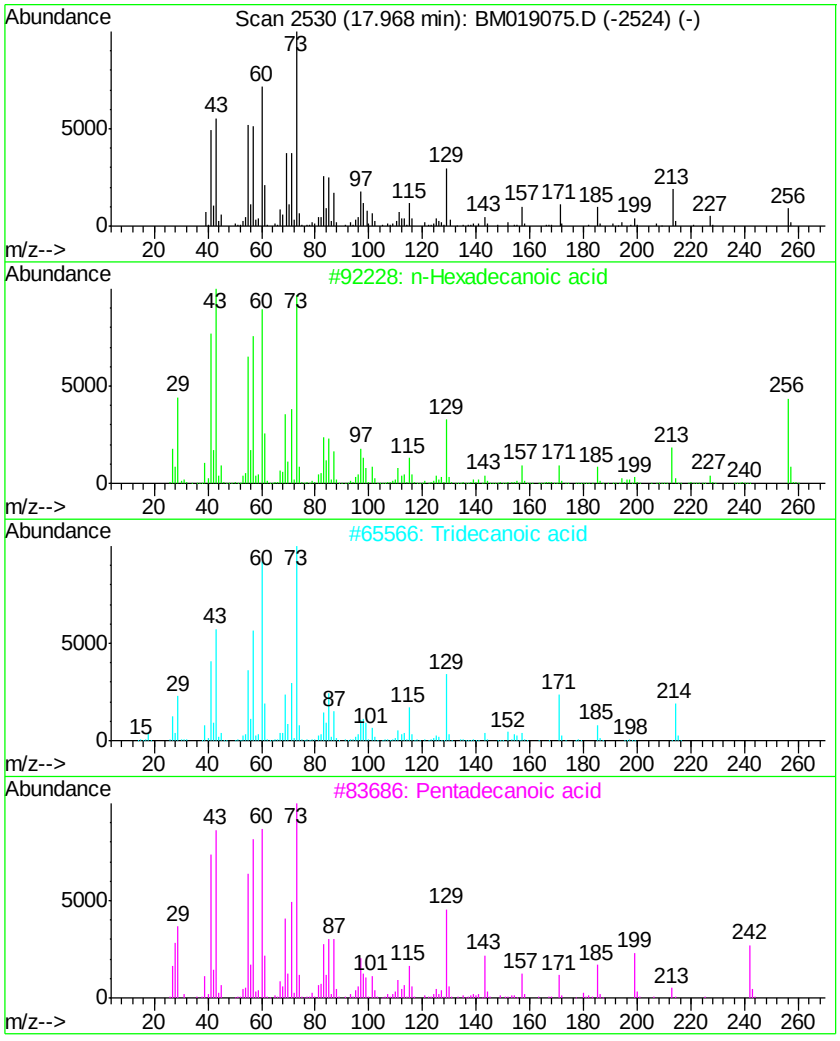
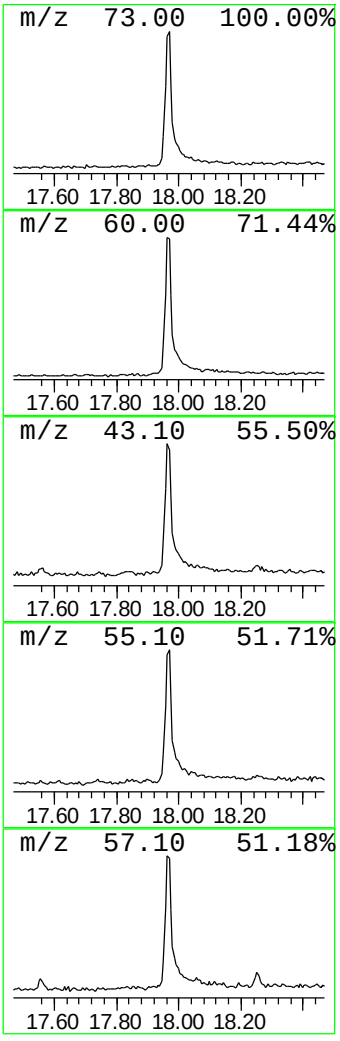
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	7.98 ng	756337	Phenanthrene-d10	17.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Undecanoic acid	186	C11H22O2	000112-37-8	37





