LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

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-BM121518.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	4.693	303	307	313	rVB2	12868	19978	1.04%	0.114%
2	5.134	377	382	392	rVB	70040	112677	5.87%	0.642%
3	6.698	643	648	649	rBV	50141	55556	2.89%	0.317%
4	6.722	649	652	666	rVB2	65679	144265	7.52%	0.822%
5	7.040	700	706	718	rBV	132579	223832	11.66%	1.276%
6	7.498	778	784	794	rBV	418634	682651	35.57%	3.891%
7	7.810	831	837	845	rBV	221125	374285	19.50%	2.134%
8	8.663	976	982	991	rBV	136651	272369	14.19%	1.553%
9	9.034	1038	1045	1052	rBV	81612	117328	6.11%	0.669%
10	10.269	1247	1255	1266	rBV	510966	968759	50.48%	5.522%
11	11.522	1460	1468	1474	rBV	122085	186055	9.69%	1.061%
12	12.769	1673	1680	1694	rBV	475285	841282	43.83%	4.796%
13	13.557	1808	1814	1820	rBV2	84487	116131	6.05%	0.662%
14	13.645	1820	1829	1841	rVV	50761	98689	5.14%	0.563%
15	14.157	1909	1916	1929	rBV2	837167	1342706	69.96%	7.654%
16	15.133	2077	2082	2087	rBV	52878	65553	3.42%	0.374%
17	15.674	2168	2174	2182	rVB	165610	273187	14.23%	1.557%
18	16.386	2290	2295	2300	rVB2	34080	47331	2.47%	0.270%
19	16.921	2379	2386	2402	rBV	917714	1444749	75.28%	8.235%
20	17.221	2432	2437	2445	rBV	71584	92062	4.80%	0.525%
21	17.457	2473	2477	2481	rVB2	28174	37059	1.93%	0.211%
22	17.833	2534	2541	2551	rBV	351148	508012	26.47%	2.896%
23	18.409	2634	2639	2643	rVB2	26444	35936	1.87%	0.205%
24	19.127	2756	2761	2772	rBV2	126858	216223	11.27%	1.233%
25	19.221	2773	2777	2781	rVB	32171	43219	2.25%	0.246%
26	19.574	2831	2837	2847	rVB	1004912	1308999	68.20%	7.462%
27	19.927	2894	2897	2901	rVB2	36137	43300	2.26%	0.247%
28	20.333	2964	2966	2969	rVB4	21111	20045	1.04%	0.114%
29	20.392	2974	2976	2979	rVB4	33641	32877	1.71%	0.187%
30	20.562	3002	3005	3009	rVB3	43782	53428	2.78%	0.305%
31	20.650	3018	3020	3024	rBV4	15131	21311	1.11%	0.121%
32	20.862	3051	3056	3063	rBV	324008	437533	22.80%	2.494%
33	21.062	3085	3090	3094	rBV	1304486	1411165	73.53%	8.044%
34	21.139	3098	3103	3113	rVV	1435633	1919272	100.00%	10.940%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

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-BM121518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.297	3126	3130	3134	rBV	157864	176273	9.18%	1.005%
36	21.721	3198	3202	3212	rBV	258895	317089	16.52%	1.807%
37	22.168	3274	3278	3281	rBV2	271597	332221	17.31%	1.894%
38	22.280	3295	3297	3304	rVB	114694	147181	7.67%	0.839%
39	22.644	3356	3359	3365	rVB	307656	448864	23.39%	2.559%
40	23.186	3446	3451	3456	rBV	247233	374806	19.53%	2.136%
41	23.297	3464	3470	3484	rVB	880020	1652462	86.10%	9.419%
42	23.791	3550	3554	3561	rVB3	157728	281270	14.66%	1.603%
43	24.486	3668	3672	3678	rVB4	131477	245128	12.77%	1.397%

