LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011519\
Data File : BM018571.D
Acq On : 15 Jan 2019 21:17
Operator : JU/SJ
Sample : K1128-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR-200053

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	4.893	302	307	320	rVB	235708	363356	1.92%	0.332%
2	5.346	377	384	396	rBV	5270160	7872815	41.52%	7.203%
3	6.928	645	653	672	rBV	5268709	8736687	46.07%	7.993%
4	7.287	707	714	727	rBV	5724016	9098211	47.98%	8.324%
5	7.751	786	793	799	rBV	1026197	1610801	8.49%	1.474%
6	8.069	840	847	856	rVB	4361977	6833250	36.04%	6.251%
7	8.922	983	992	1004	rBV	3174891	5371516	28.33%	4.914%
8	10.539	1260	1267	1281	rBV	1230600	2109081	11.12%	1.930%
9	13.016	1681	1688	1708	rBV	8194179	11945966	63.00%	10.929%
10	13.857	1825	1831	1842	rBV	1804036	2569328	13.55%	2.351%
11	14.398	1916	1923	1932	rBV2	1839212	2816676	14.85%	2.577%
12	15.898	2170	2178	2198	rBV	7235202	10812015	57.02%	9.891%
13	17.151	2384	2391	2396	rBV	2547238	3560536	18.78%	3.257%
14	18.033	2536	2541	2553	rBV2	320848	581962	3.07%	0.532%
15	19.209	2732	2741	2747	rBV	258267	373026	1.97%	0.341%
16	19.321	2755	2760	2770	rBV3	115136	217519	1.15%	0.199%
17	19.580	2800	2804	2811	rVB2	265270	402200	2.12%	0.368%
18	19.780	2832	2838	2846	rBV	15460887	18961894	100.00%	17.347%
19	20.574	2969	2973	2977	rBV	230176	258009	1.36%	0.236%
20	21.039	3048	3052	3061	rBV	581915	702745	3.71%	0.643%
21	21.339	3097	3103	3108	rBV	4033631	5123966	27.02%	4.688%
22	21.474	3123	3126	3132	rBV	426158	452066	2.38%	0.414%
23	21.915	3197	3201	3208	rBV	472561	596407	3.15%	0.546%
24	22.386	3277	3281	3288	rBV	532355	692844	3.65%	0.634%
25	22.897	3364	3368	3372	rBV	490410	721971	3.81%	0.661%
26	23.474	3462	3466	3471	rBV	421726	687951	3.63%	0.629%
27	23.621	3484	3491	3504	rVB	2660019	5129457	27.05%	4.693%
28	24.133	3574	3578	3587	rVB	379505	704146	3.71%	0.644%

Sum of corrected areas: 109306401

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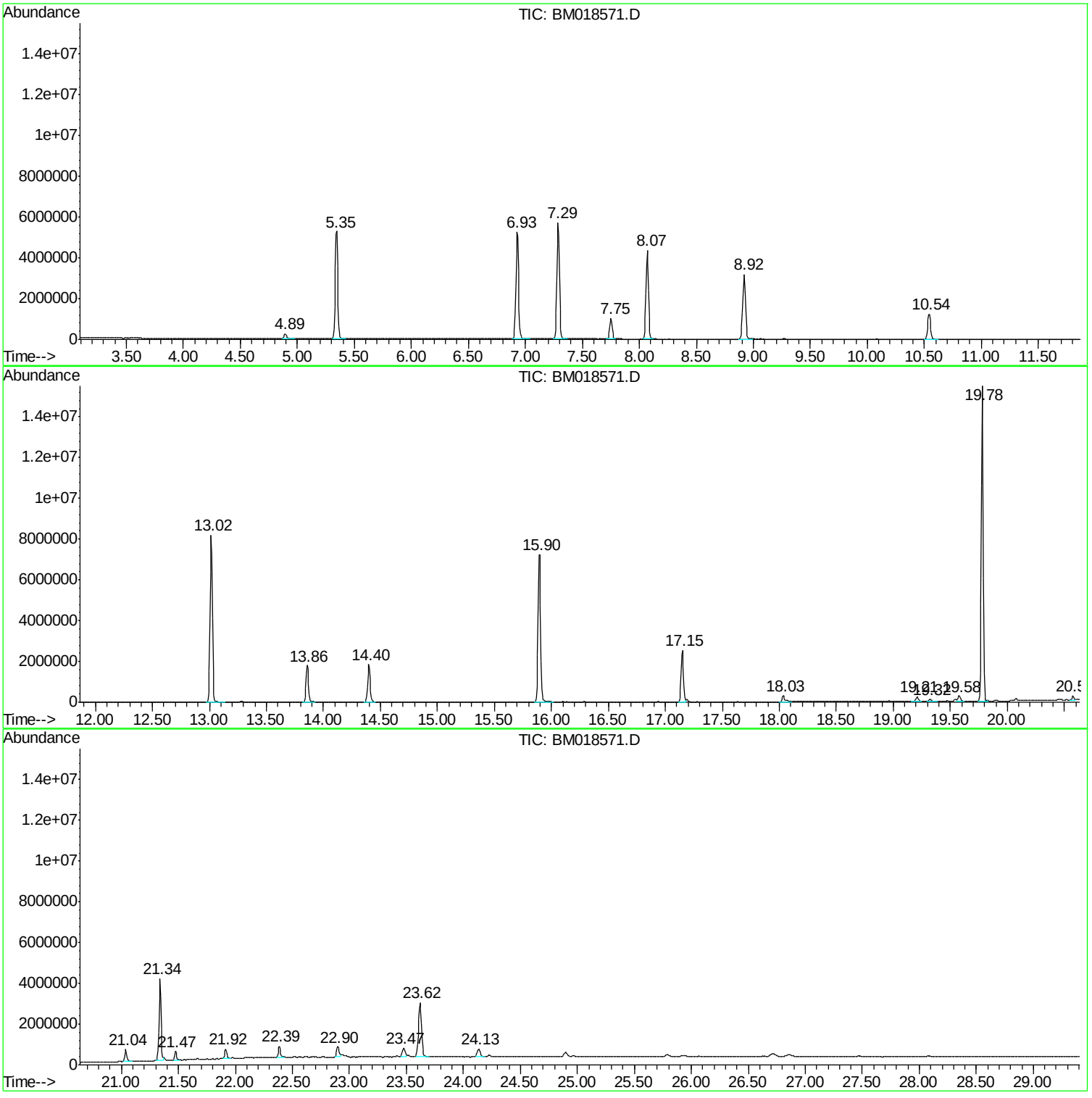
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200053

