LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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	4.881	300	305	314	rBV	275728	404996	3.04%	0.362%
2	5.328	375	381	395	rBV	5516702	8028508	60.35%	7.175%
3	6.916	643	651	665	rBV	5510941	8918057	67.04%	7.970%
4	7.275	704	712	729	rVB	6014356	9474733	71.23%	8.468%
5	7.739	784	791	798	rBV	1465897	2277100	17.12%	2.035%
6	8.057	837	845	854	rBV	4349303	6920500	52.02%	6.185%
7	8.910	982	990	1001	rBV	3283277	5559876	41.80%	4.969%
8	10.527	1254	1265	1273	rBV	1872969	3164724	23.79%	2.828%
9	13.004	1679	1686	1697	rBV	8282838	11824701	88.89%	10.568%
10	13.845	1822	1829	1837	rBV	542223	782457	5.88%	0.699%
11	14.257	1892	1899	1911	rBV3	50869	144920	1.09%	0.130%
12	14.386	1914	1921	1928	rVV2	2834912	4205497	31.61%	3.759%
13	14.451	1928	1932	1938	rVB	87739	133924	1.01%	0.120%
14	15.439	2093	2100	2112	rVB3	61122	148734	1.12%	0.133%
15	15.886	2165	2176	2186	rBV	7169187	10455703	78.60%	9.345%
16	16.786	2324	2329	2337	rVB2	186605	290971	2.19%	0.260%
17	17.139	2382	2389	2393	rBV	3355624	4803816	36.11%	4.293%
18	17.180	2393	2396	2403	rVV	483413	645855	4.86%	0.577%
19	17.268	2407	2411	2416	rVV	98195	136069	1.02%	0.122%
20	17.509	2446	2452	2455	rBV2	117888	172550	1.30%	0.154%
21	18.027	2533	2540	2544	rBV2	886780	1260434	9.48%	1.126%
22	18.209	2565	2571	2575	rBV3	128368	216735	1.63%	0.194%
23	19.197	2734	2739	2745	rVB	1115405	1496206	11.25%	1.337%
24	19.309	2753	2758	2769	rBV4	195994	343602	2.58%	0.307%
25	19.533	2791	2796	2798	rBV3	204170	296806	2.23%	0.265%
26	19.562	2798	2801	2810	rVB	895154	1244191	9.35%	1.112%
27	19.768	2830	2836	2842	rBV	10835793	13302497	100.00%	11.889%
28	20.039	2875	2882	2883	rBV6	101119	164532	1.24%	0.147%
29	20.062	2883	2886	2891	rVB2	151600	231224	1.74%	0.207%
30	21.027	3046	3050	3060	rBV3	1409236	1642873	12.35%	1.468%
31	21.238	3082	3086	3090	rVB	559843	626898	4.71%	0.560%
32	21.327	3095	3101	3106	rVV	2963308	4633720	34.83%	4.141%
33	21.368	3106	3108	3115	rVB	444371	474189	3.56%	0.424%
34	21.468	3123	3125	3131	rVB3	164066	224070	1.68%	0.200%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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

35	21.903	3197	3199	3202	rBV2	152217	170262	1.28%	0.152%
36	22.374	3275	3279	3285	rBV	353028	490373	3.69%	0.438%
37	22.885	3362	3366	3369	rBV	532441	831220	6.25%	0.743%
38	23.462	3460	3464	3468	rBV	548165	838543	6.30%	0.749%
39	23.603	3482	3488	3495	rBV2	1746493	3212886	24.15%	2.871%
40	24.121	3571	3576	3584	rVB	568072	1086477	8.17%	0.971%
41	24.879	3701	3705	3711	rVB	313797	609091	4.58%	0.544%

