LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

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-BM010919.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	4.887	301	306	319	rVB	290688	451237	1.99%	0.293%
2	5.340	376	383	396	rBV	6198142	8845352	38.97%	5.747%
3	6.928	645	653	670	rBV	6219335	10089924	44.45%	6.556%
4	7.287	706	714	722	rBV	6501705	10559930	46.52%	6.861%
5	7.745	785	792	799	rBV	1288325	1969531	8.68%	1.280%
6	8.063	838	846	854	rBV	5071397	8020513	35.33%	5.211%
7	8.916	982	991	1004	rBV	3851125	6318903	27.84%	4.106%
8	10.539	1259	1267	1274	rBV	1645648	2784459	12.27%	1.809%
9	13.010	1680	1687	1702	rBV	10863305	15964325	70.33%	10.373%
10	13.851	1824	1830	1840	rBV	2061380	2842025	12.52%	1.847%
11	14.392	1916	1922	1939	rVB2	2498332	3912519	17.24%	2.542%
12	15.892	2168	2177	2195	rBV	9115761	12934250	56.98%	8.404%
13	17.145	2384	2390	2395	rBV2	3169853	4608839	20.30%	2.995%
14	17.186	2395	2397	2402	rVB	199993	234278	1.03%	0.152%
15	18.039	2536	2542	2559	rBV	2702071	4079017	17.97%	2.650%
16	19.198	2735	2739	2752	rVB2	770833	1246588	5.49%	0.810%
17	19.315	2755	2759	2779	rBV	1116984	1736209	7.65%	1.128%
18	19.574	2799	2803	2810	rVB	252435	368834	1.62%	0.240%
19	19.780	2832	2838	2843	rBV	18469372	22700754	100.00%	14.750%
20	20.574	2969	2973	2977	rVB	278864	308720	1.36%	0.201%
21	21.033	3047	3051	3061	rBV	2466426	2783668	12.26%	1.809%
22	21.339	3097	3103	3108	rBV	3641223	4858436	21.40%	3.157%
23	21.439	3117	3120	3122	rBV2	257702	278558	1.23%	0.181%
24	21.474	3122	3126	3131	rVB	1466684	1541550	6.79%	1.002%
25	21.909	3196	3200	3208	rBV	2150593	3100239	13.66%	2.014%
26	22.380	3275	3280	3287	rBV	2968348	3984538	17.55%	2.589%
27	22.509	3299	3302	3306	rVB	266374	312856	1.38%	0.203%
28	22.897	3362	3368	3373	rBV	3049274	4427715	19.50%	2.877%
29	23.474	3460	3466	3482	rVB	2567135	4319246	19.03%	2.806%
30	23.615	3484	3490	3498	rVB	1797928	3427799	15.10%	2.227%
31	24.127	3572	3577	3586	rVB	1656396	3222746	14.20%	2.094%
32	24.891	3702	3707	3715	rVB	834278	1670874	7.36%	1.086%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

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-BM010919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