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

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Data File : BM018571.D
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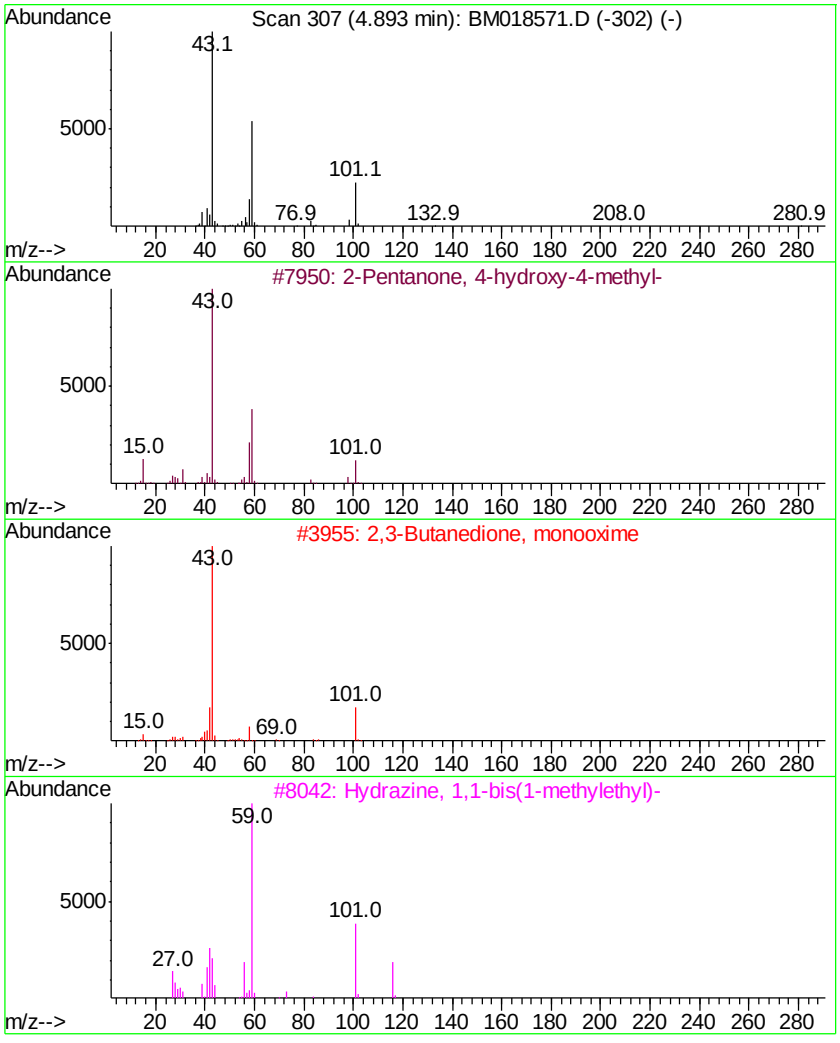
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

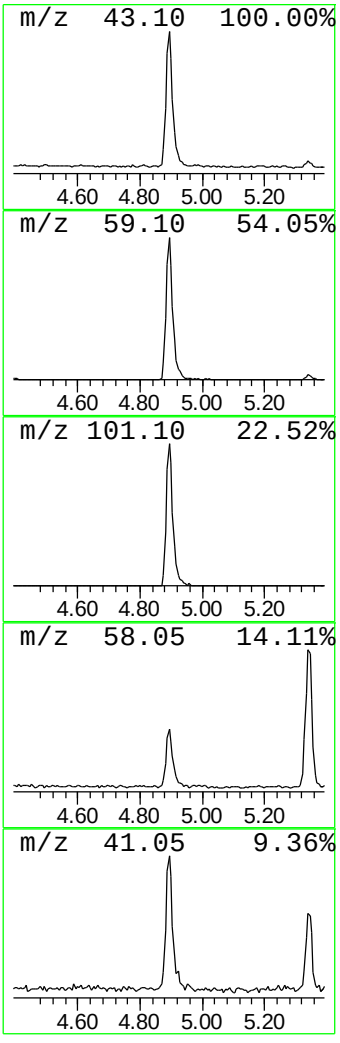
****

Peak Number 1 unknown4.89 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	4.51 ng	363356	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	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	17
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





Library Search Compound Report

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Data File : BM018571.D
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Operator : JU/SJ
Sample : K1128-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR-200053