Sum of corrected areas: 111890520

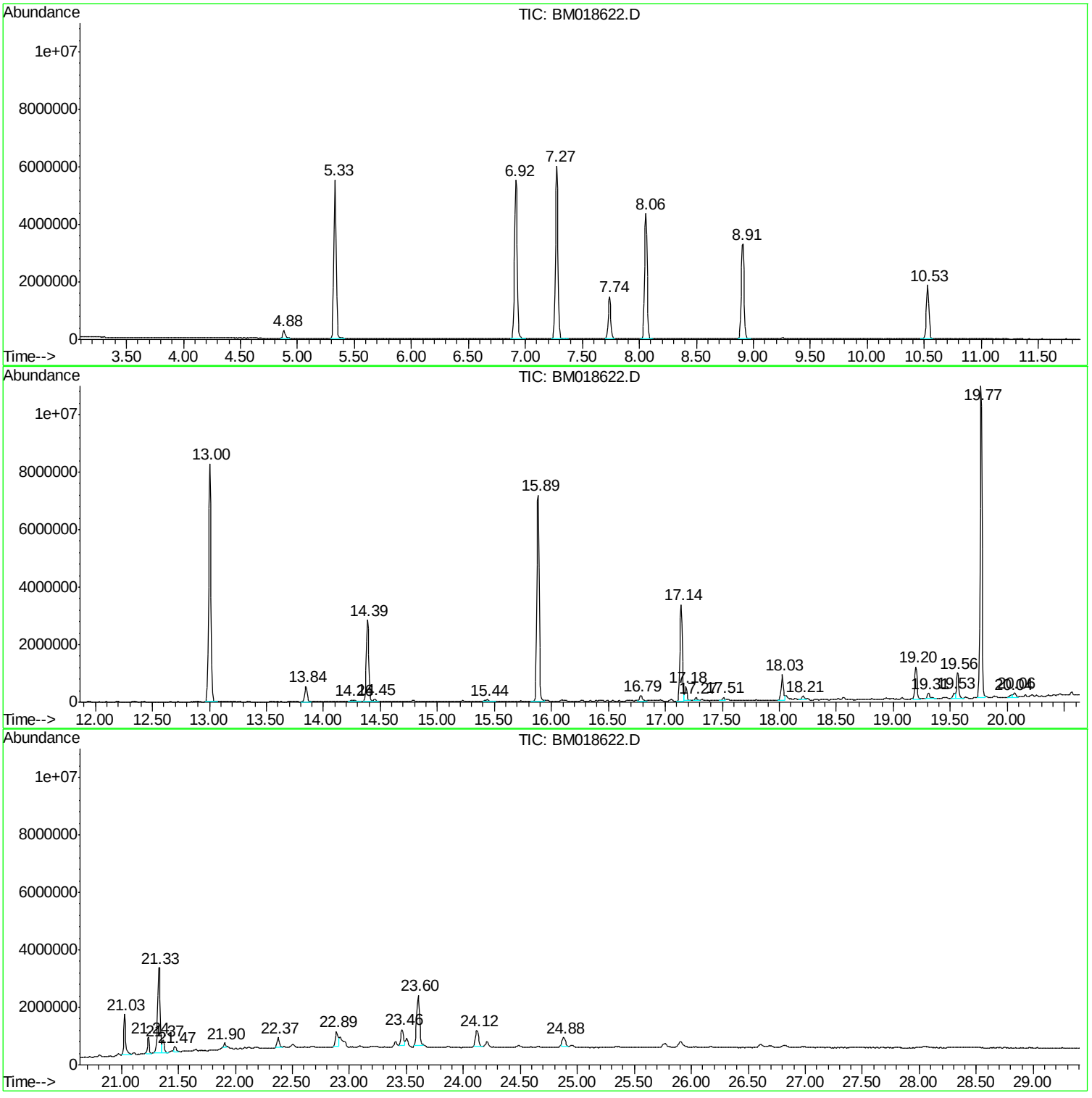
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR200044-RBR200027

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\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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

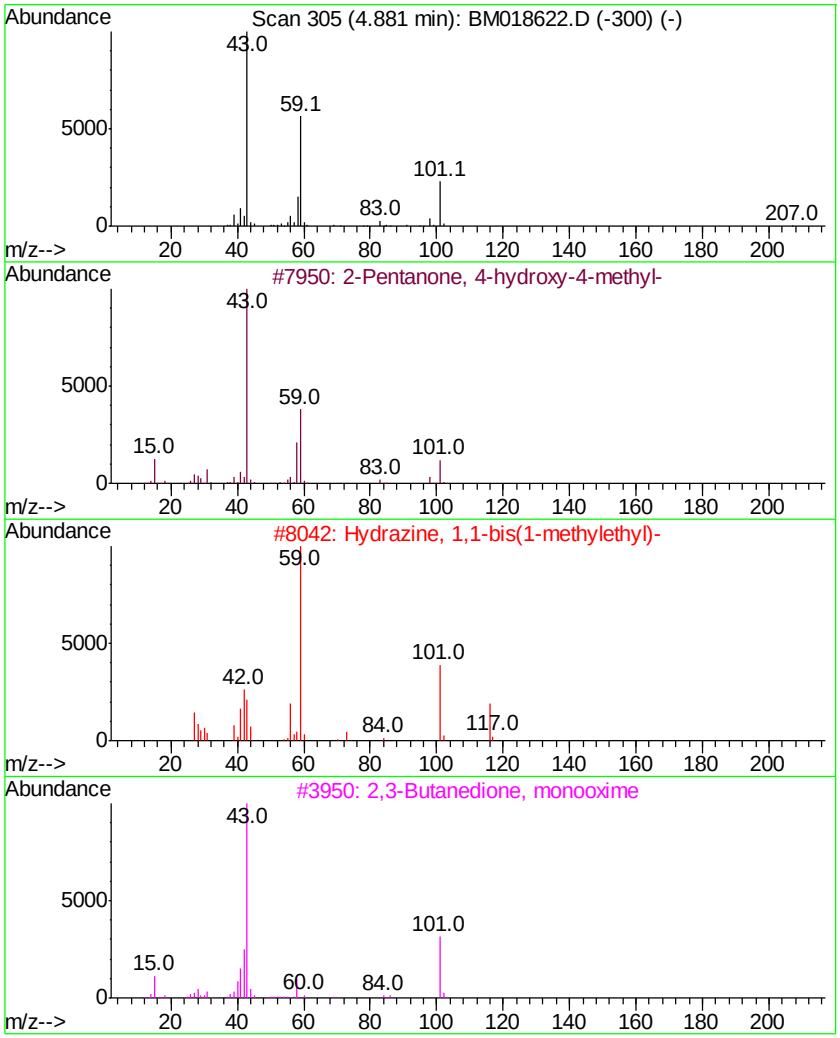
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