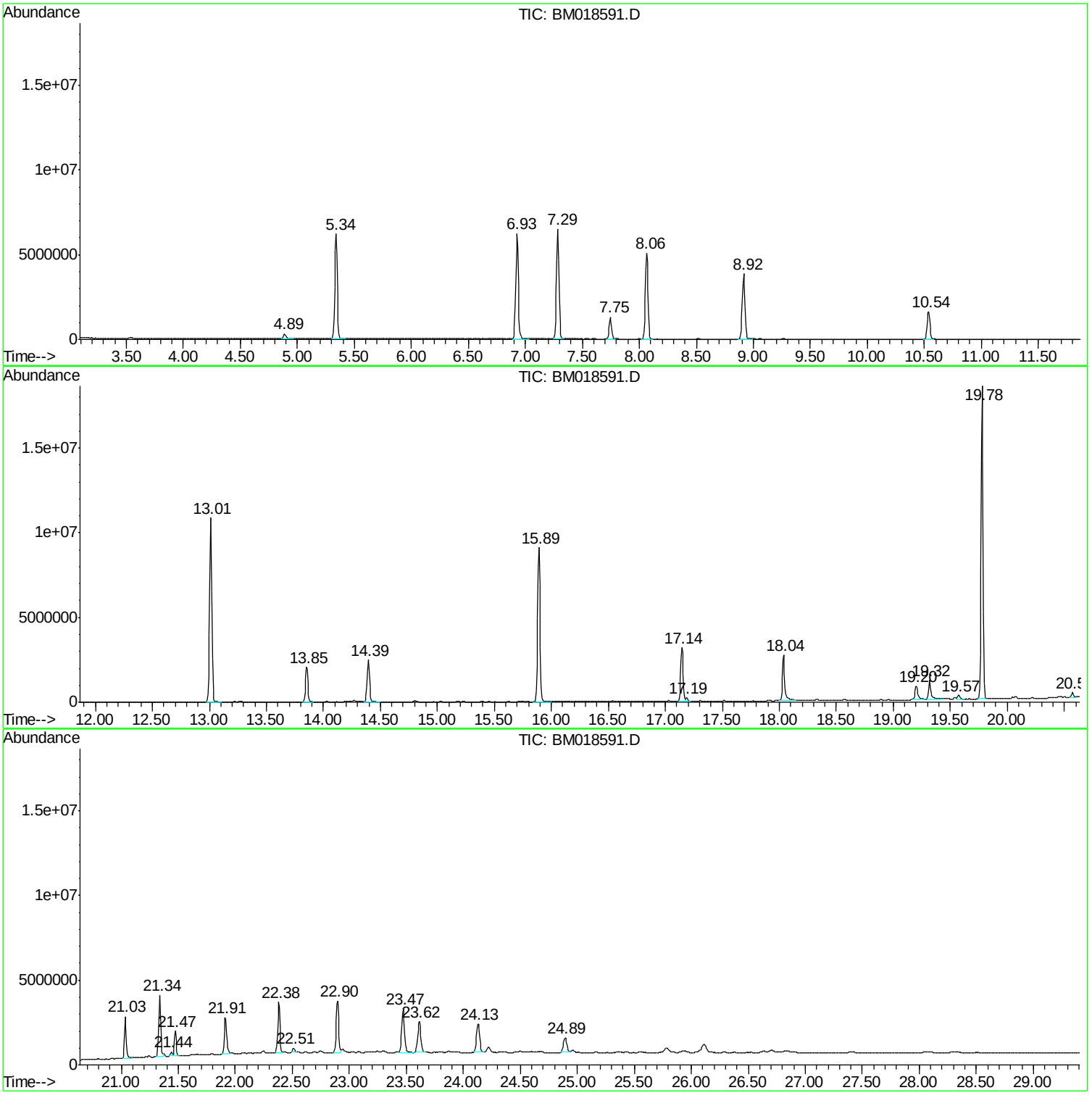
Sum of corrected areas: 153904432

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

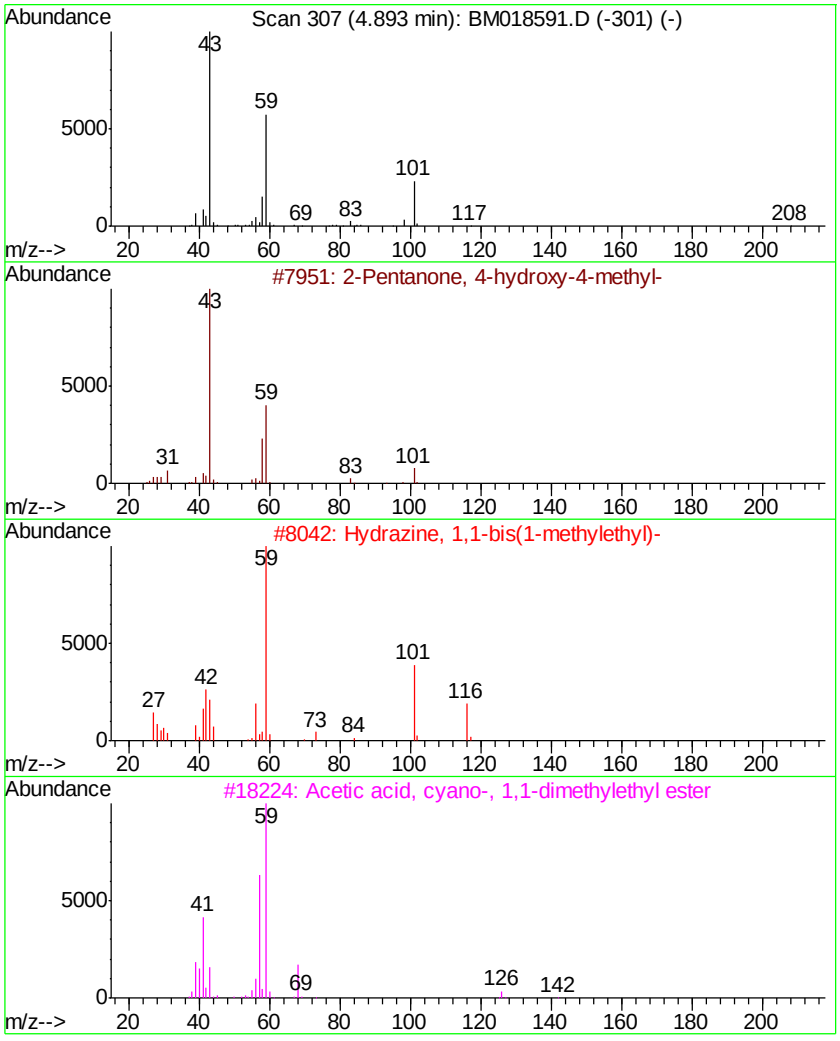
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

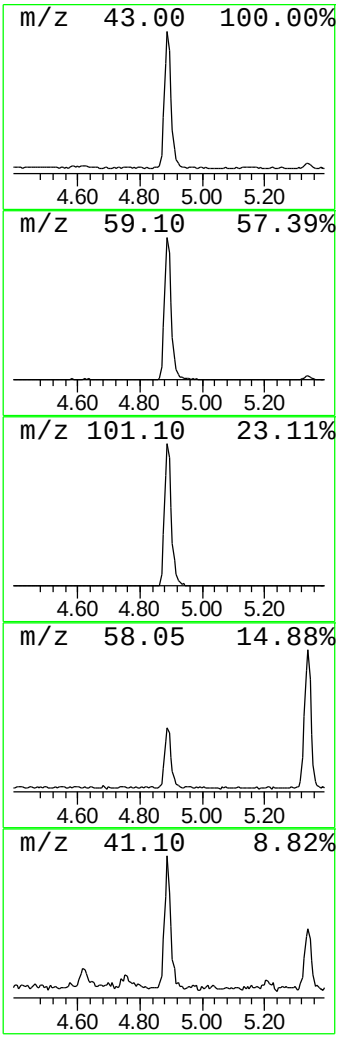
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	4.58 ng	451237	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

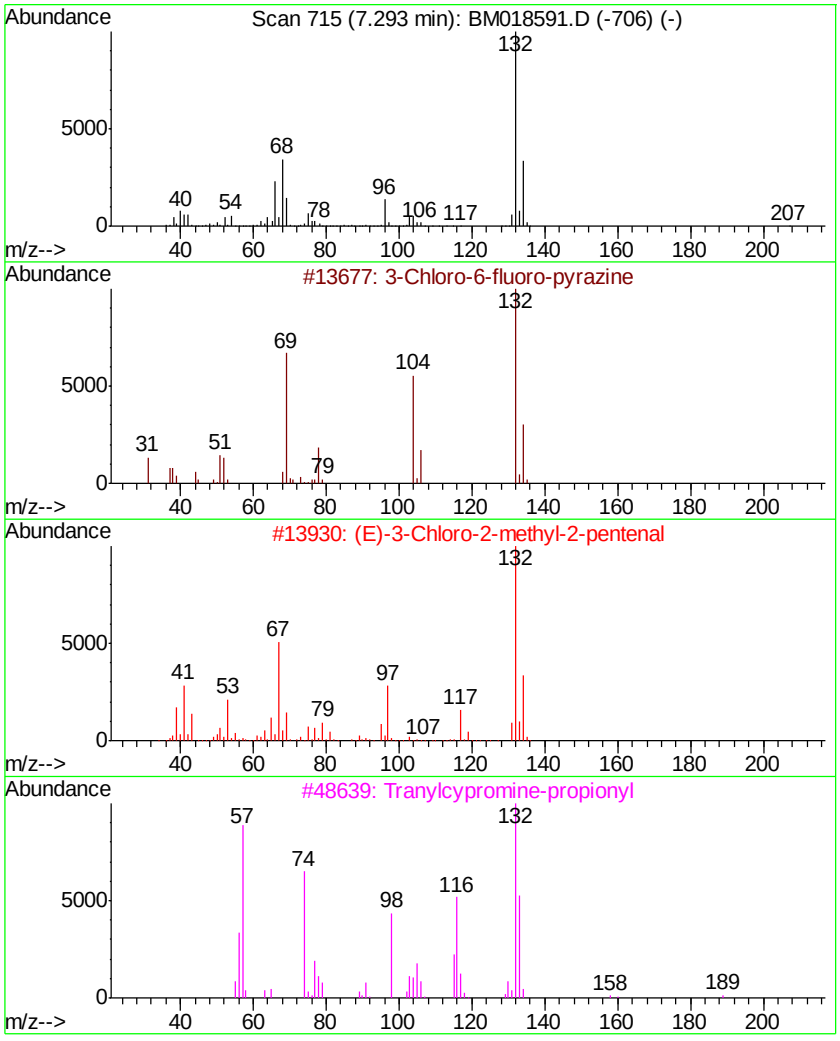
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