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
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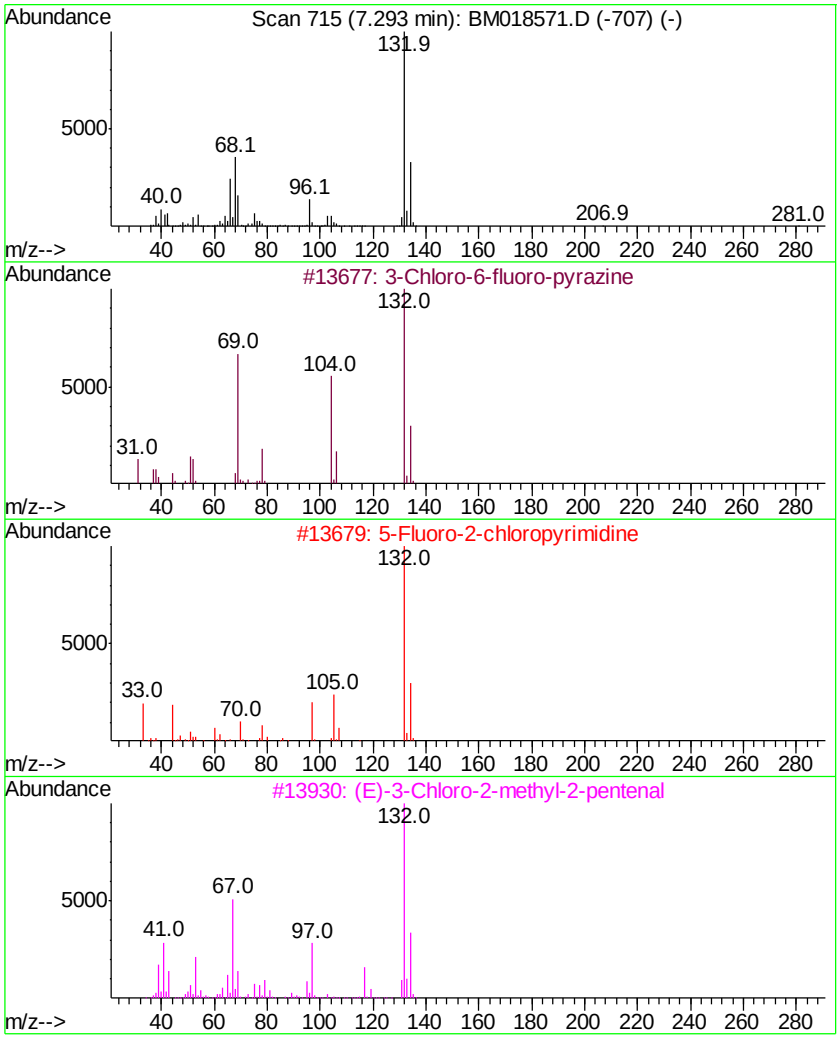
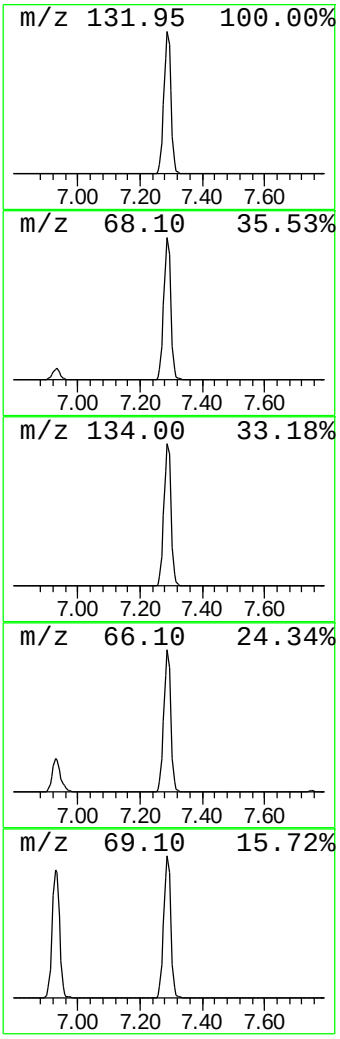
Peak Number 2 unknown7.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	112.97 ng	9098210	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Sample : K1128-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR-200053

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
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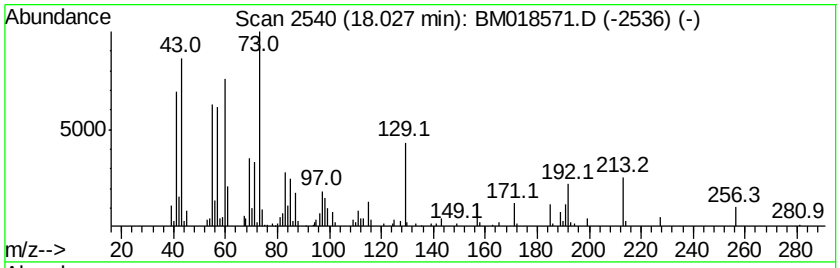
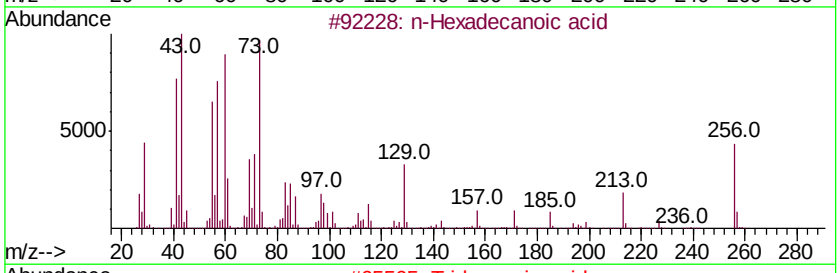
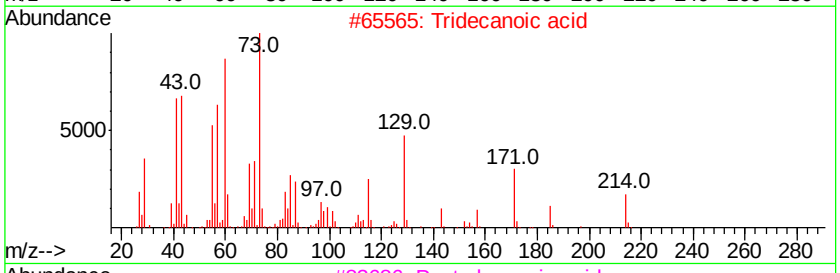
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