Library Search Compound Report

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Operator : JU/SJ
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Misc :
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Instrument : BNA_M
ClientSampleId : TP-17

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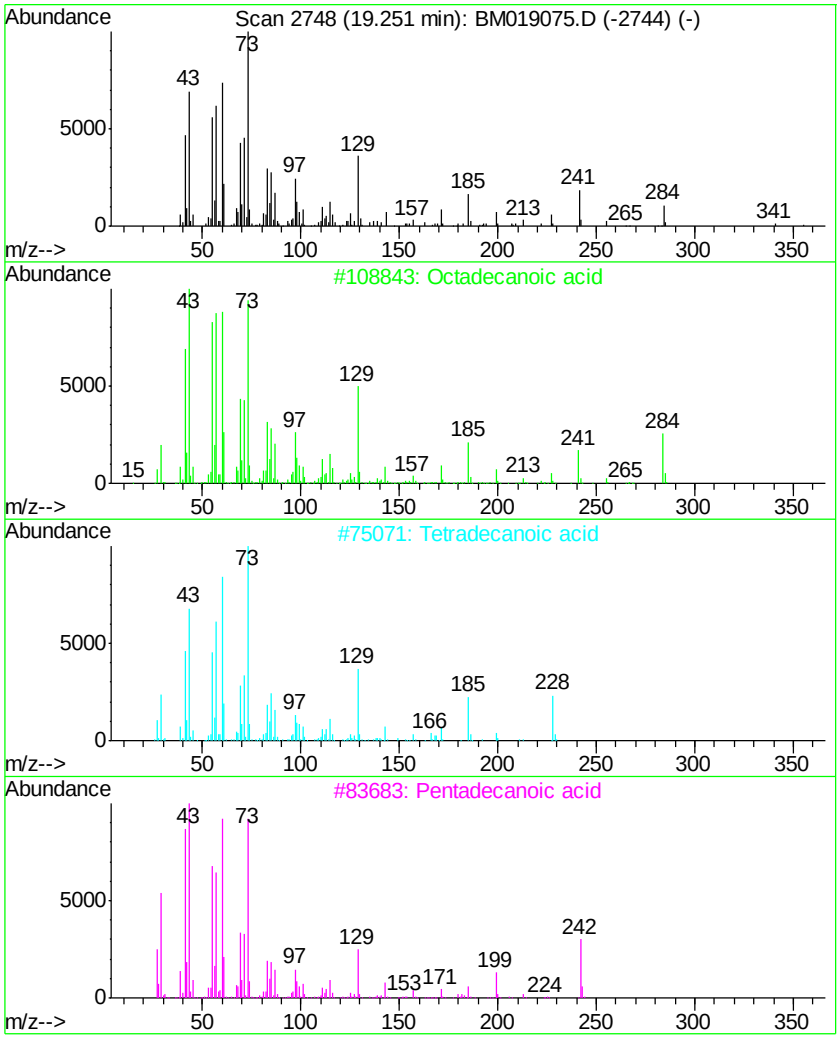
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