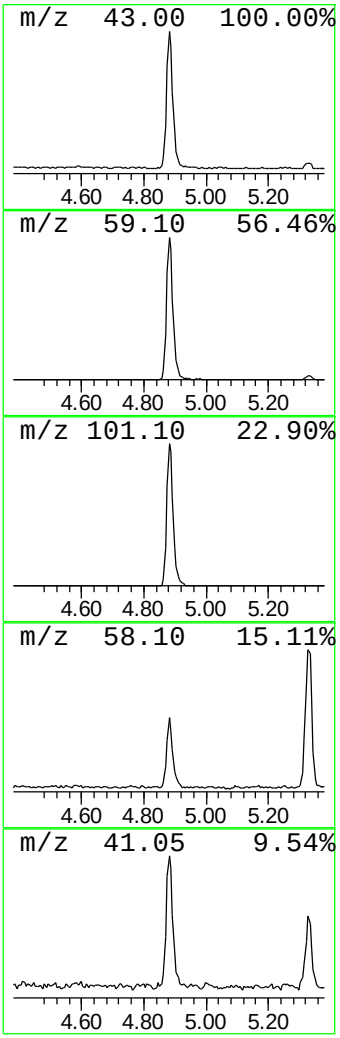
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	3.56 ng	404996	1,4-Dichlorobenzene-d4	7.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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

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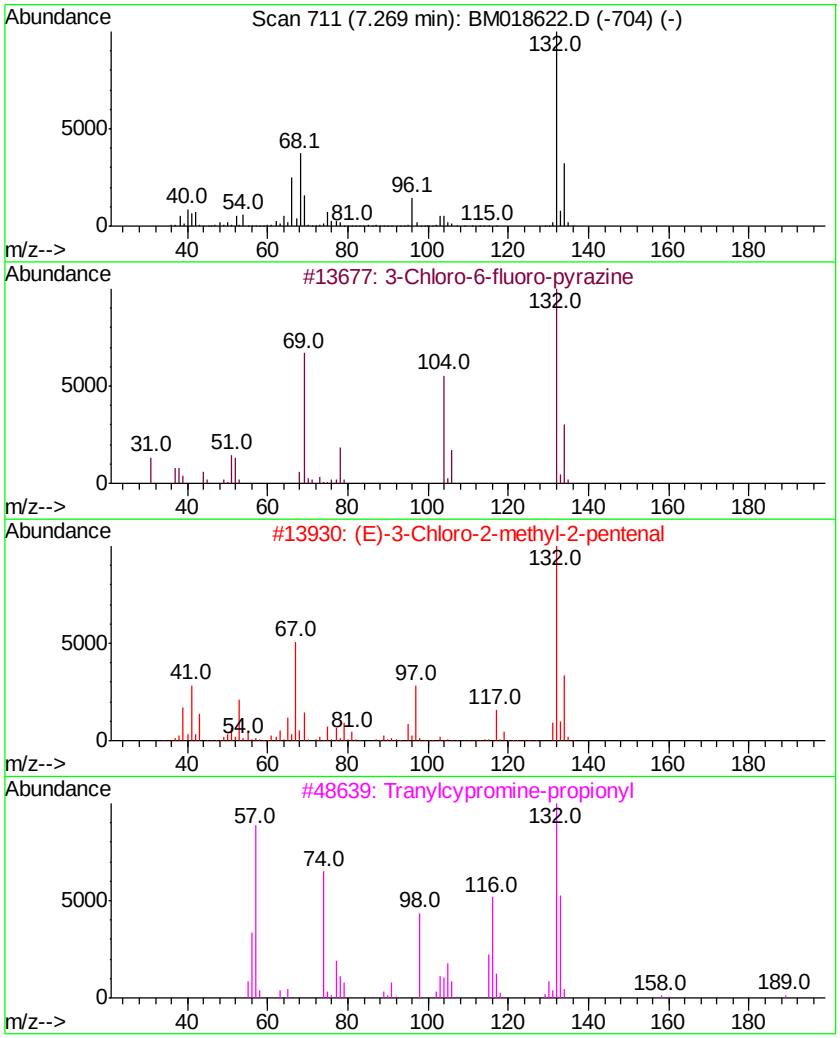
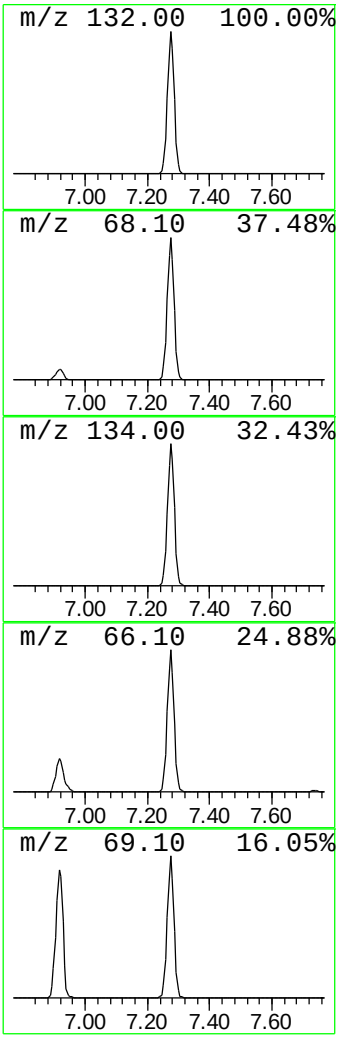
Peak Number 2 unknown7.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	83.22 ng	9474730	1,4-Dichlorobenzene-d4	7.74