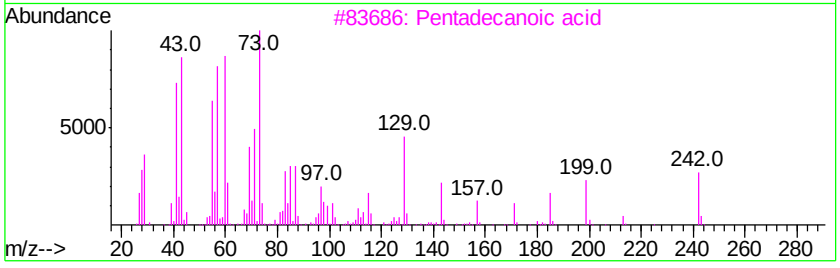
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	3.27 ng	581962	Phenanthrene-d10	17.15

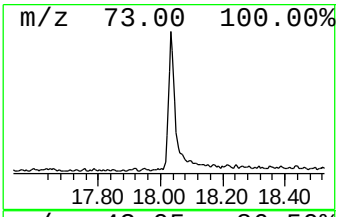
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53

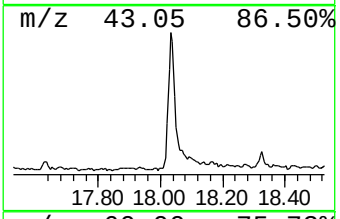


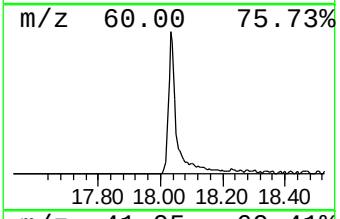


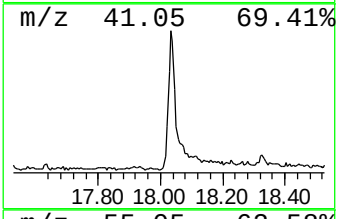


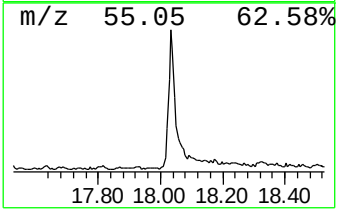












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011519\
Data File : BM018571.D
Acq On : 15 Jan 2019 21:17
Operator : JU/SJ
Sample : K1128-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR-200053

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

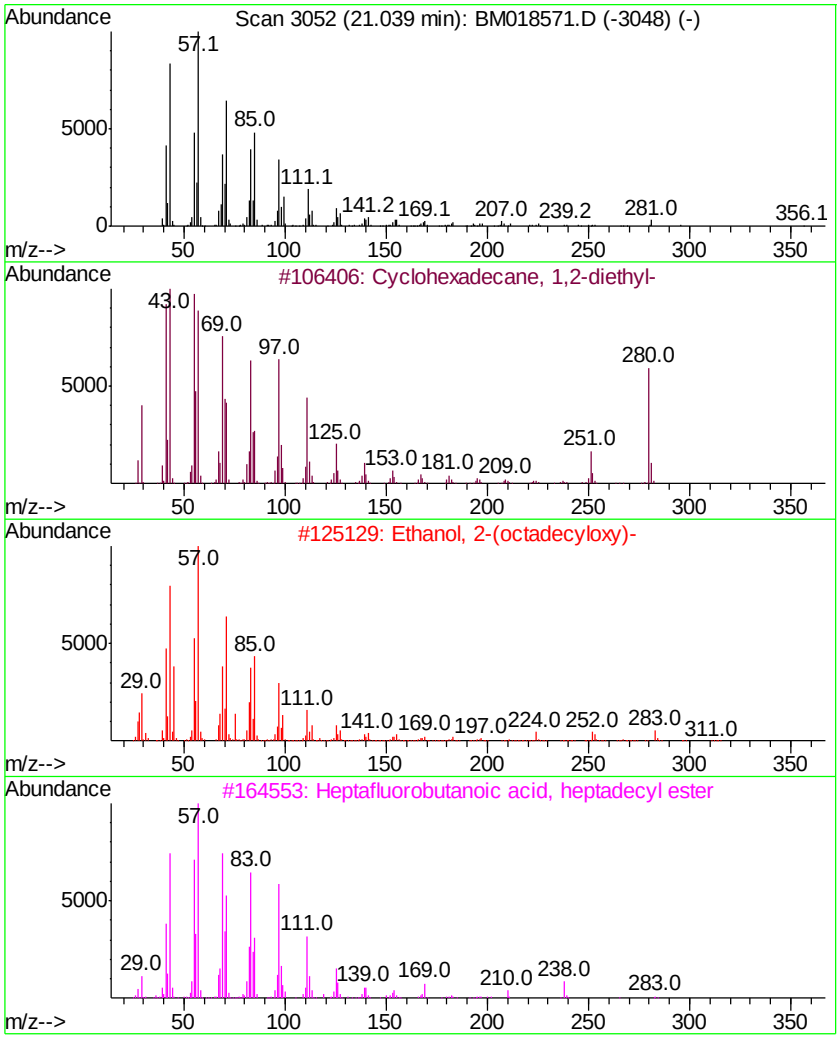
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

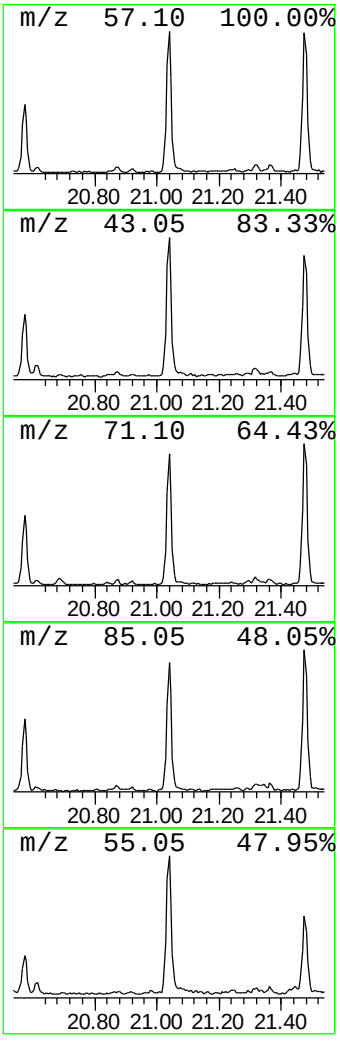
****

Peak Number 6 Cyclohexadecane, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	2.74 ng	702745	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
2	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	87
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	70
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	70
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	70