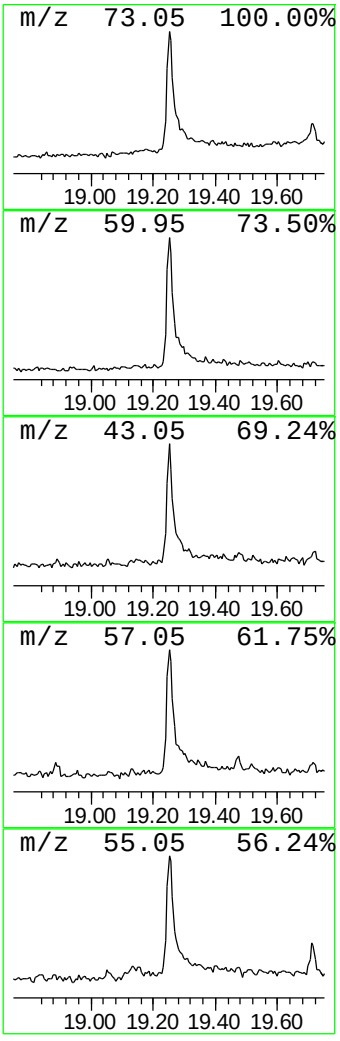
****

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.25	3.90 ng	477672	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	30





Library Search Compound Report

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Sample : K1807-23
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-17

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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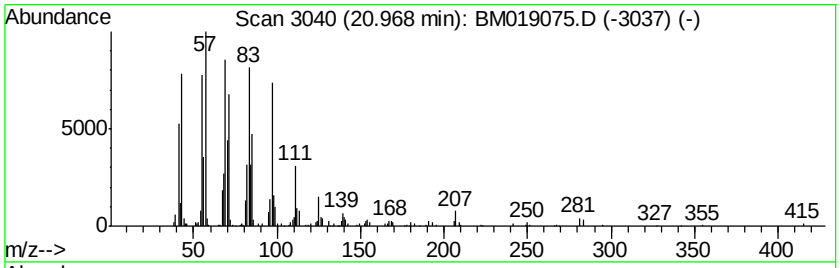
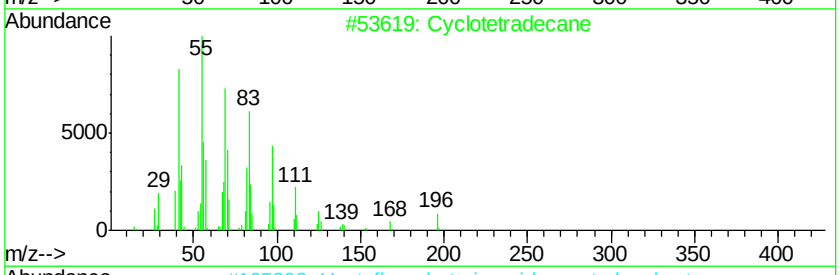
****

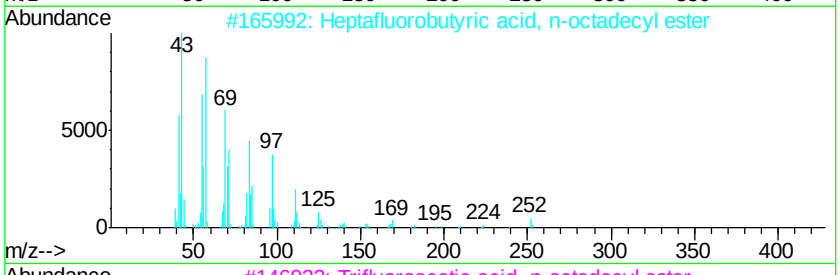
Peak Number 6 Cyclotetradecane Concentration Rank 6

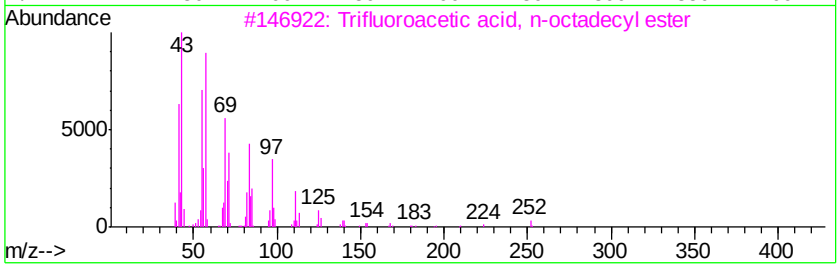
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	3.06 ng	375313	Chrysene-d12	21.27