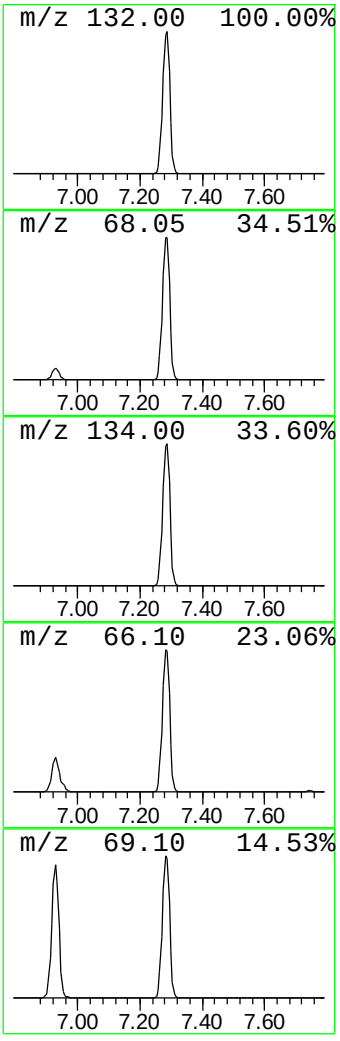
****

Peak Number 2 unknown7.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	107.23 ng	10559900	1,4-Dichlorobenzene-d4	7.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

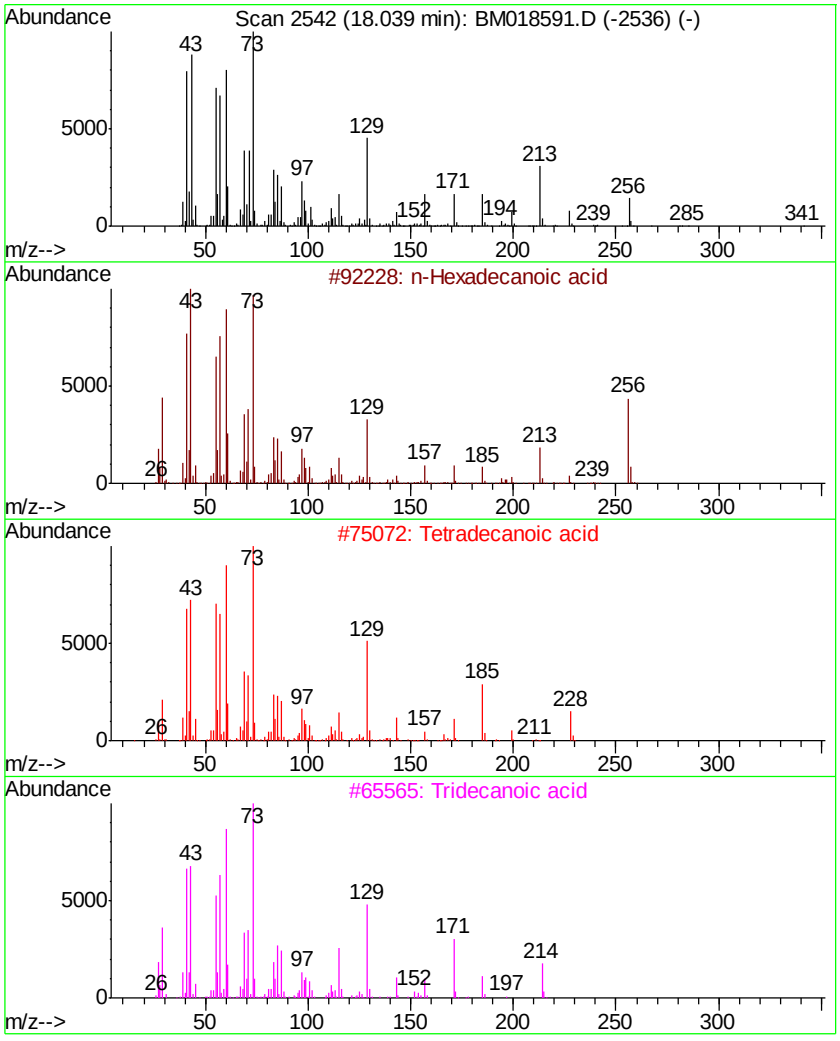
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

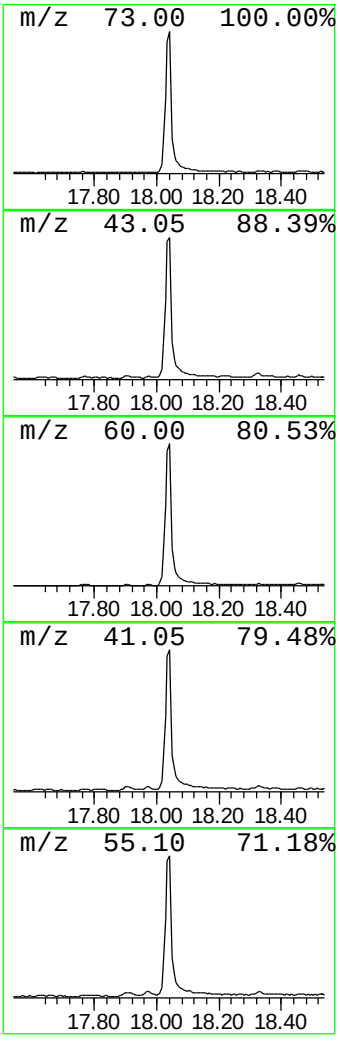
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	17.70 ng	4079020	Phenanthrene-d10	17.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Undecanoic acid	186	C11H22O2	000112-37-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