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Sample : K1128-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR-200053

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
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TIC Library : C:\DATABASE\NIST02.L
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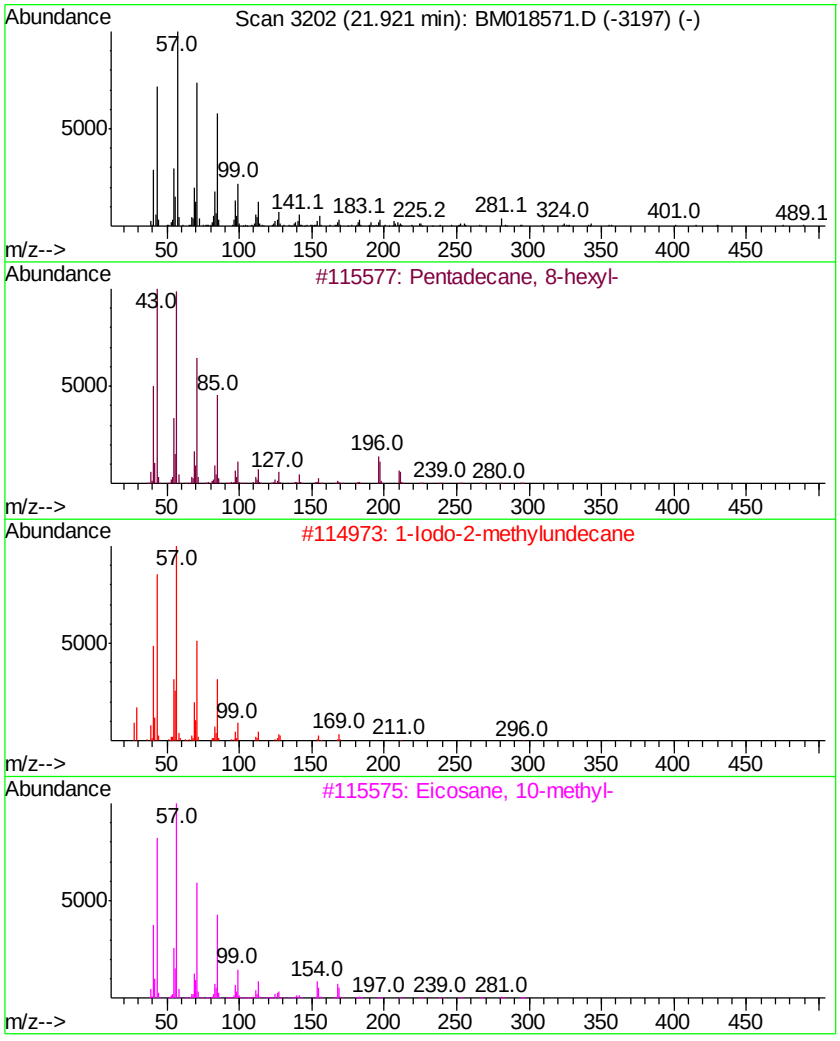
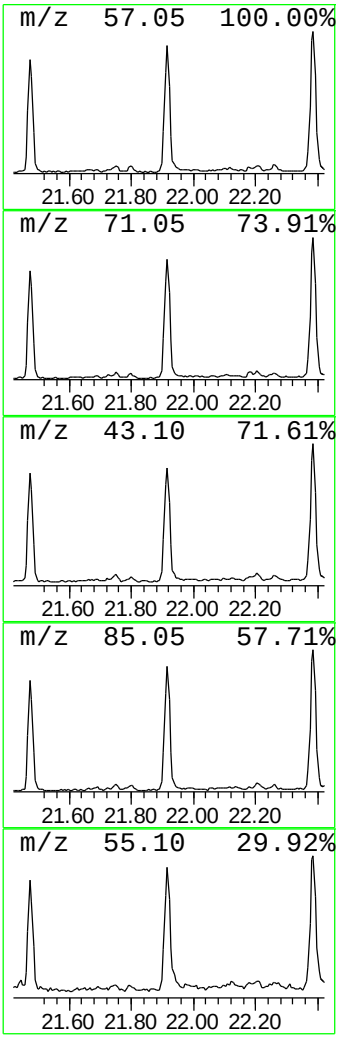
****

Peak Number 7 Pentadecane, 8-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.92	2.33 ng	596407	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	93
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





Library Search Compound Report

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Sample : K1128-01
Misc :
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Instrument : BNA_M
ClientSampleId : RBR-200053