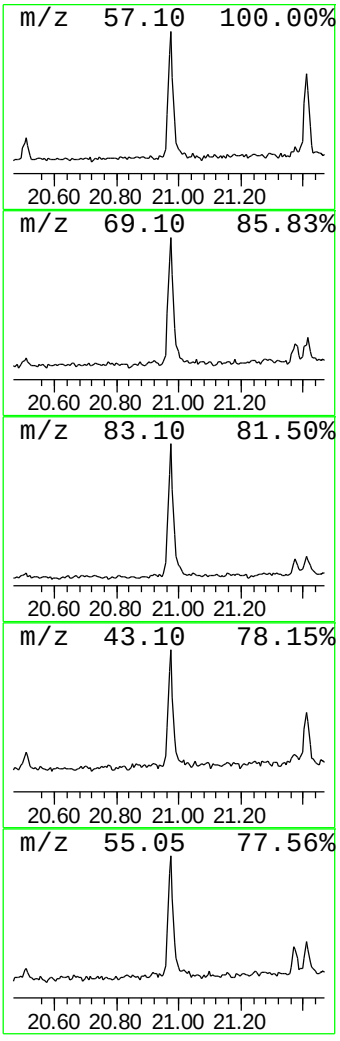
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	93
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91











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Misc :
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Instrument :
BNA_M
ClientSampleId :
TP-17

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

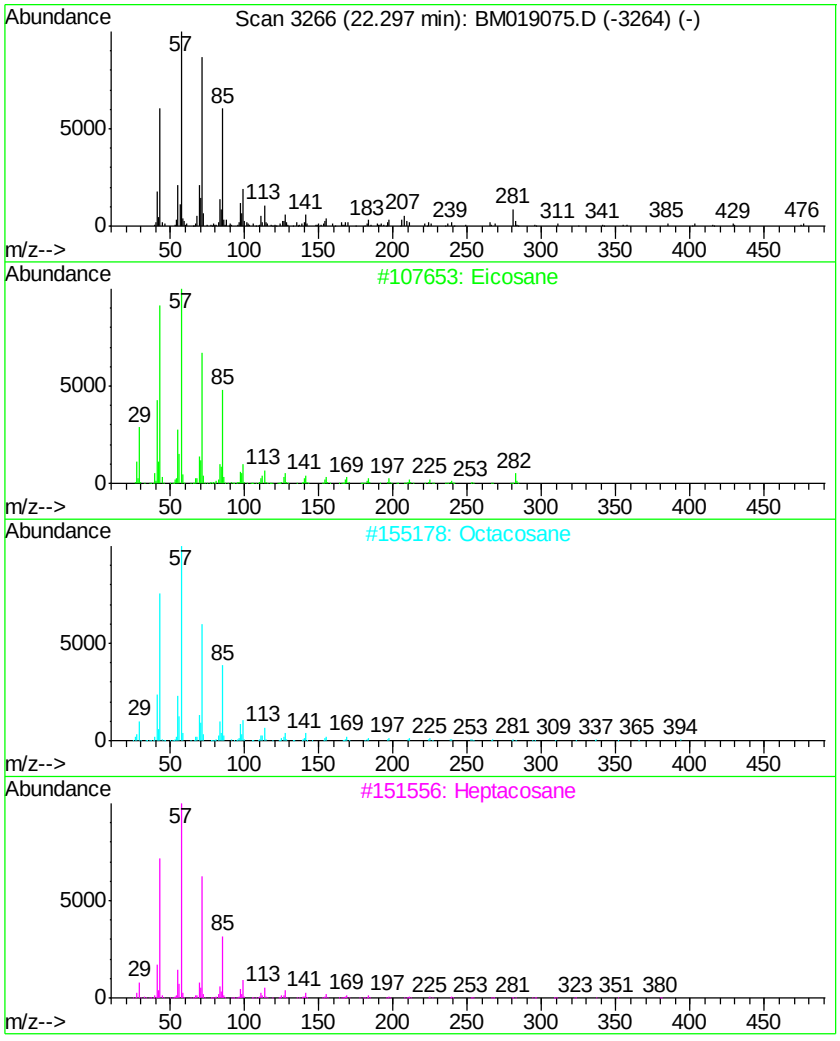
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