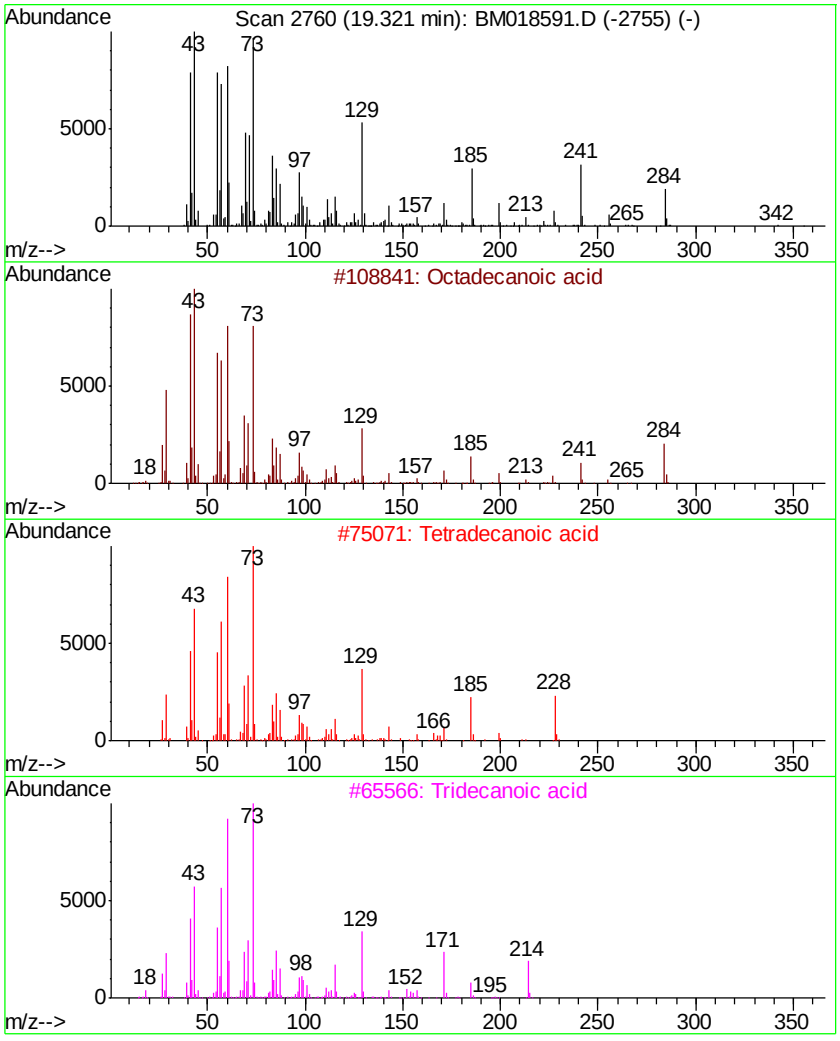
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

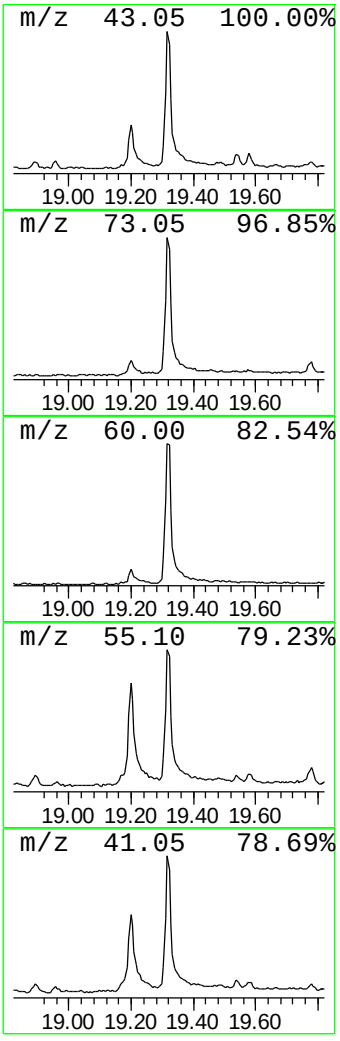
****

Peak Number 6 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	7.15 ng	1736210	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

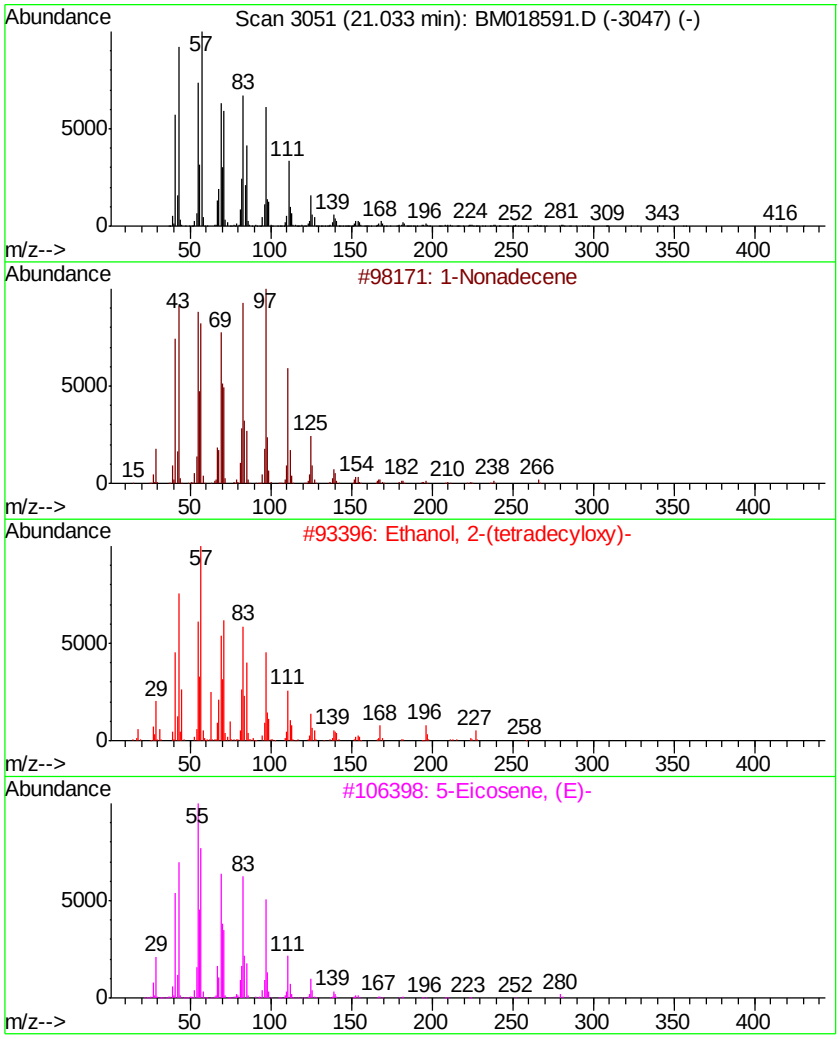
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