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.M
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TIC Library : C:\DATABASE\NIST02.L
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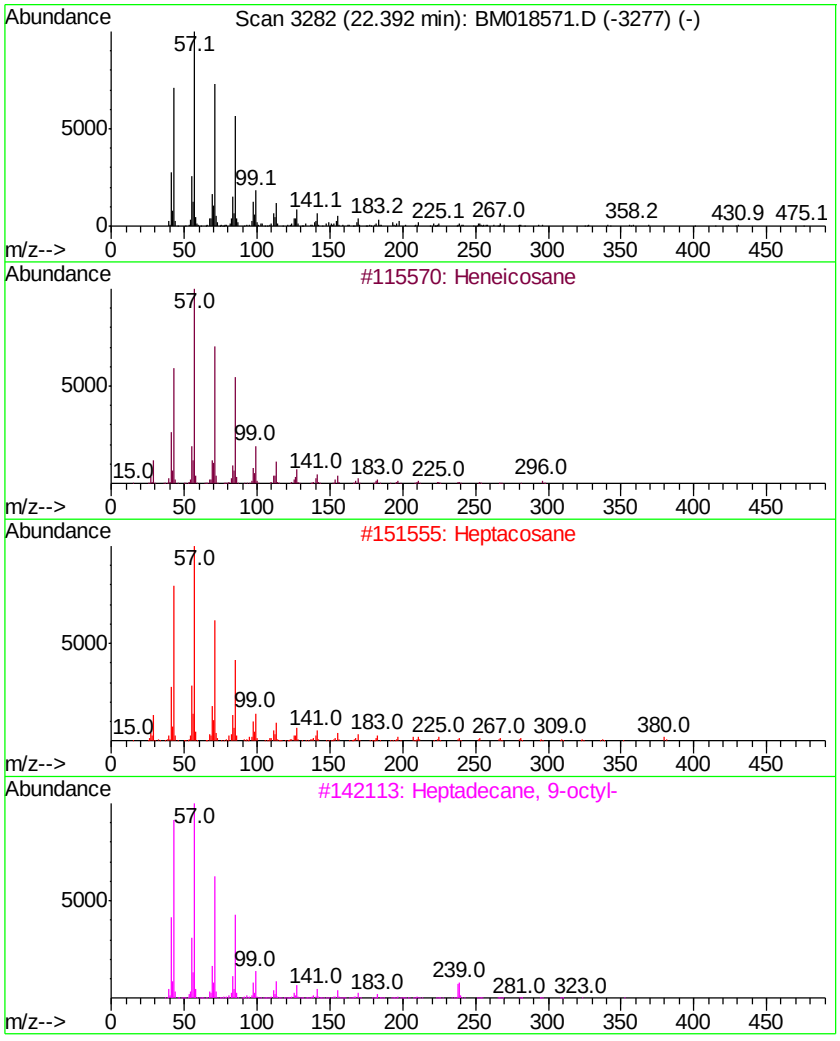
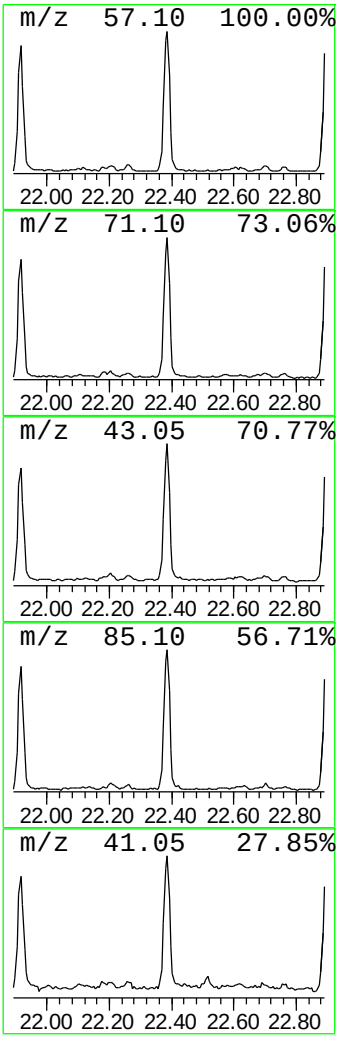
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	2.70 ng	692844	Chrysene-d12	21.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
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	Triacontane	422	C30H62	000638-68-6	91





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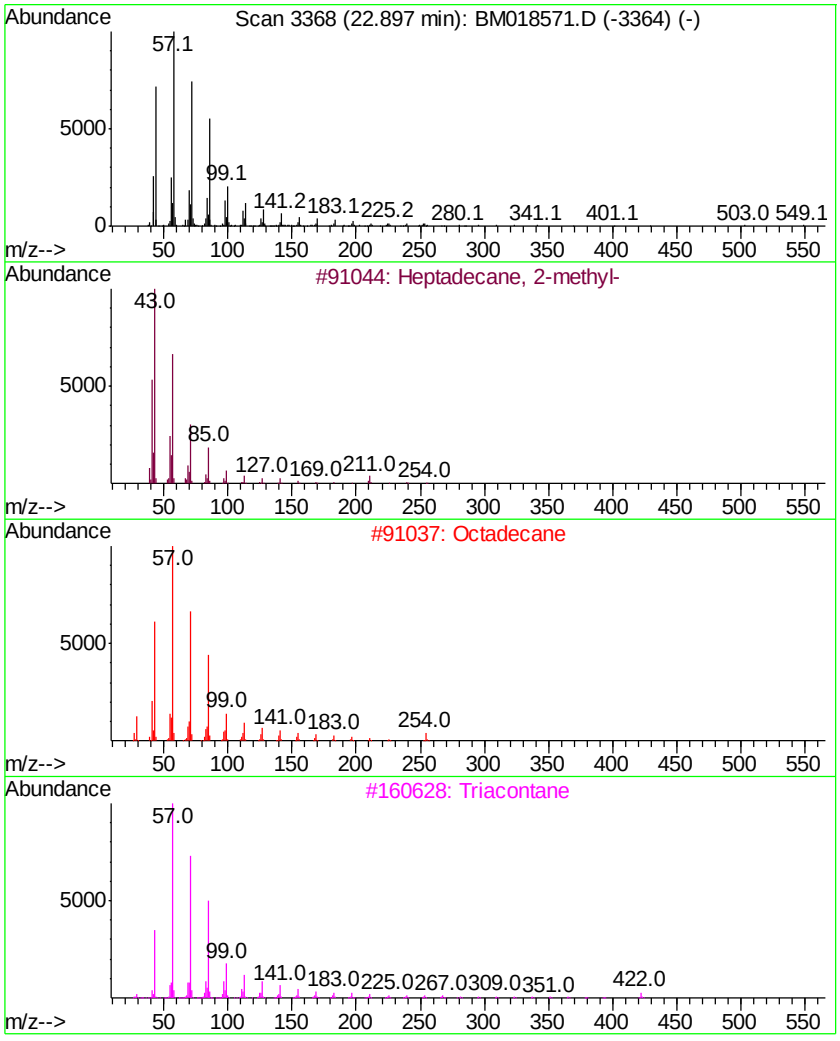
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