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	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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

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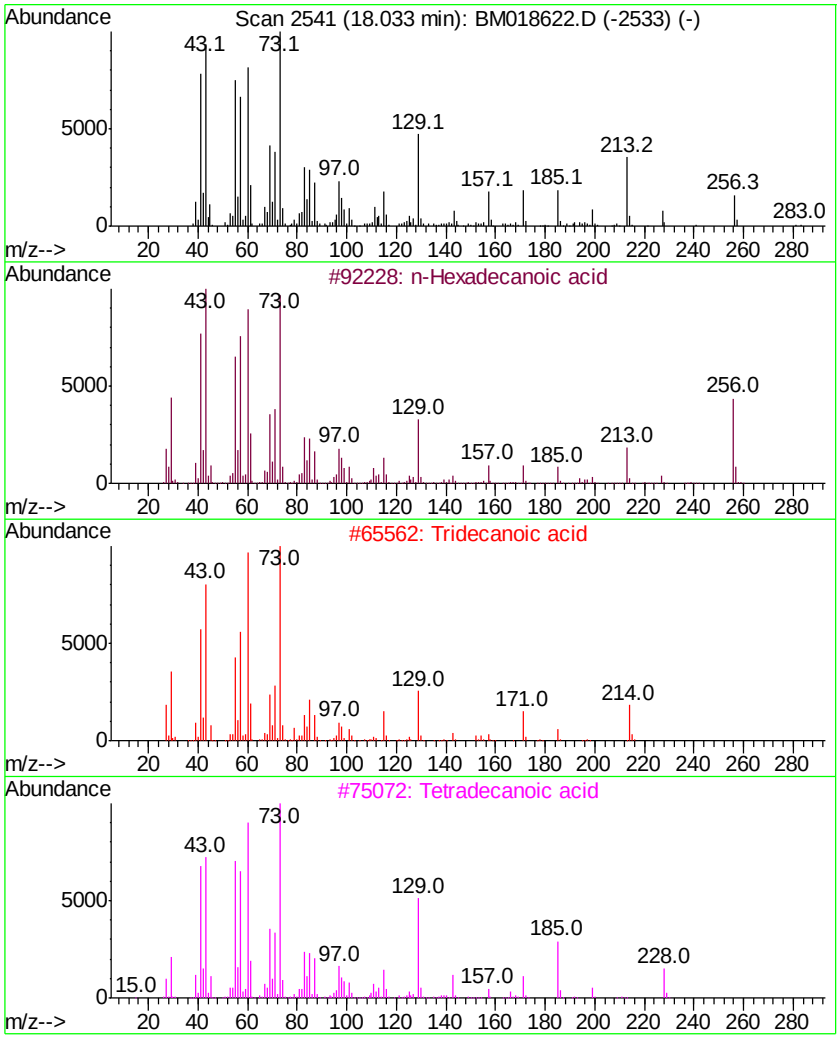
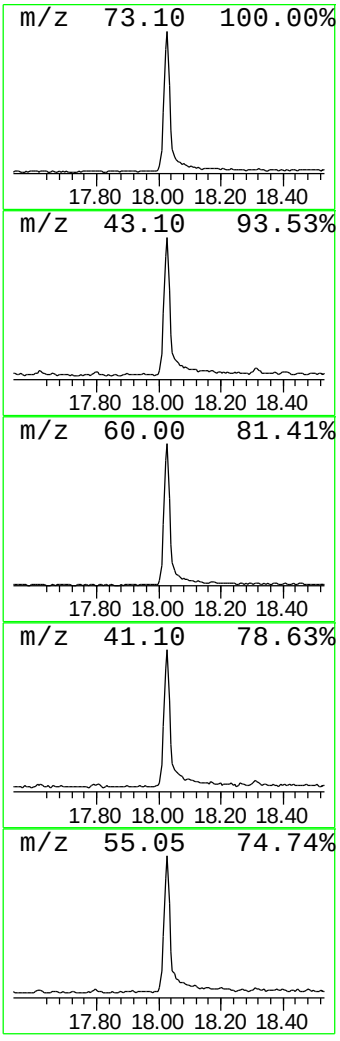
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	5.25 ng	1260430	Phenanthrene-d10	17.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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