Sum of corrected areas: 17543118

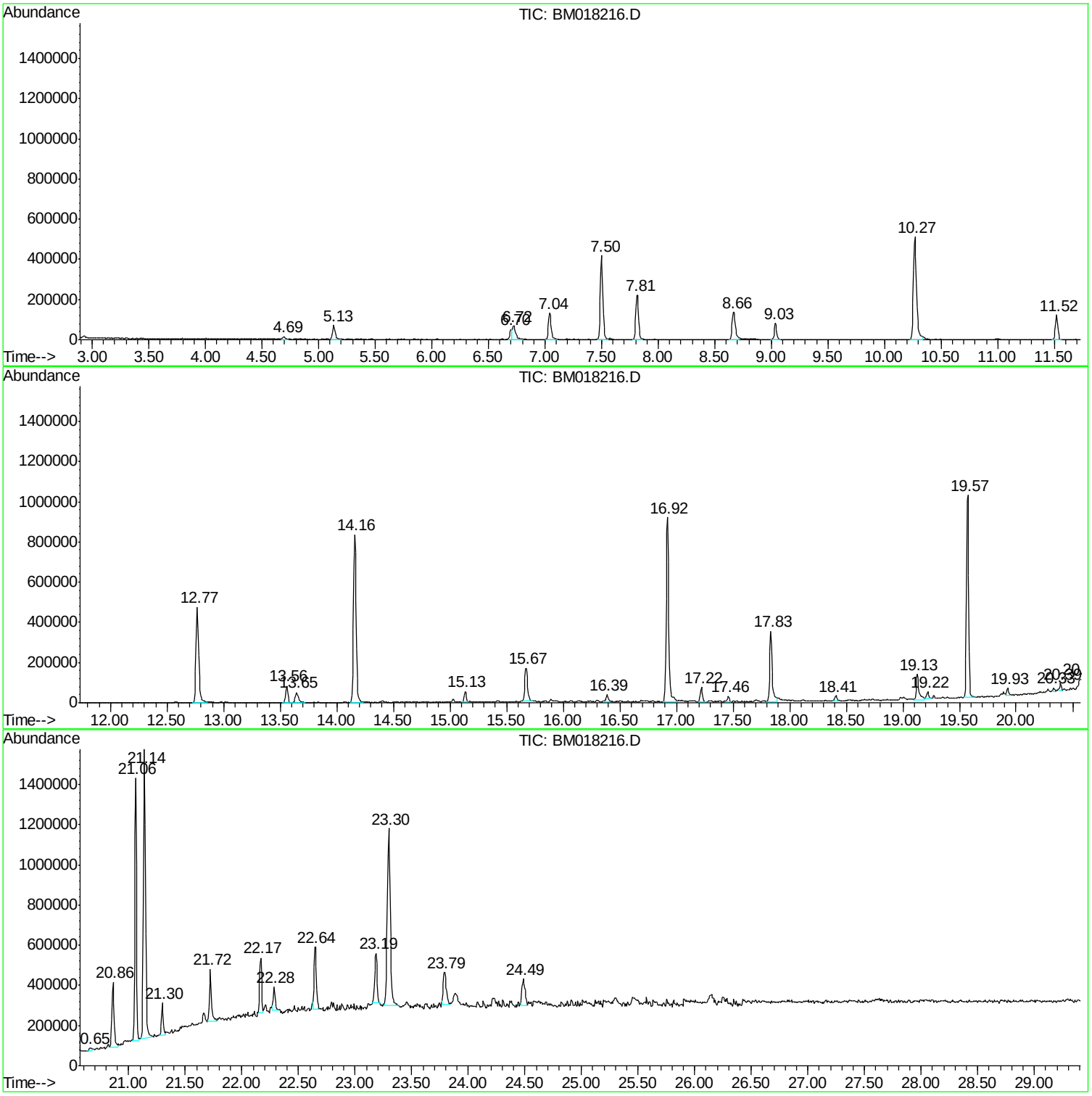
LSC Report - Integrated Chromatogram

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

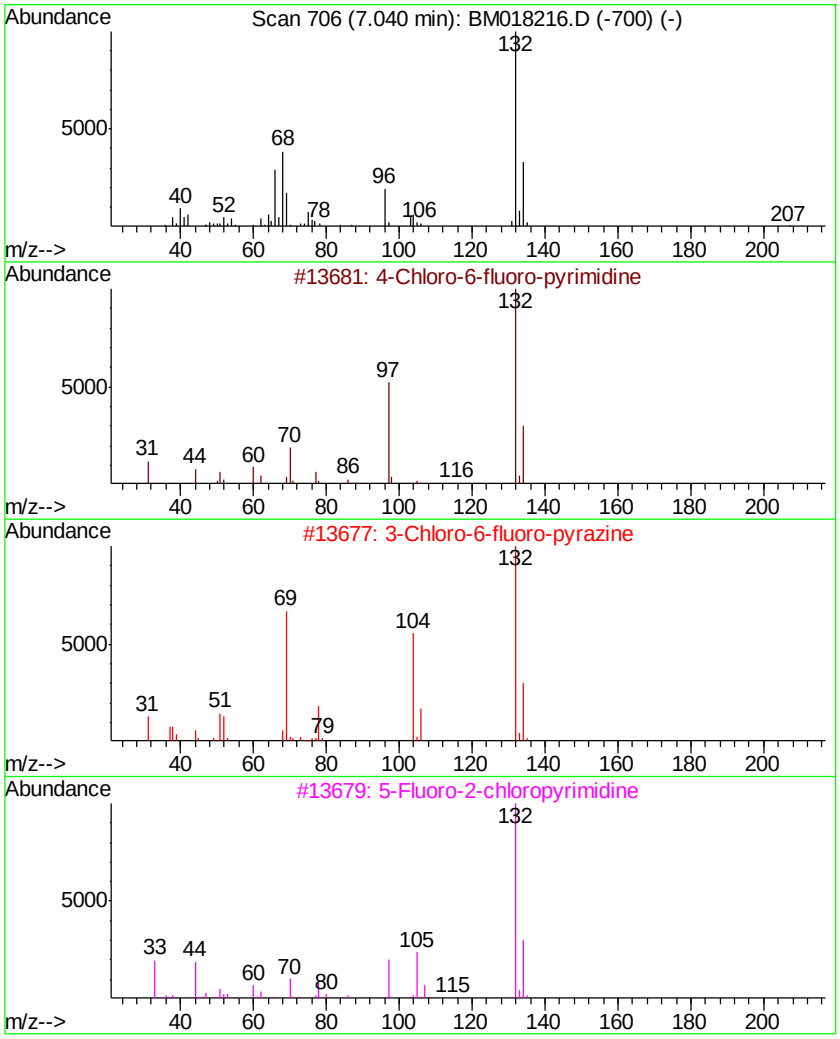
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