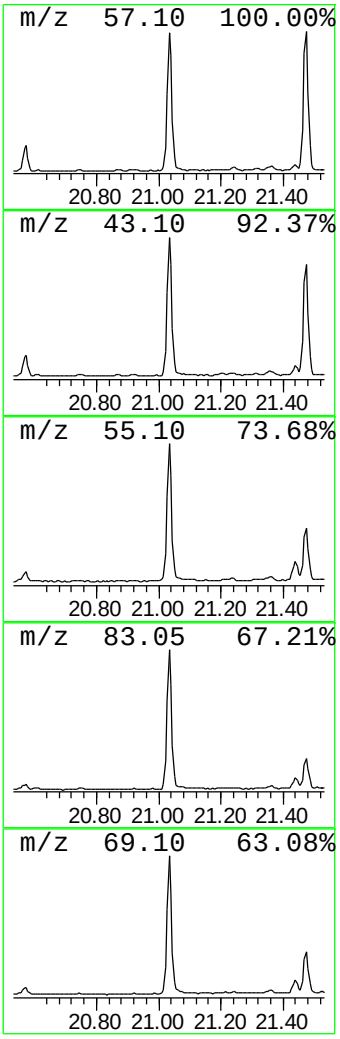
****

Peak Number 7 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	11.46 ng	2783670	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	97
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	96
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
4	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	94
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

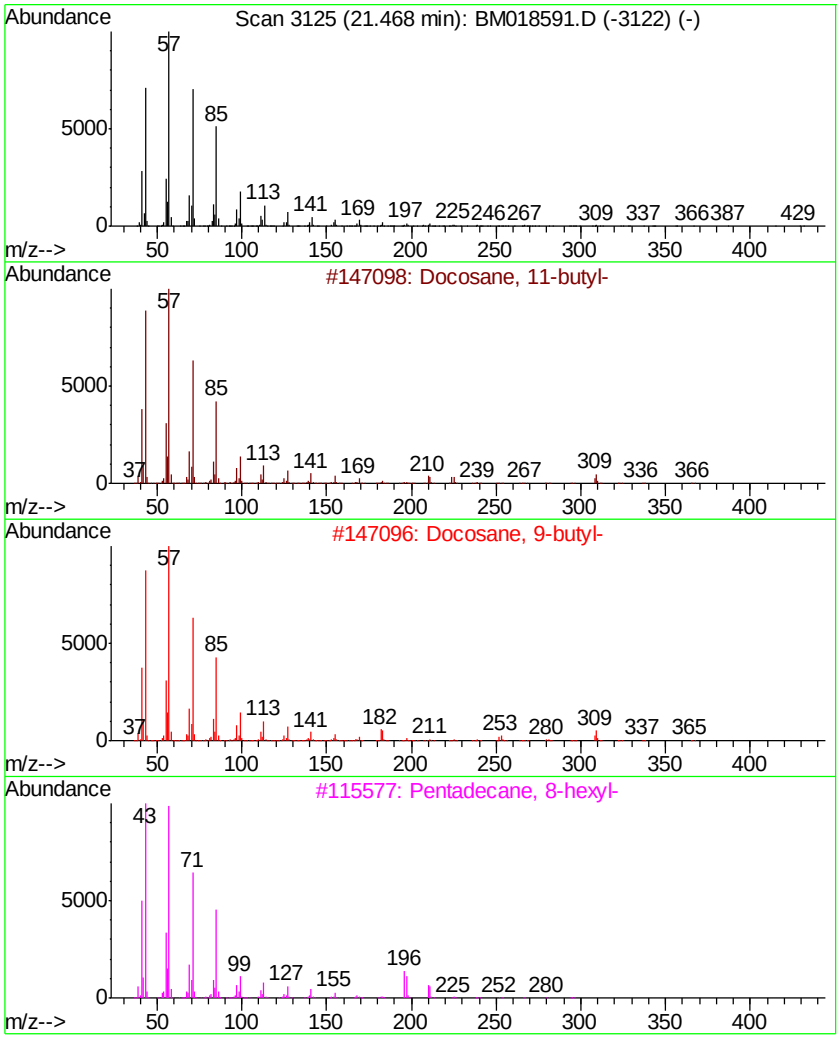
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

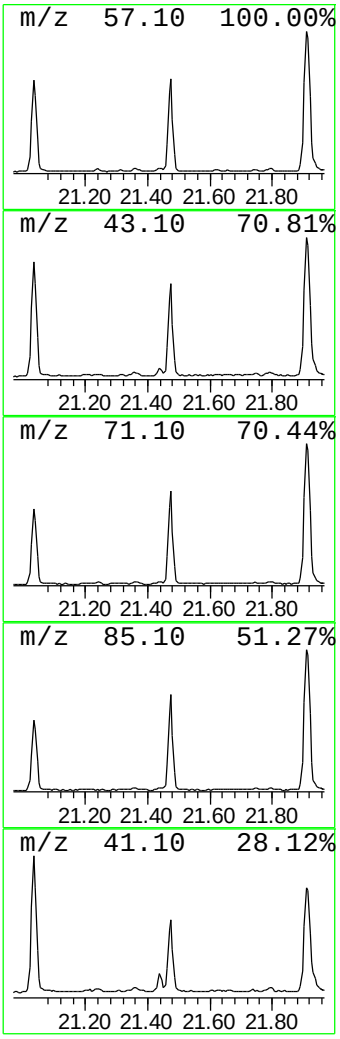
****

Peak Number 8 Docosane, 11-butyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	6.35 ng	1541550	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	95
2	Docosane, 9-butyl-	366	C26H54	055282-14-9	94
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