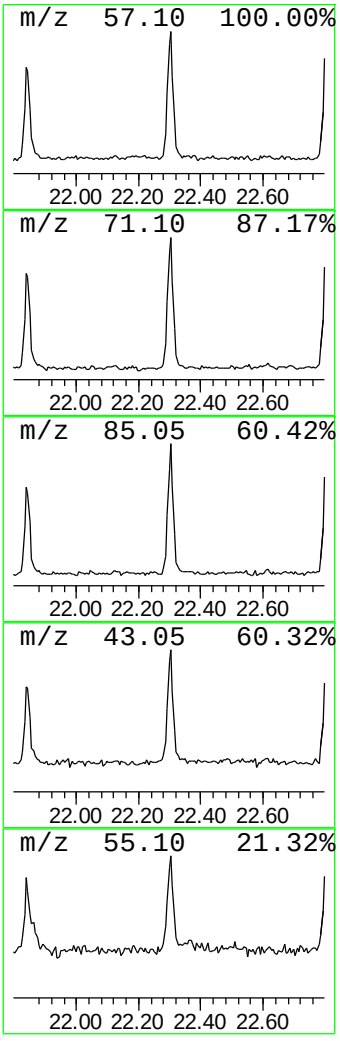
****

Peak Number 7 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.30	2.14 ng	262005	Chrysene-d12	21.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Octacosane	394	C28H58	000630-02-4	83
3	Heptacosane	380	C27H56	000593-49-7	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83





Library Search Compound Report

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Sample : K1807-23
Misc :
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Instrument : BNA_M
ClientSampleId : TP-17