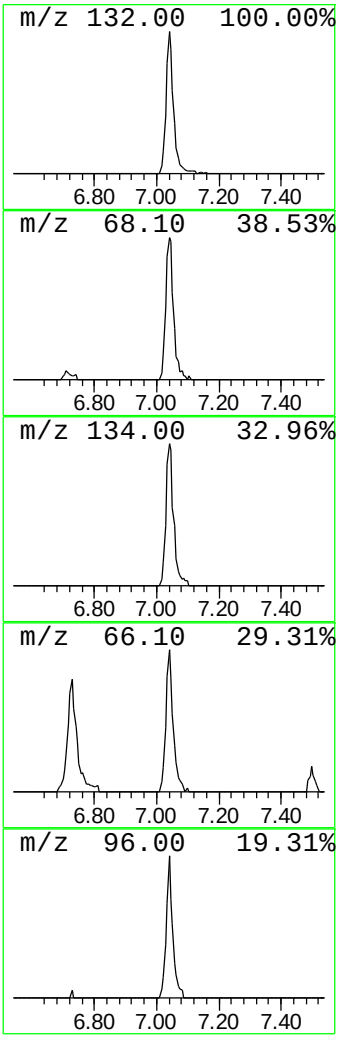
****

Peak Number 1 unknown7.04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	6.56 ng	223832	1,4-Dichlorobenzene-d4	7.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

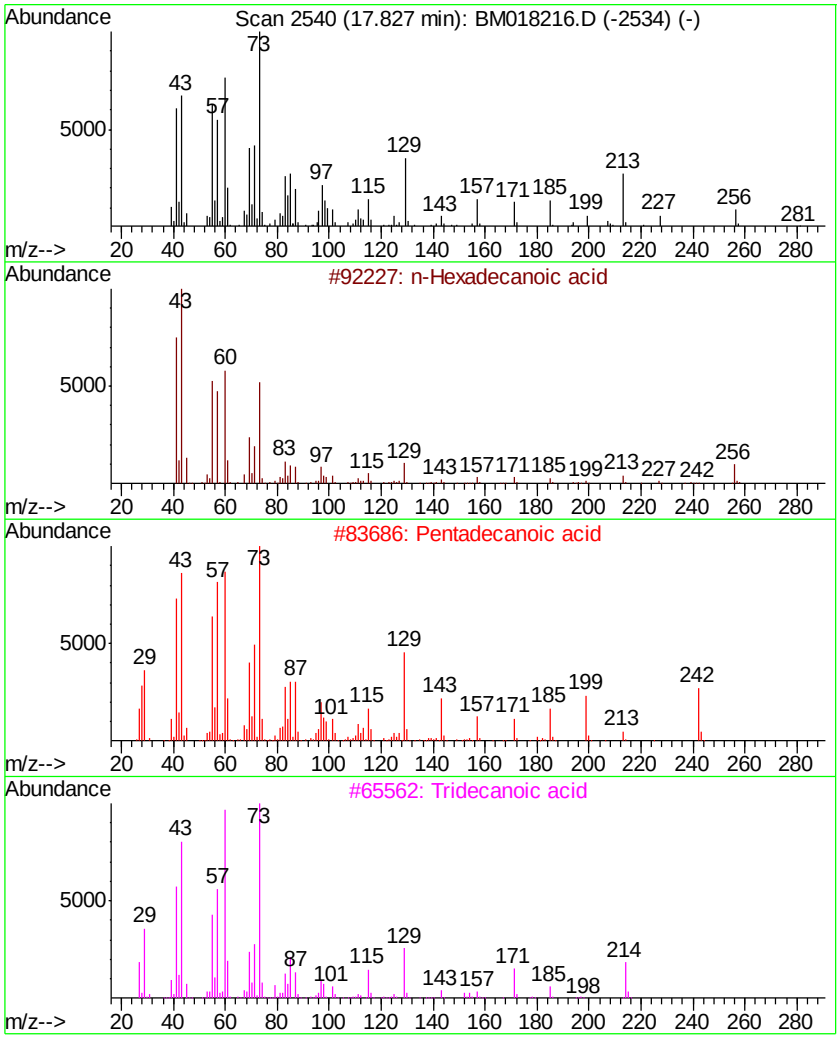
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