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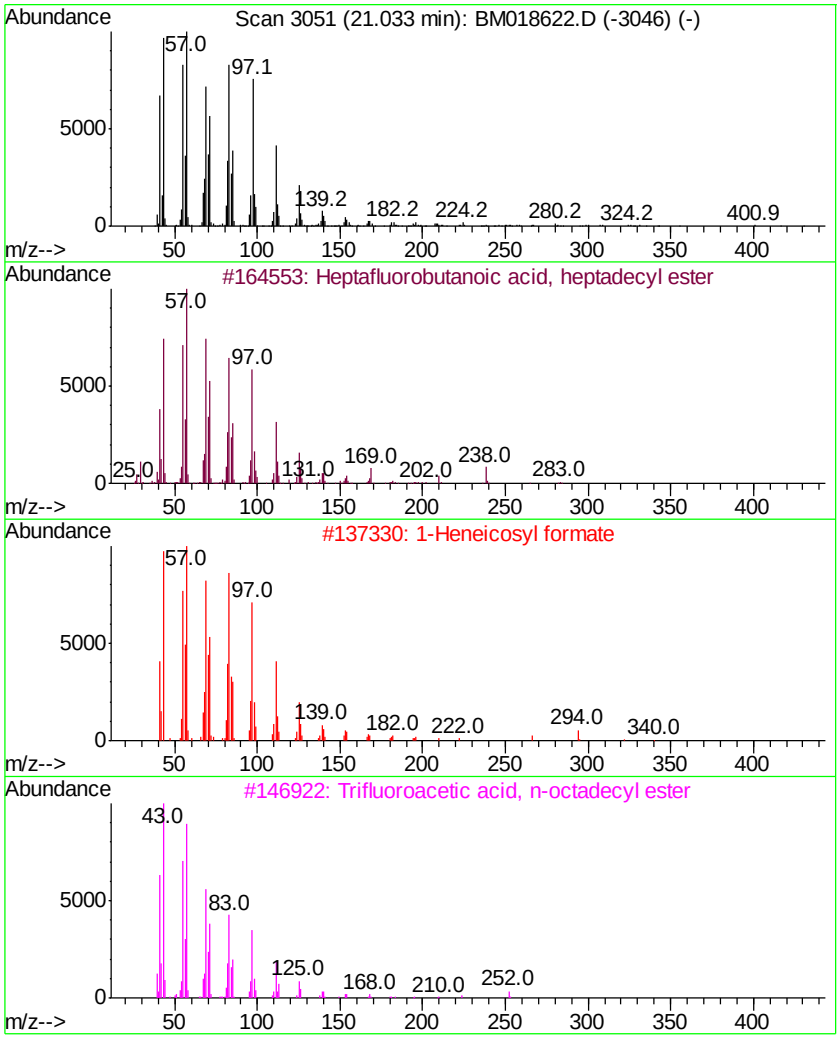
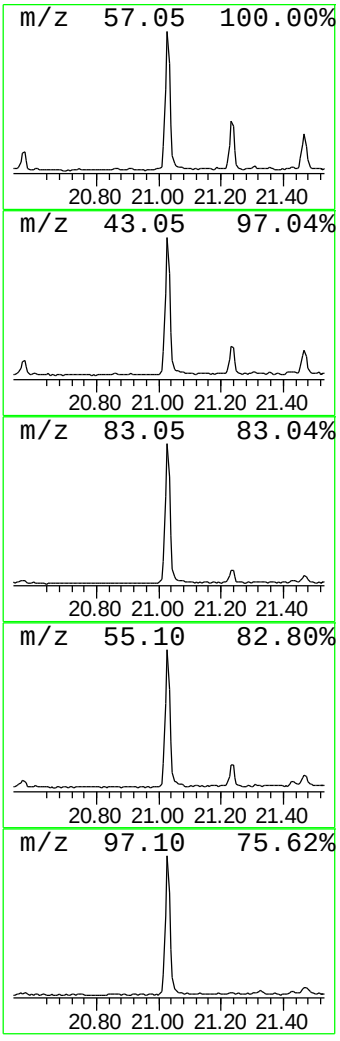
Peak Number 5 Heptafluorobutanoic acid, h... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	7.09 ng	1642870	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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