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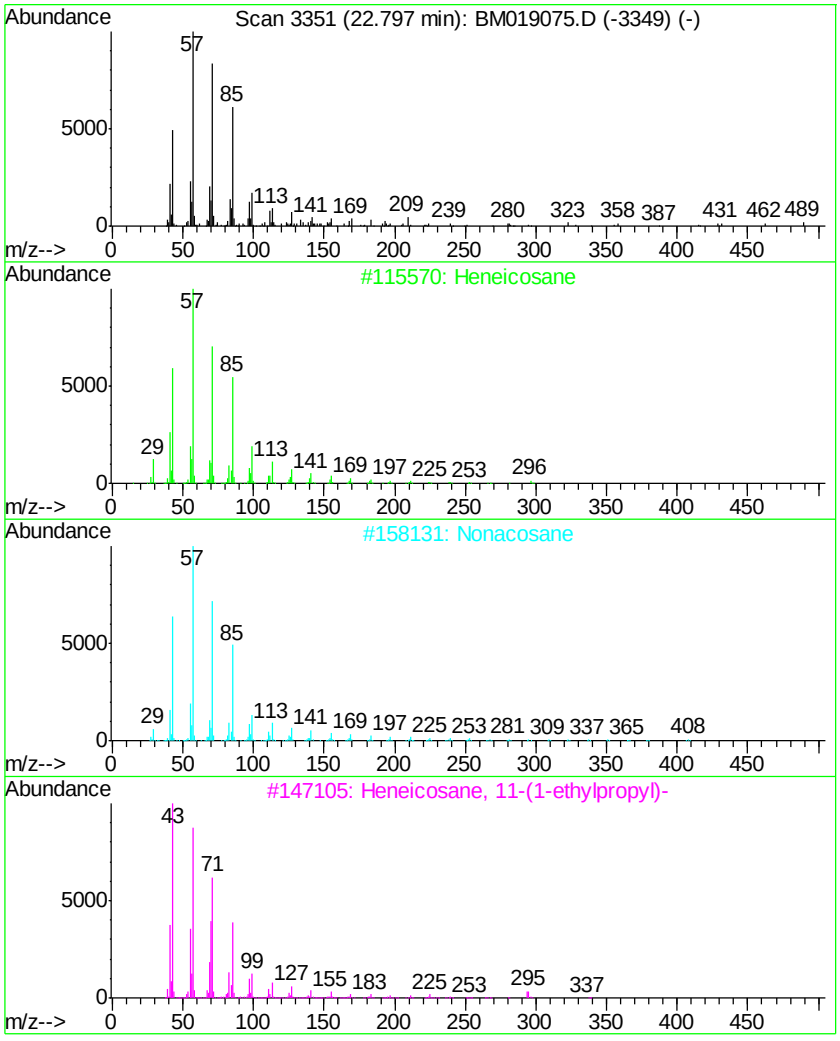
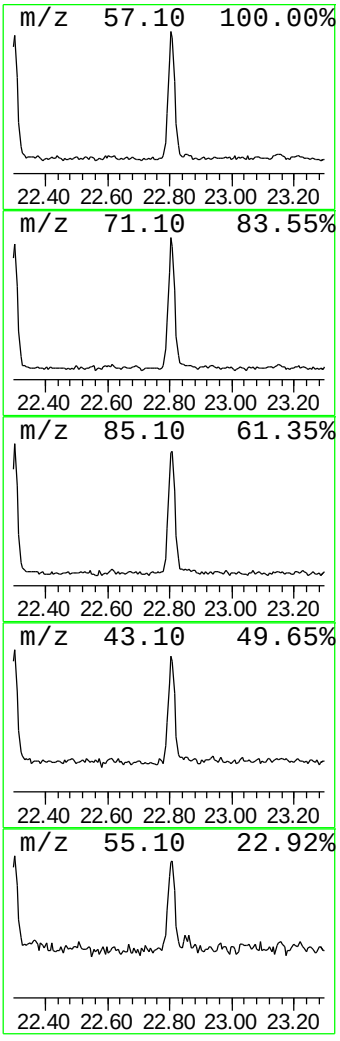
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.80	2.31 ng	300424	Perylene-d12	23.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Nonacosane	408	C29H60	000630-03-5	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90