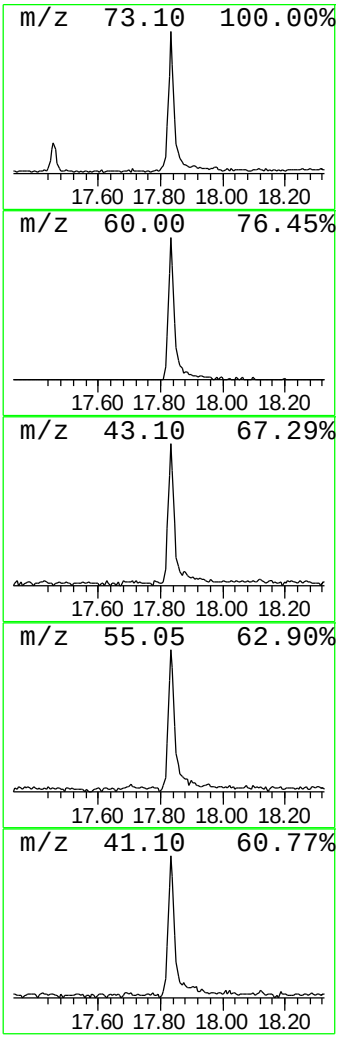
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	7.03 ng	508012	Phenanthrene-d10	16.92

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	70
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	41





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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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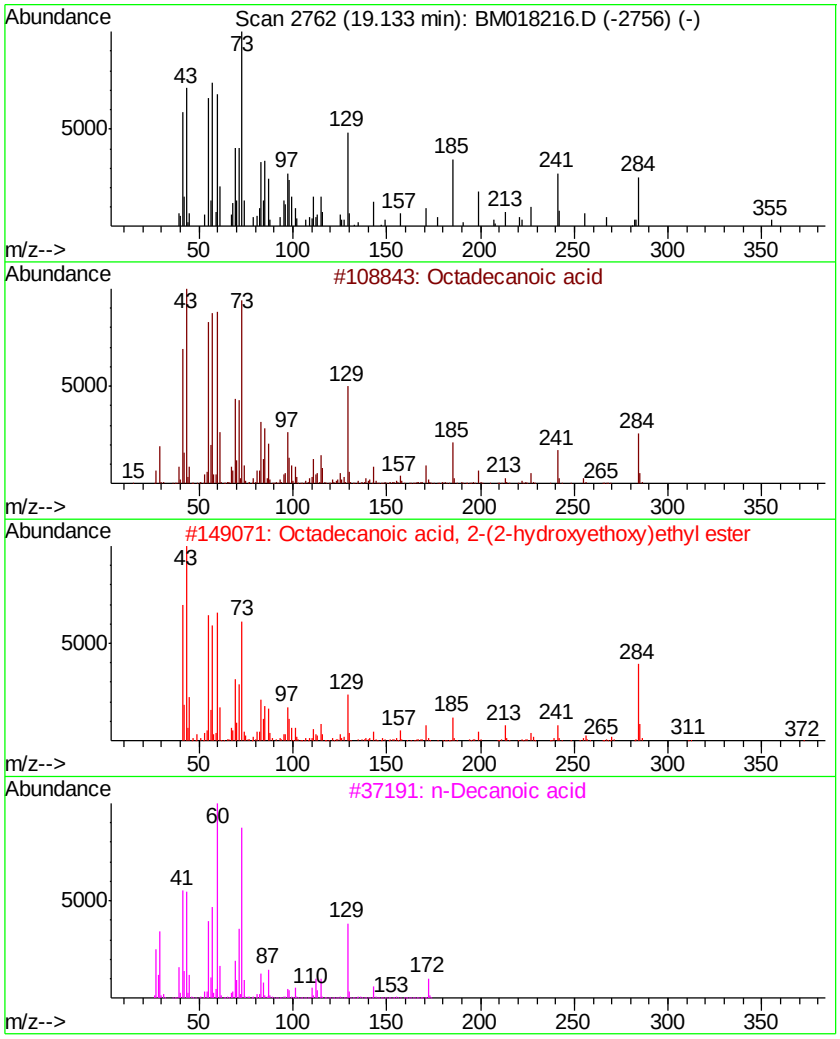
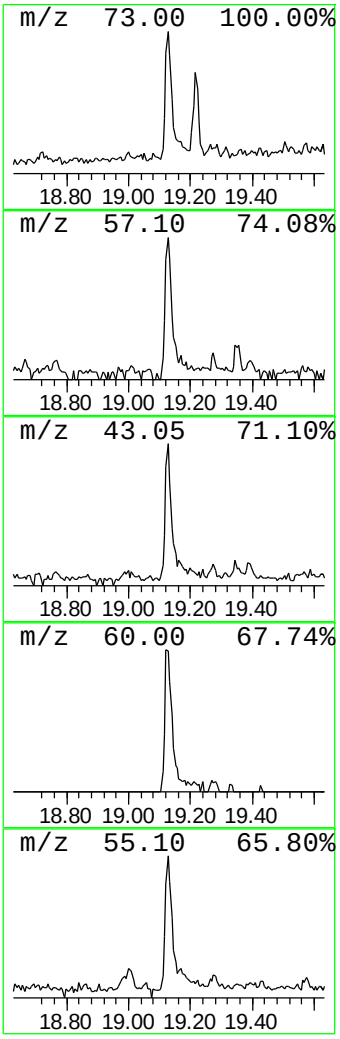
Peak Number 6 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	2.25 ng	216223	Chrysene-d12	21.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	n-Decanoic acid	172	C10H20O2	000334-48-5	55
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52