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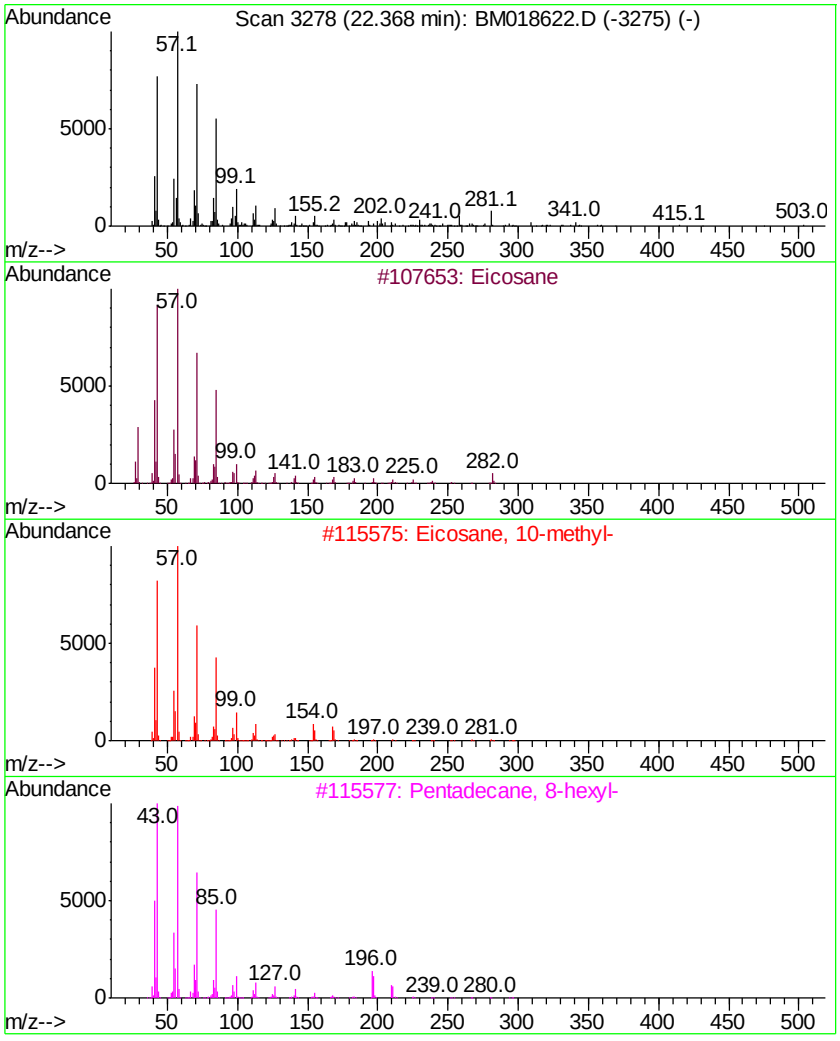
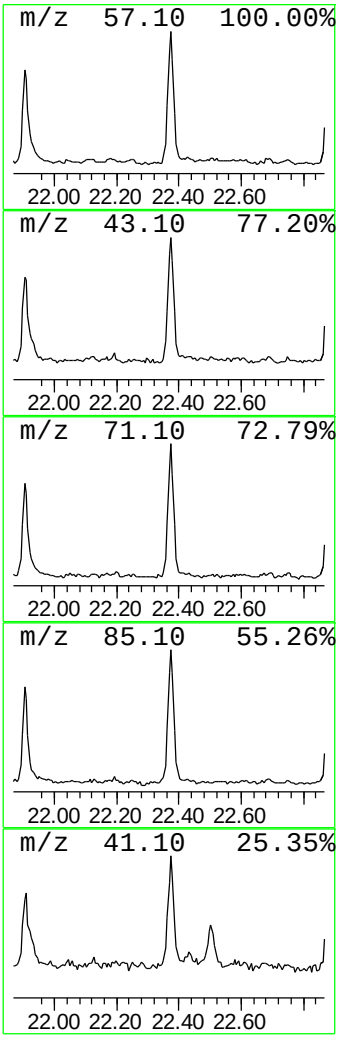
Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	2.12 ng	490373	Chrysene-d12	21.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	Triacontane	422	C30H62	000638-68-6	91





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Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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

