LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099797.D
Acq On : 24 Oct 2017 19:28
Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	5.028	496	500	517	rBV	193250	313632	14.42%	1.801%
2	5.428	565	568	592	rBV	1822235	1894819	87.13%	10.881%
3	6.451	737	742	759	rBV	1808186	1901416	87.44%	10.918%
4	6.581	759	764	767	rBV	2057608	1993362	91.67%	11.446%
5	6.804	799	802	811	rBV	590833	489776	22.52%	2.812%
6	6.957	824	828	845	rBB	1624604	1556825	71.59%	8.940%
7	7.375	895	899	902	rBV	1299206	1145574	52.68%	6.578%
8	8.086	1016	1020	1037	rBV	824808	657775	30.25%	3.777%
9	8.645	1112	1115	1122	rBB	27618	24404	1.12%	0.140%
10	9.163	1198	1203	1206	rBV	2476458	2174593	100.00%	12.487%
11	9.557	1267	1270	1276	rBV	43666	33945	1.56%	0.195%
12	9.839	1315	1318	1329	rVB2	729176	652241	29.99%	3.745%
13	10.557	1436	1440	1445	rVB	81903	67903	3.12%	0.390%
14	10.633	1450	1453	1464	rBV	1004266	950399	43.70%	5.457%
15	11.333	1568	1572	1581	rBV	615367	515194	23.69%	2.958%
16	11.851	1655	1660	1668	rBV2	30282	42665	1.96%	0.245%
17	12.915	1837	1841	1844	rBV	1543104	1320107	60.71%	7.580%
18	13.792	1986	1990	2000	rBV	89931	111621	5.13%	0.641%
19	13.980	2018	2022	2028	rBV	522181	441464	20.30%	2.535%
20	15.051	2200	2204	2209	rBV	34342	37561	1.73%	0.216%
21	15.421	2263	2267	2268	rBV	56166	61320	2.82%	0.352%
22	15.451	2268	2272	2278	rVB	336311	436259	20.06%	2.505%
23	15.845	2334	2339	2344	rBV	69309	93240	4.29%	0.535%
24	16.333	2416	2422	2435	rVB3	69514	133590	6.14%	0.767%
25	16.909	2512	2520	2527	rBV	56795	127131	5.85%	0.730%
26	17.586	2627	2635	2643	rBV3	47372	114918	5.28%	0.660%
27	18.392	2764	2772	2779	rBV4	24775	67234	3.09%	0.386%
28	19.350	2928	2935	2943	rBV3	19536	55667	2.56%	0.320%

Sum of corrected areas: 17414635

LSC Report - Integrated Chromatogram

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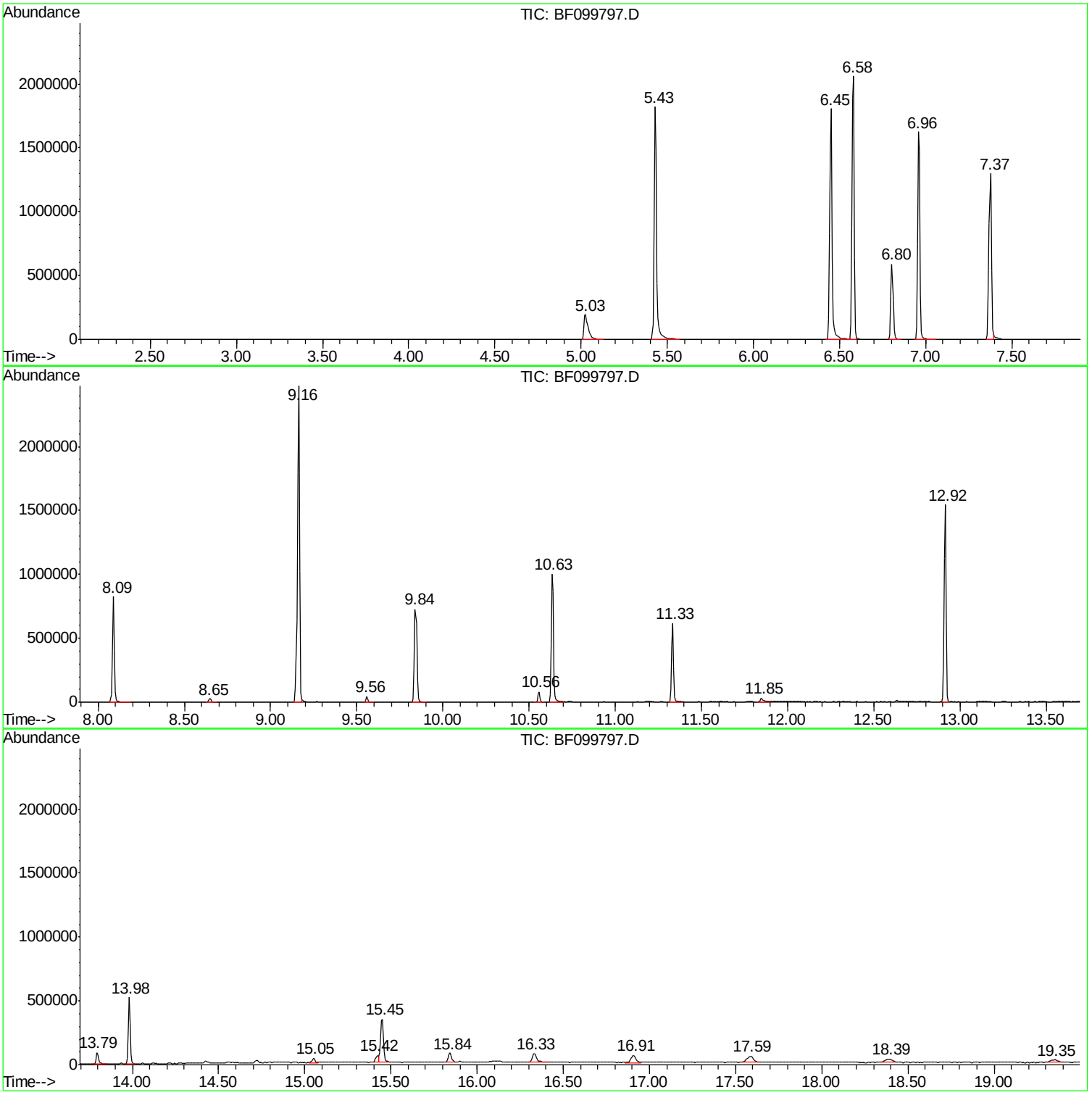
Data File : BF099797.D
Acq On : 24 Oct 2017 19:28
Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099797.D
Acq On : 24 Oct 2017 19:28
Operator : SJ/JU
Sample : I5956-01
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ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