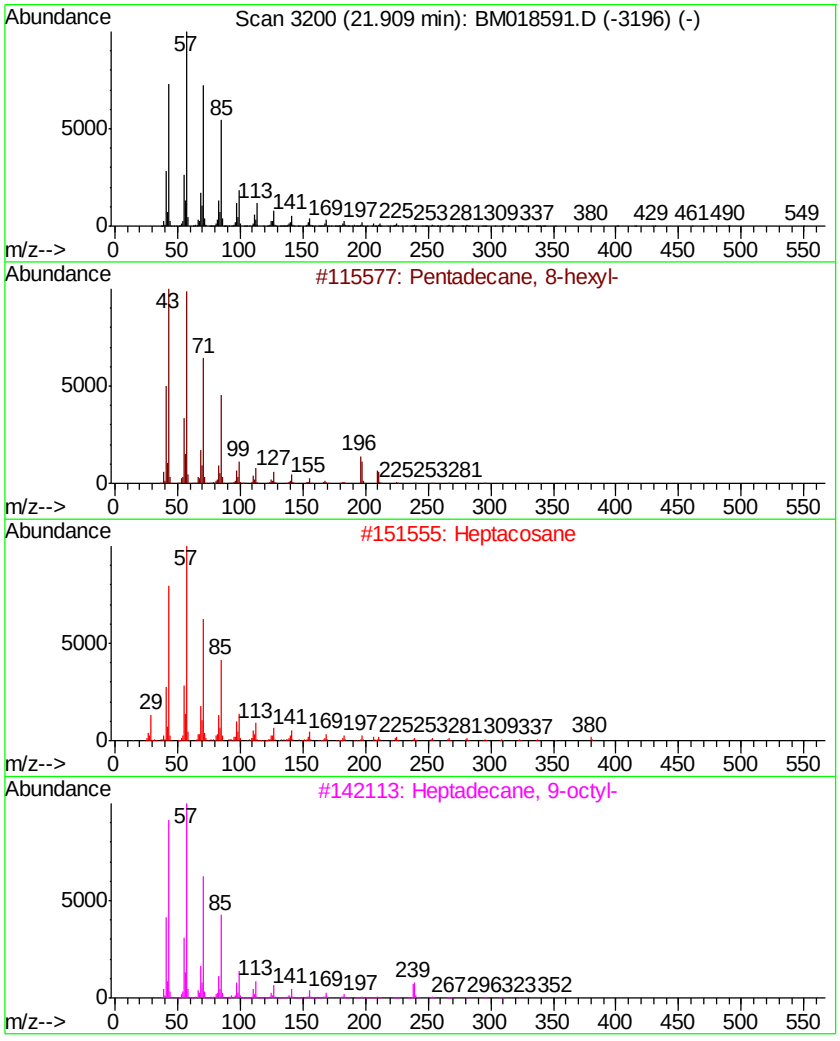
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

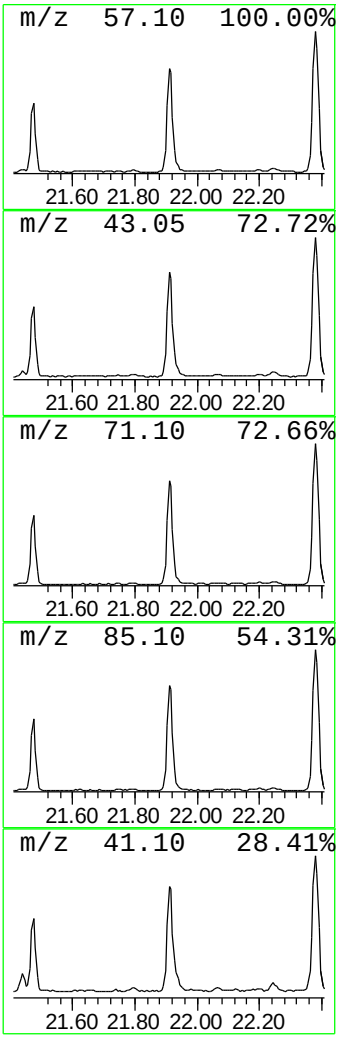
****

Peak Number 9 Pentadecane, 8-hexyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.91	12.76 ng	3100240	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

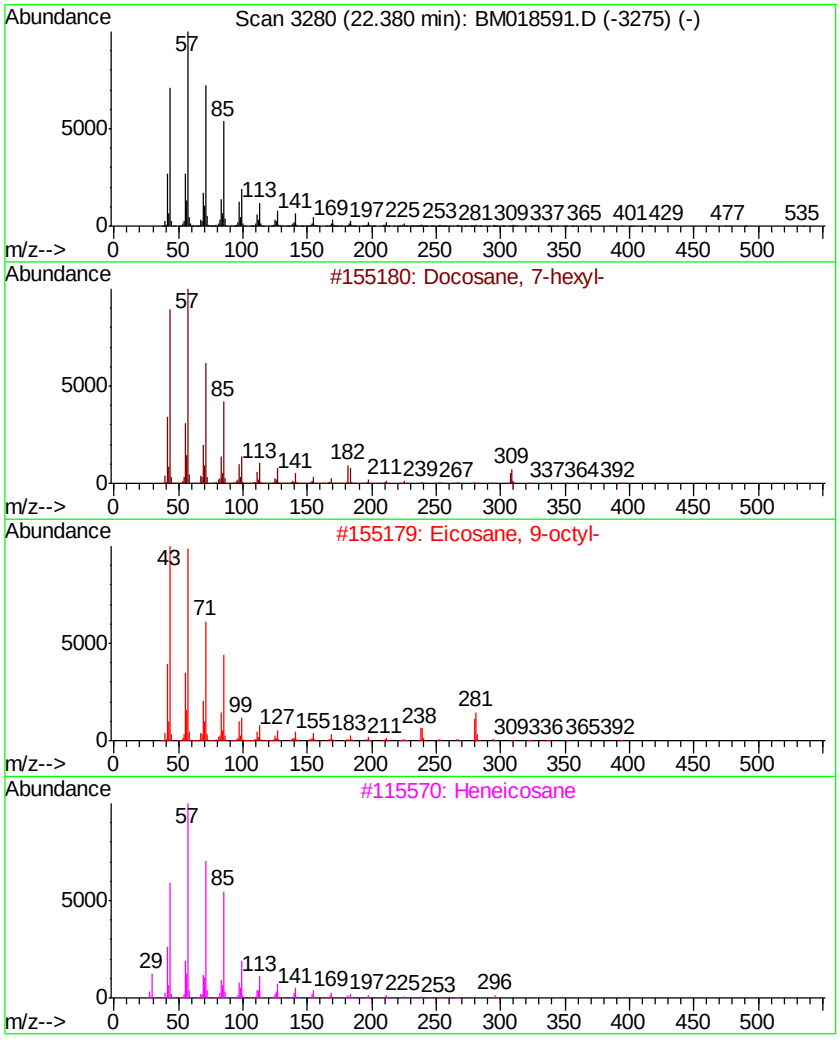
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