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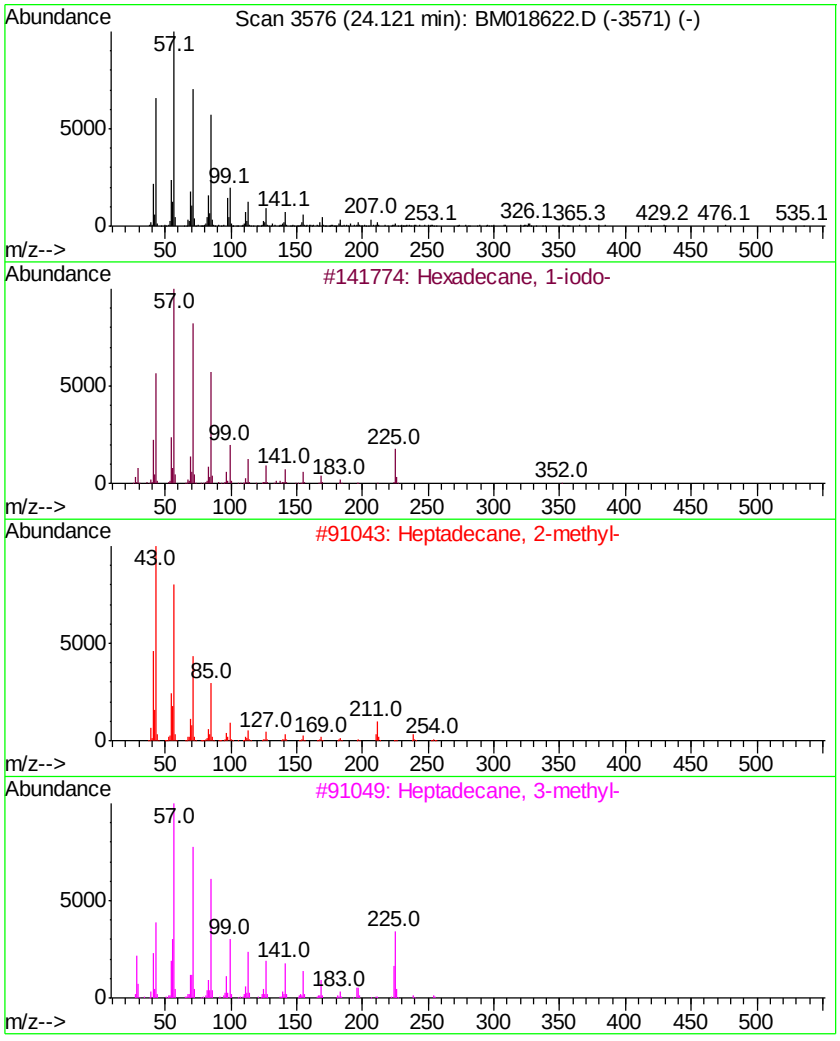
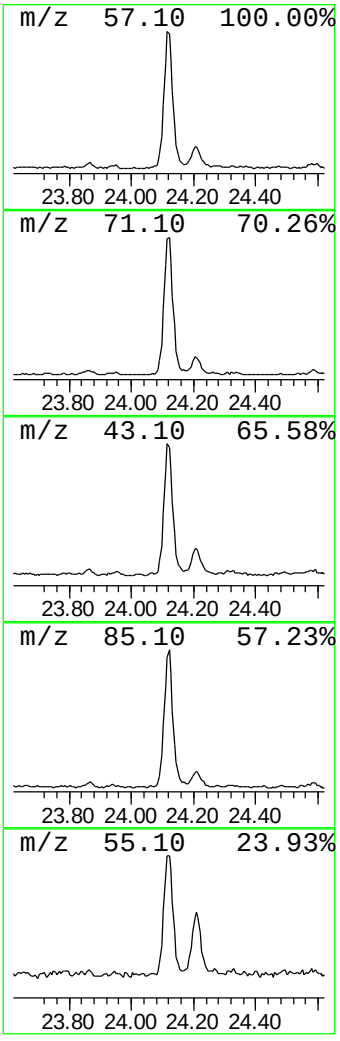
Peak Number 7 Hexadecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.12	6.76 ng	1086480	Perylene-d12	23.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	96
2	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	94
3	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	93
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	91





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Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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

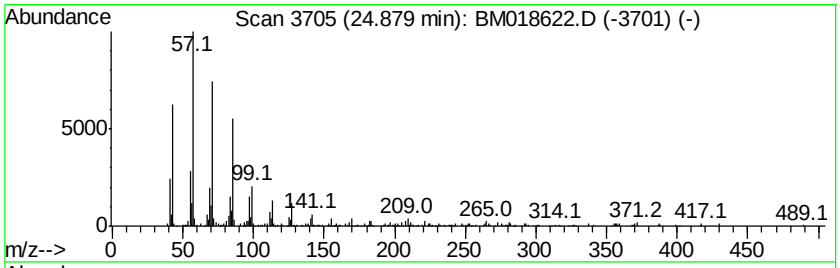
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