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

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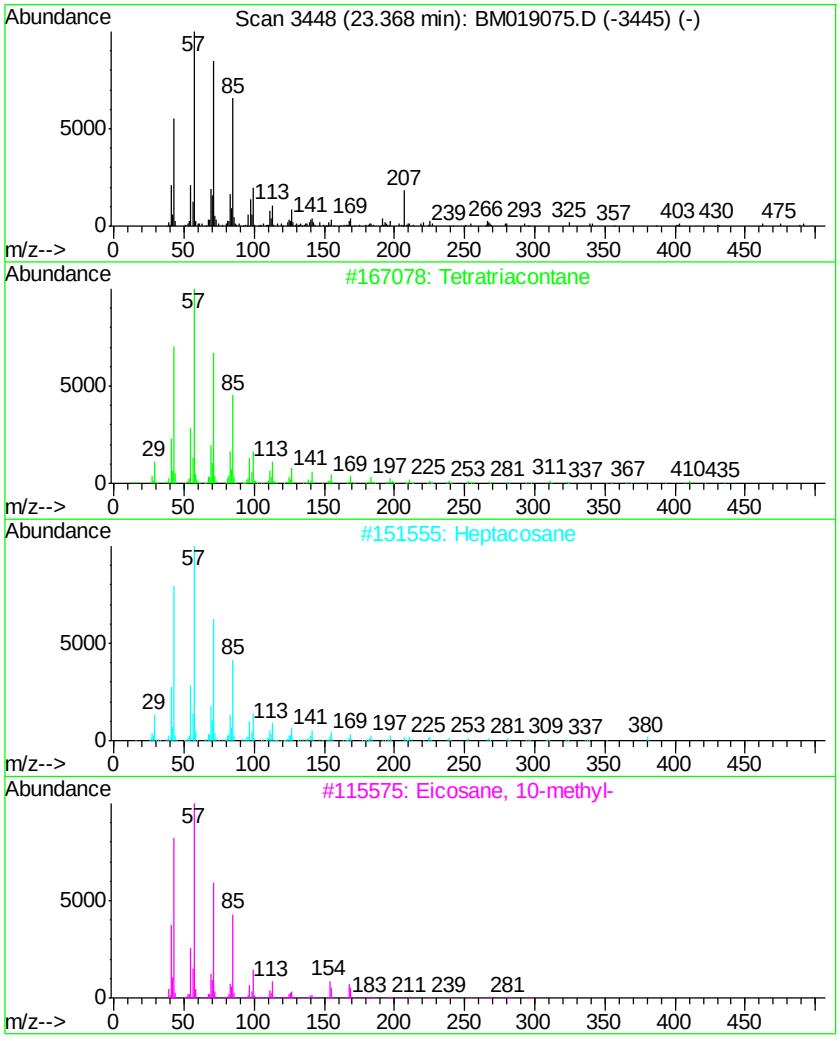
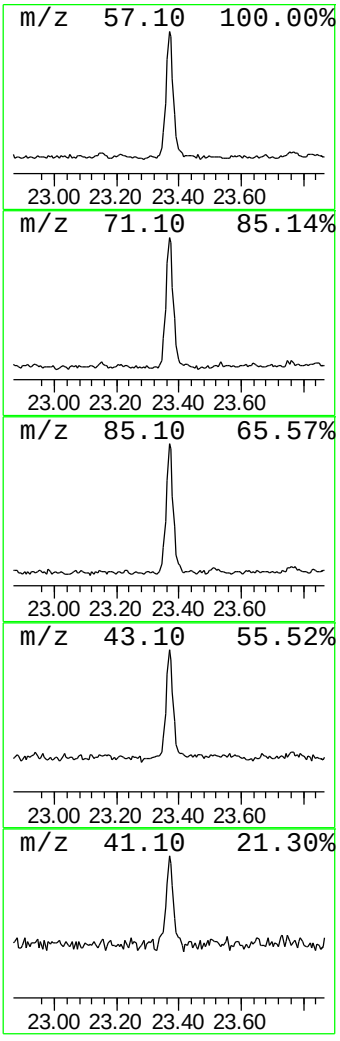
Peak Number 9 Tetratriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.37	2.47 ng	320767	Perylene-d12	23.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	83
2	Heptacosane	380	C27H56	000593-49-7	80
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
4	Heneicosane	296	C21H44	000629-94-7	80
5	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	80





Tentatively Identified Compound (LSC) summary

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Acq On : 08 Mar 2019 16:06
Operator : JU/SJ
Sample : K1807-23
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Instrument : BNA_M
ClientSampleId : TP-17

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.20	7.20	103.2	ng	5696820	1	7.67	1104100	20.0
1,6-Anhydro-.beta...	14.20	3.2	ng	265591	3	14.32	1641270	20.0
n-Hexadecanoic acid	17.97	8.0	ng	756337	4	17.08	1895670	20.0
Octadecanoic acid	19.25	3.9	ng	477672	5	21.27	2452420	20.0
Cyclotetradecane	20.97	3.1	ng	375313	5	21.27	2452420	20.0
Eicosane	22.30	2.1	ng	262005	5	21.27	2452420	20.0
Heneicosane	22.80	2.3	ng	300424	6	23.52	2595990	20.0
Tetratriacontane	23.37	2.5	ng	320767	6	23.52	2595990	20.0