Library Search Compound Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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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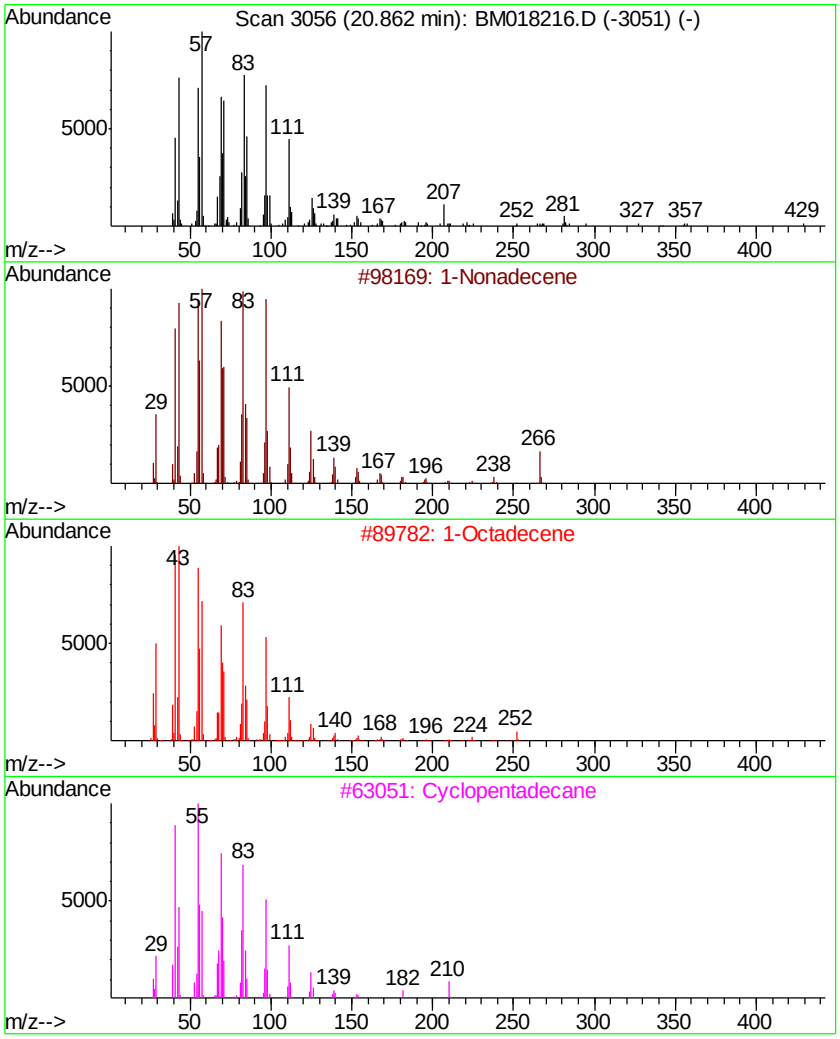
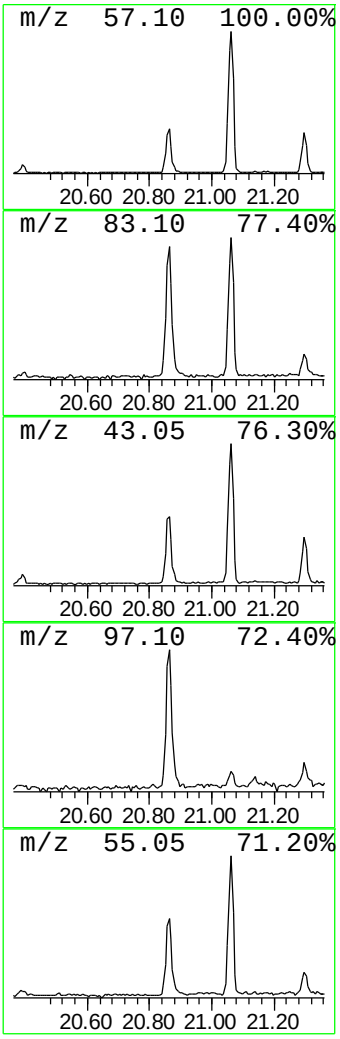
Peak Number 7 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	4.56 ng	437533	Chrysene-d12	21.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	95
2	1-Octadecene	252	C18H36	000112-88-9	93
3	Cyclopentadecane	210	C15H30	000295-48-7	91
4	1-Eicosene	280	C20H40	003452-07-1	89
5	Cyclotetradecane	196	C14H28	000295-17-0	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