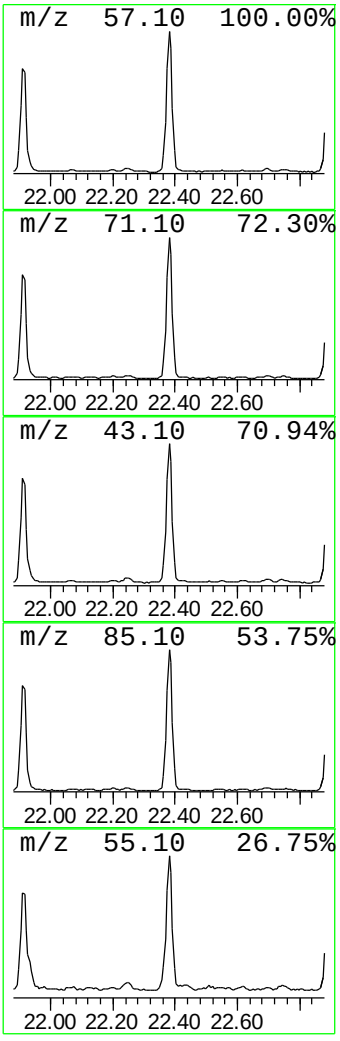
****

Peak Number 10 Docosane, 7-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.38	16.40 ng	3984540	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	95
2	Eicosane, 9-octyl-	394	C28H58	013475-77-9	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetratriacontane	479	C34H70	014167-59-0	91
5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

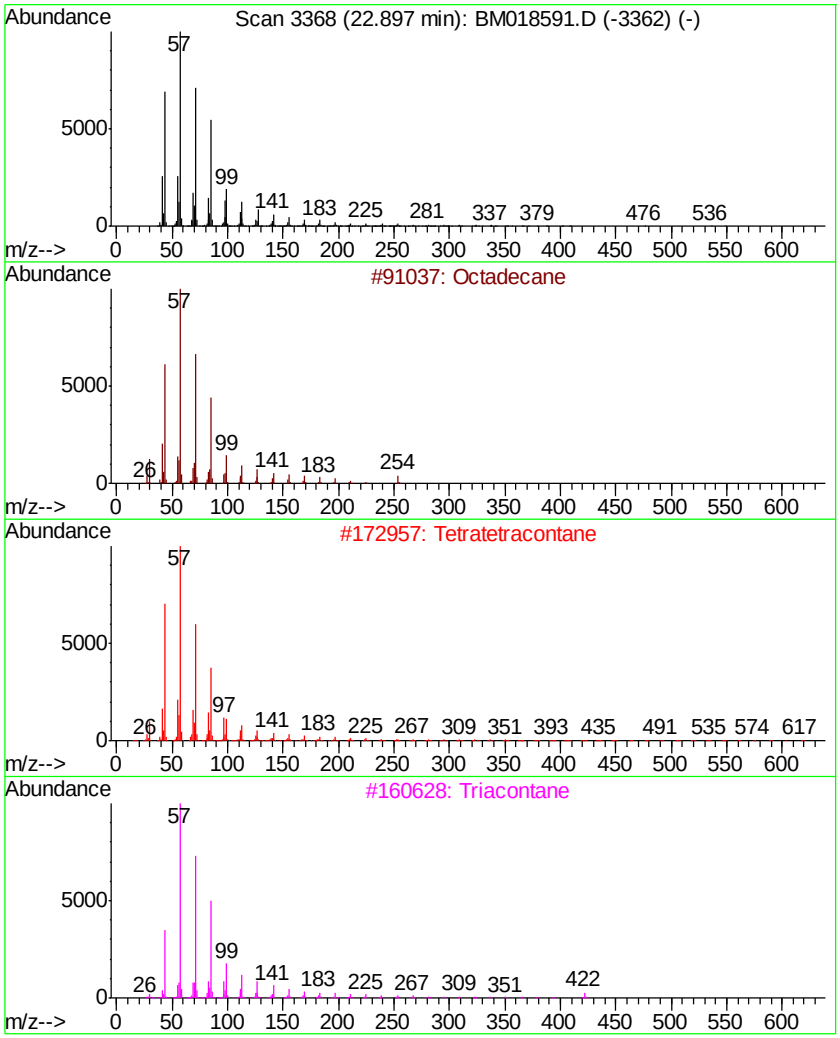
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