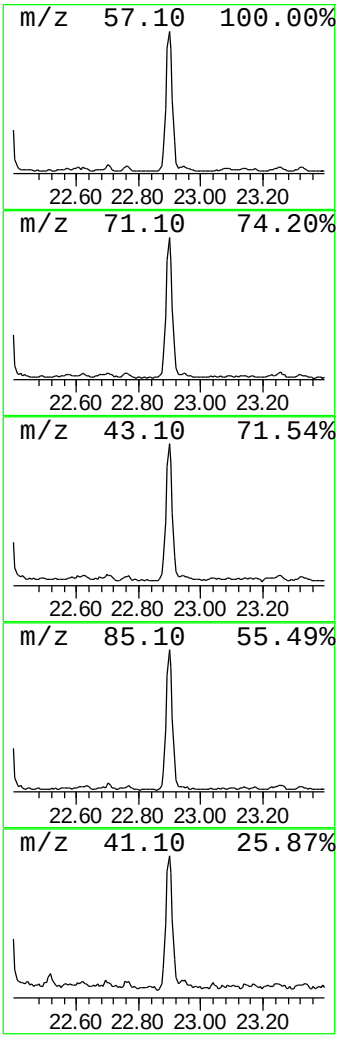
****

Peak Number 9 Heptadecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.90	2.82 ng	721971	Perylene-d12	23.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	94
2	Octadecane	254	C18H38	000593-45-3	93
3	Triacontane	422	C30H62	000638-68-6	91
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
5	Heneicosane	296	C21H44	000629-94-7	91





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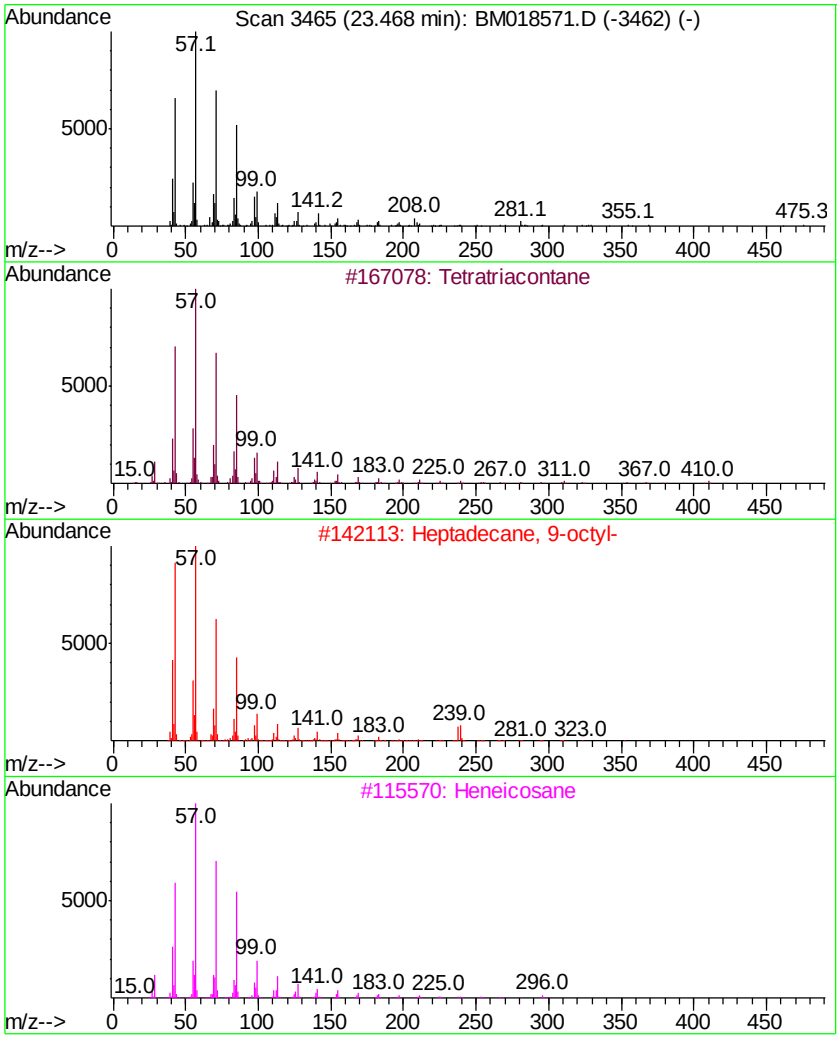
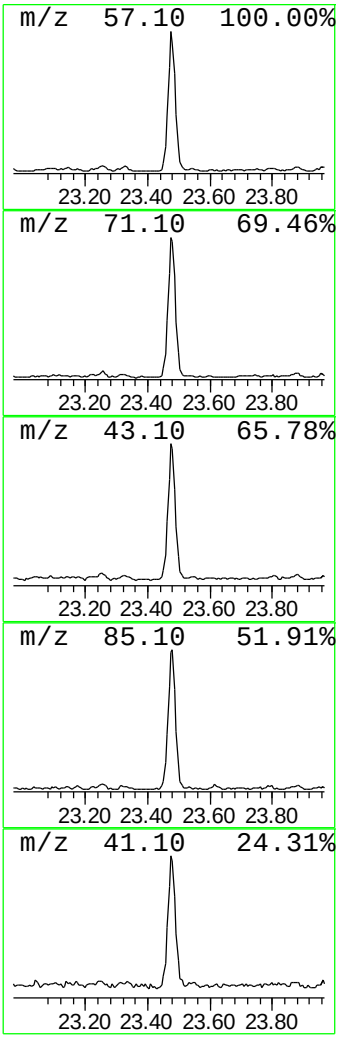
****