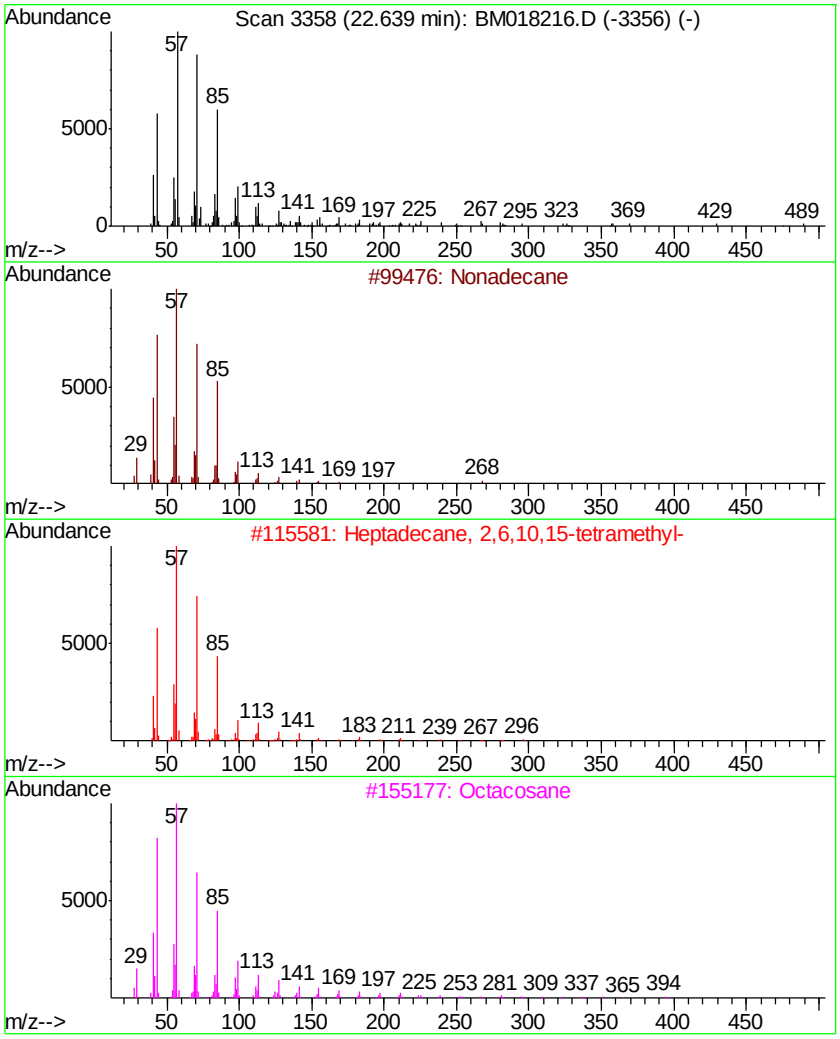
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