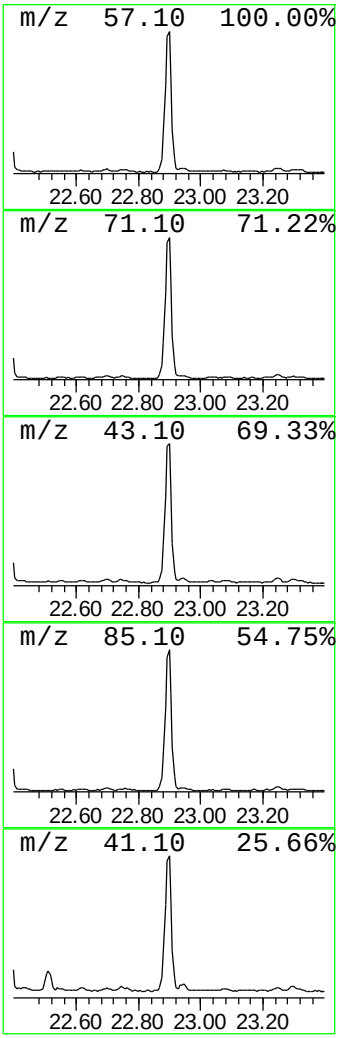
****

Peak Number 11 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.90	25.83 ng	4427720	Perylene-d12	23.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	94
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

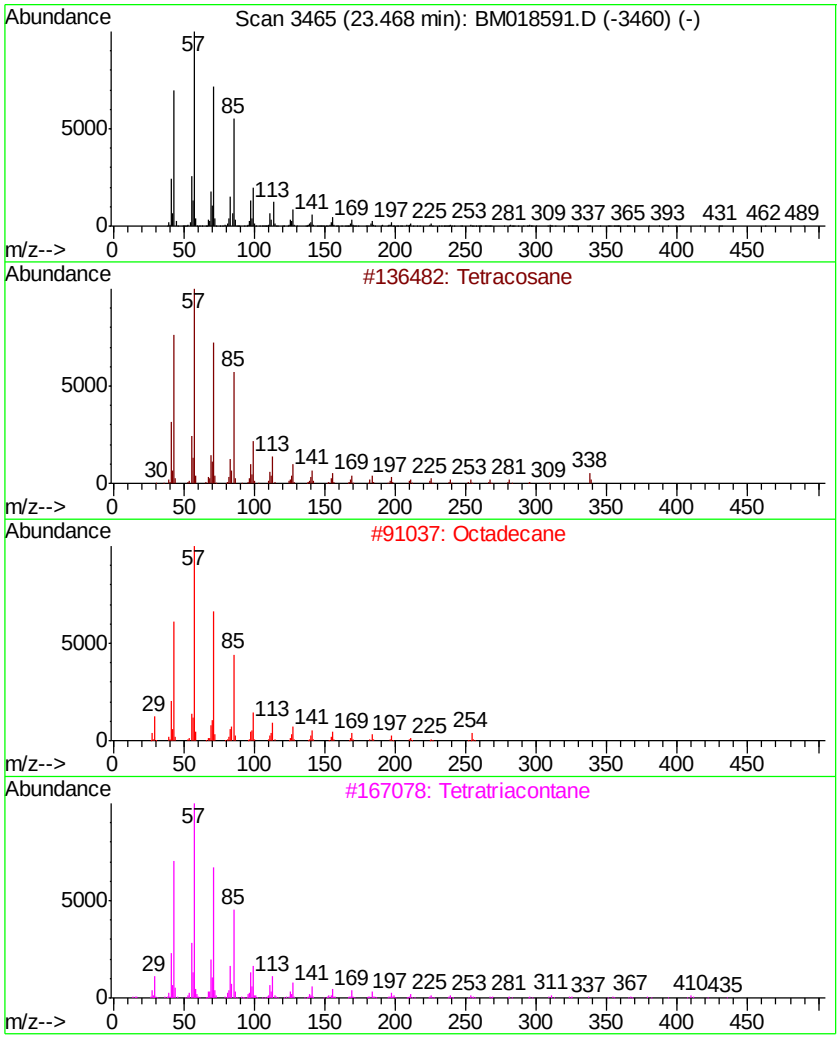
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

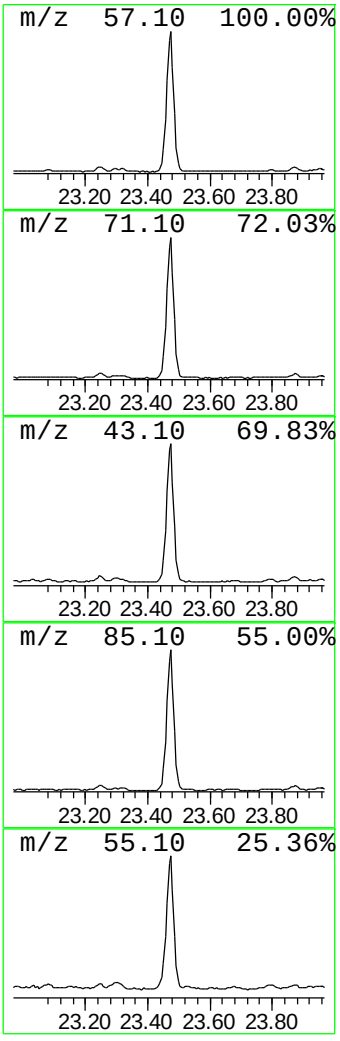
****

Peak Number 12 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.47	25.20 ng	4319250	Perylene-d12	23.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	98
2	Octadecane	254	C18H38	000593-45-3	94
3	Tetratriacontane	479	C34H70	014167-59-0	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane	296	C21H44	000629-94-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011619\
Data File : BM018591.D
Acq On : 16 Jan 2019 19:50
Operator : JU/SJ
Sample : K1147-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : TP-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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
2-Pentanone, 4-hy...	4.89	4.6	ng	451237	1	7.75	1969530	20.0
unknown7.29	7.29	107.2	ng	10559900	1	7.75	1969530	20.0
n-Hexadecanoic acid	18.04	17.7	ng	4079020	4	17.14	4608840	20.0
Octadecanoic acid	19.32	7.2	ng	1736210	5	21.34	4858440	20.0
1-Nonadecene	21.03	11.5	ng	2783670	5	21.34	4858440	20.0
Docosane, 11-butyl-	21.47	6.3	ng	1541550	5	21.34	4858440	20.0
Pentadecane, 8-he...	21.91	12.8	ng	3100240	5	21.34	4858440	20.0
Docosane, 7-hexyl-	22.38	16.4	ng	3984540	5	21.34	4858440	20.0
Octadecane	22.90	25.8	ng	4427720	6	23.62	3427800	20.0
Tetracosane	23.47	25.2	ng	4319250	6	23.62	3427800	20.0