Peak Number 10 Tetratriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.47	2.68 ng	687951	Perylene-d12	23.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane	479	C34H70	014167-59-0	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011519\
Data File : BM018571.D
Acq On : 15 Jan 2019 21:17
Operator : JU/SJ
Sample : K1128-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR-200053

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

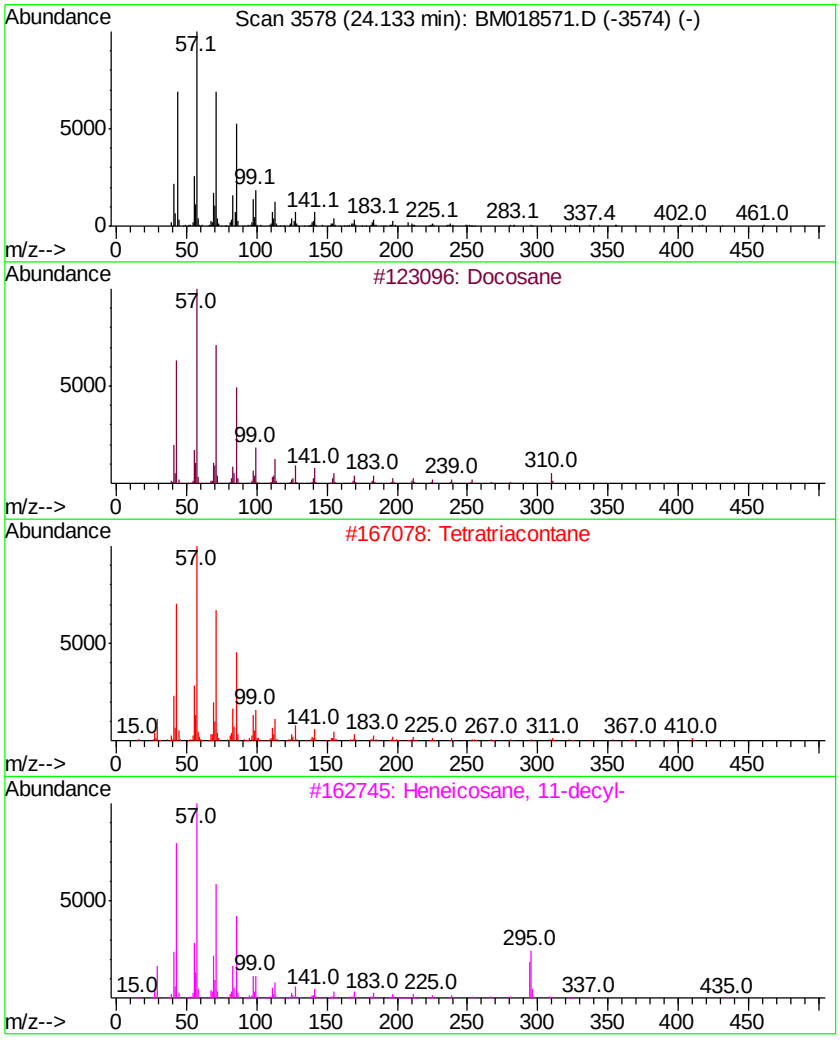
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

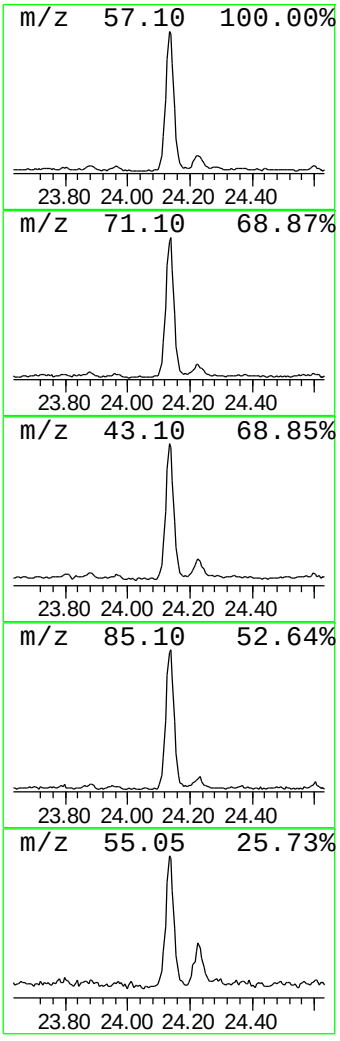
****

Peak Number 11 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.13	2.75 ng	704146	Perylene-d12	23.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Tetratriacontane	479	C34H70	014167-59-0	90
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011519\
Data File : BM018571.D
Acq On : 15 Jan 2019 21:17
Operator : JU/SJ
Sample : K1128-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RBR-200053

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
unknown4.89	4.89	4.5	ng	363356	1	7.75	1610800	20.0
unknown7.29	7.29	113.0	ng	9098210	1	7.75	1610800	20.0
n-Hexadecanoic acid	18.03	3.3	ng	581962	4	17.15	3560540	20.0
Cyclohexadecane, ...	21.04	2.7	ng	702745	5	21.34	5123970	20.0
Pentadecane, 8-he...	21.92	2.3	ng	596407	5	21.34	5123970	20.0
Heneicosane	22.39	2.7	ng	692844	5	21.34	5123970	20.0
Heptadecane, 2-me...	22.90	2.8	ng	721971	6	23.62	5129460	20.0
Tetratriacontane	23.47	2.7	ng	687951	6	23.62	5129460	20.0
Docosane	24.13	2.8	ng	704146	6	23.62	5129460	20.0