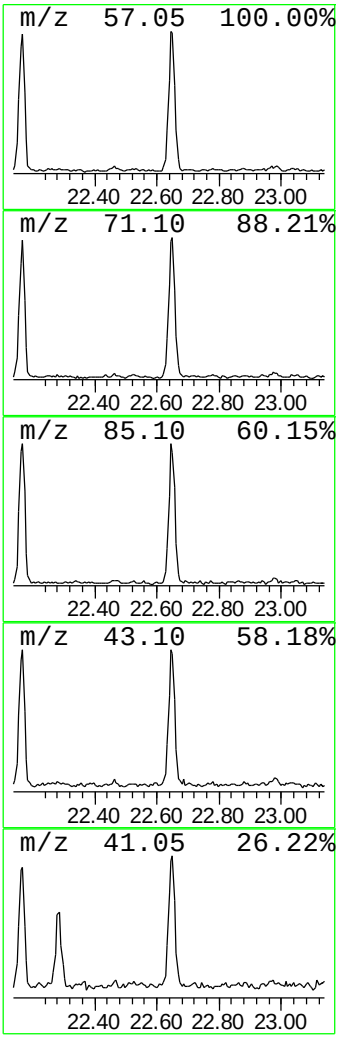
****

Peak Number 10 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.64	5.43 ng	448864	Perylene-d12	23.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetratriacontane	479	C34H70	014167-59-0	91
5	Pentacosane	352	C25H52	000629-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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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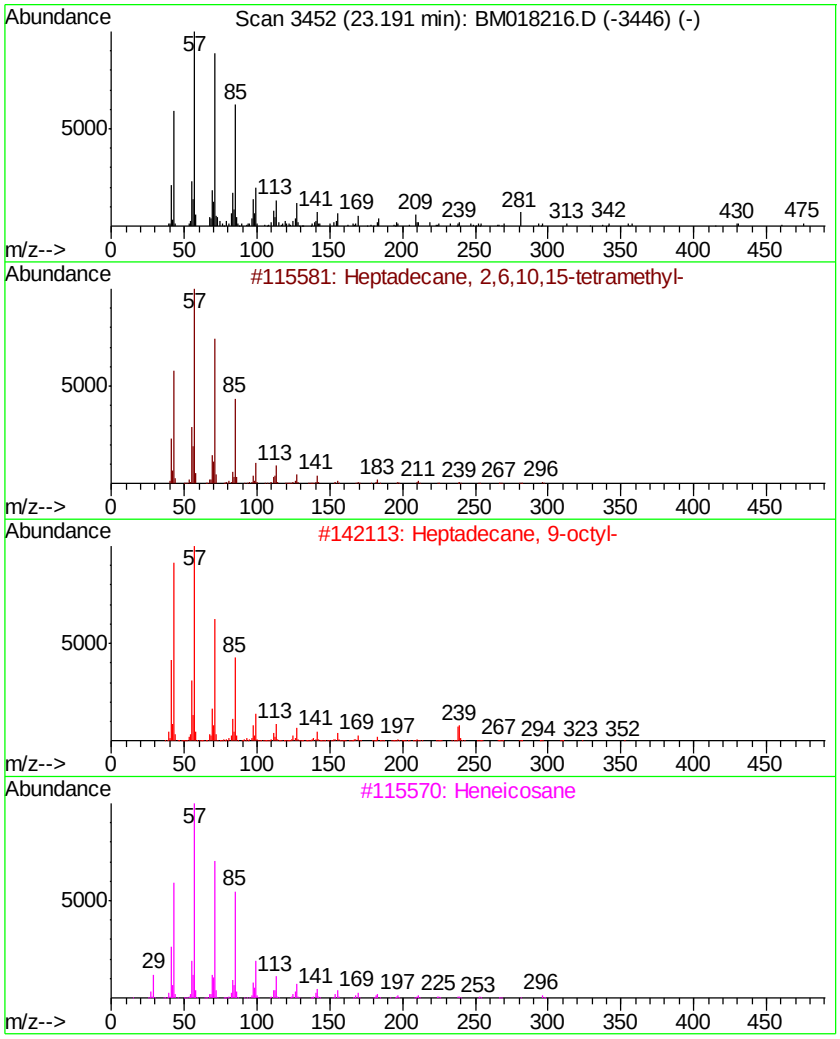
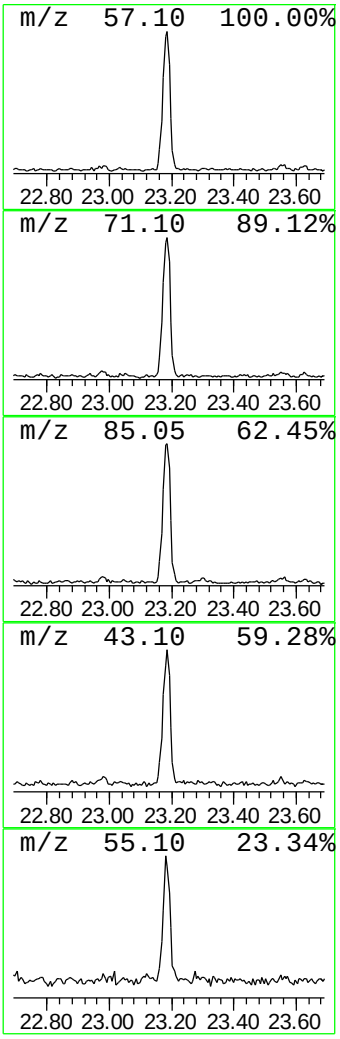
Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	4.54 ng	374806	Perylene-d12	23.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91