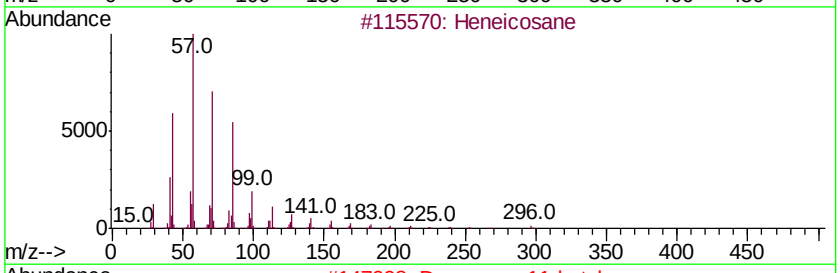
****

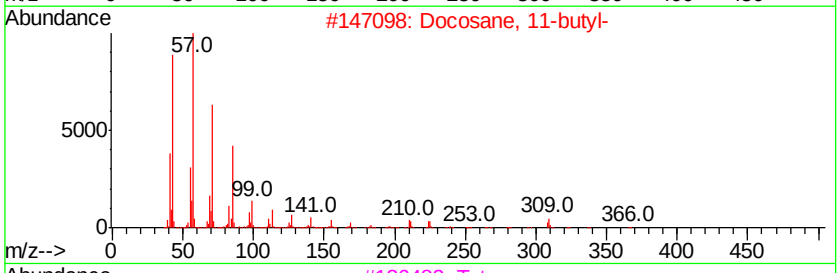
Peak Number 8 Heneicosane Concentration Rank 6

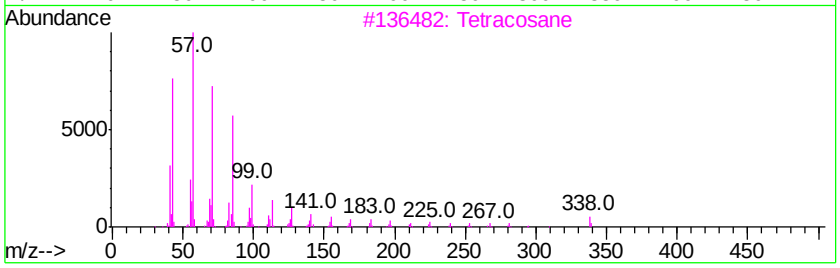
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.88	3.79 ng	609091	Perylene-d12	23.60

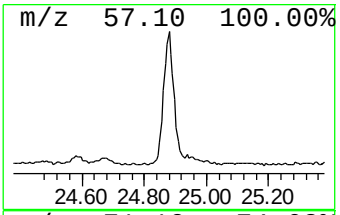
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90

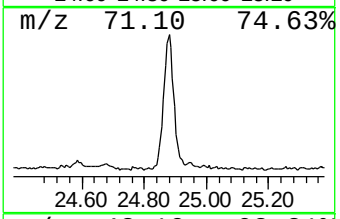


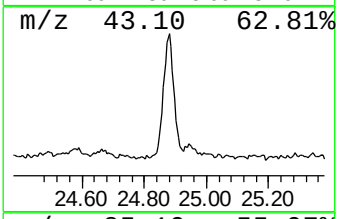


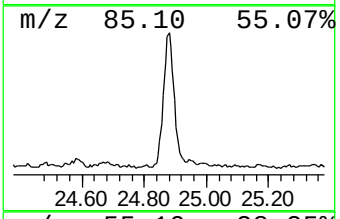


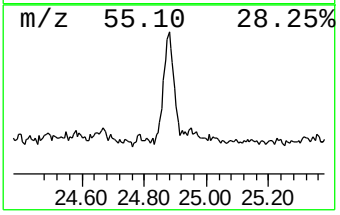












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011719\
Data File : BM018622.D
Acq On : 17 Jan 2019 19:58
Operator : JU/SJ
Sample : K1153-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR200044-RBR200027

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...	4.88	3.6	ng	404996	1	7.74	2277100	20.0
unknown7.27	7.27	83.2	ng	9474730	1	7.74	2277100	20.0
n-Hexadecanoic acid	18.03	5.3	ng	1260430	4	17.14	4803820	20.0
Heptafluorobutano...	21.03	7.1	ng	1642870	5	21.33	4633720	20.0
Eicosane	22.37	2.1	ng	490373	5	21.33	4633720	20.0
Hexadecane, 1-iodo-	24.12	6.8	ng	1086480	6	23.60	3212890	20.0
Heneicosane	24.88	3.8	ng	609091	6	23.60	3212890	20.0