Library Search Compound Report

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Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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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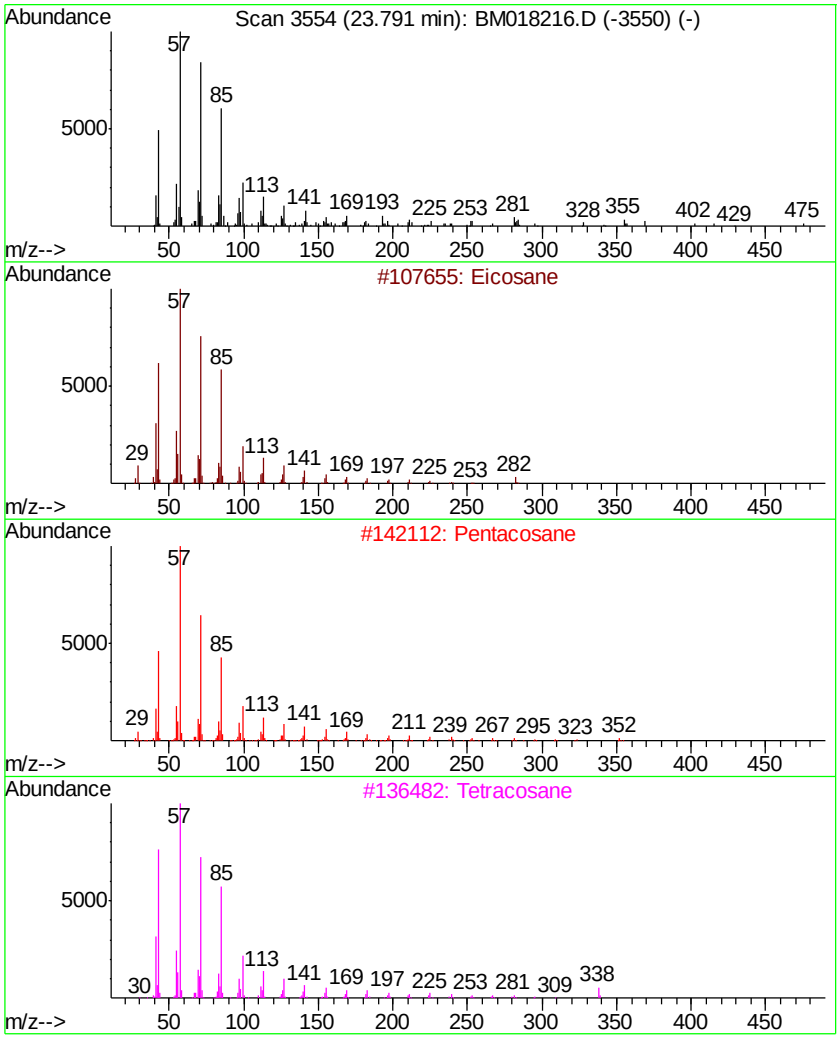
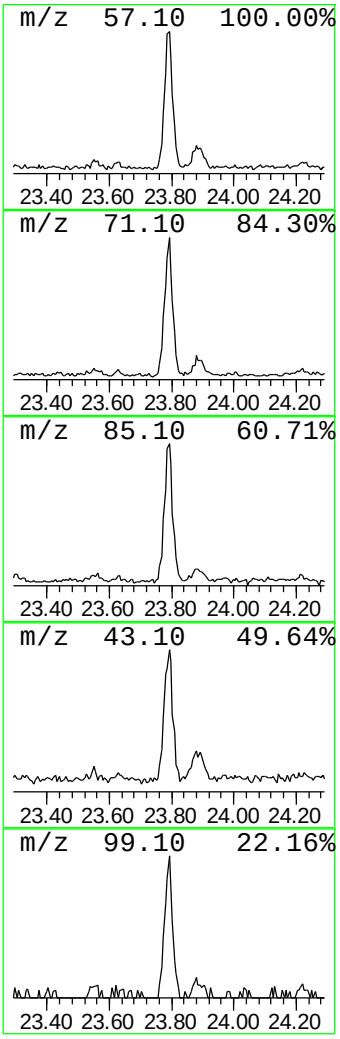
Peak Number 12 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.79	3.40 ng	281270	Perylene-d12	23.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Pentacosane	352	C25H52	000629-99-2	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Tetratriacontane	479	C34H70	014167-59-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121518\
Data File : BM018216.D
Acq On : 15 Dec 2018 22:35
Operator : JU/SJ
Sample : J6347-10
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P001-SW002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown7.04	7.04	6.6	ng	223832	1	7.50	682651	20.0
n-Hexadecanoic acid	17.83	7.0	ng	508012	4	16.92	1444750	20.0
Octadecanoic acid	19.13	2.3	ng	216223	5	21.14	1919270	20.0
1-Nonadecene	20.86	4.6	ng	437533	5	21.14	1919270	20.0
Nonadecane	22.64	5.4	ng	448864	6	23.30	1652460	20.0
Heptadecane, 2,6,...	23.19	4.5	ng	374806	6	23.30	1652460	20.0
Eicosane	23.79	3.4	ng	281270	6	23.30	1652460	20.0