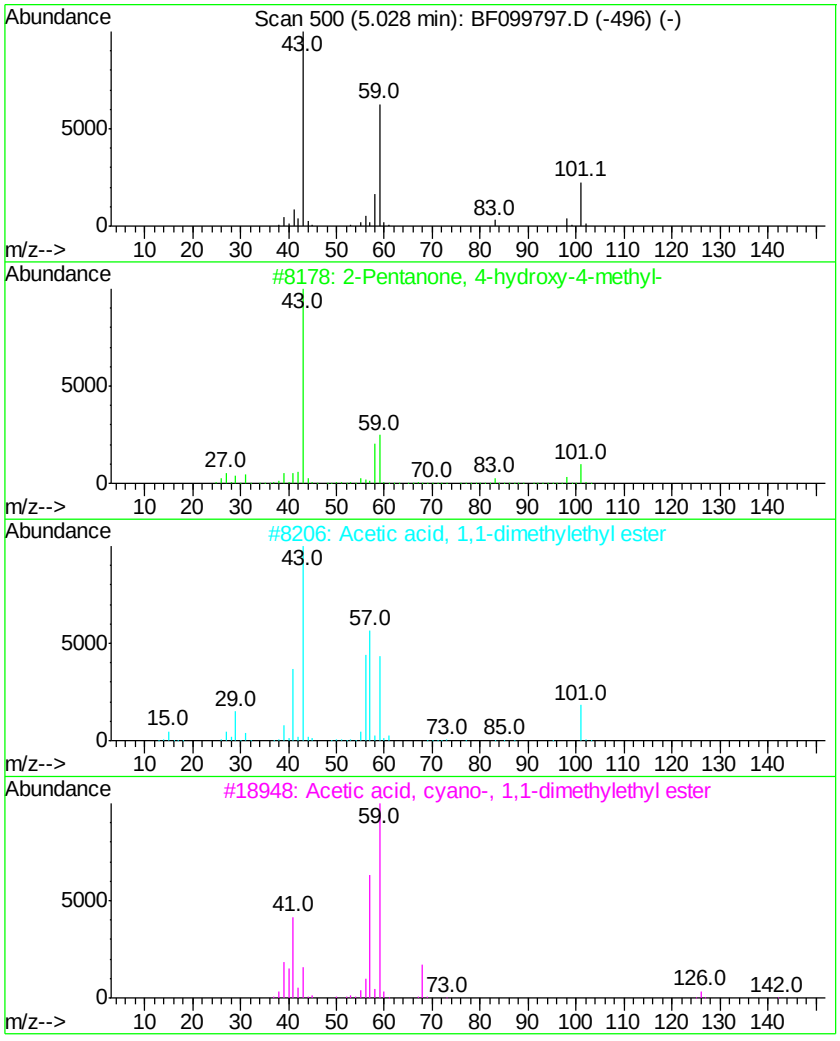
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

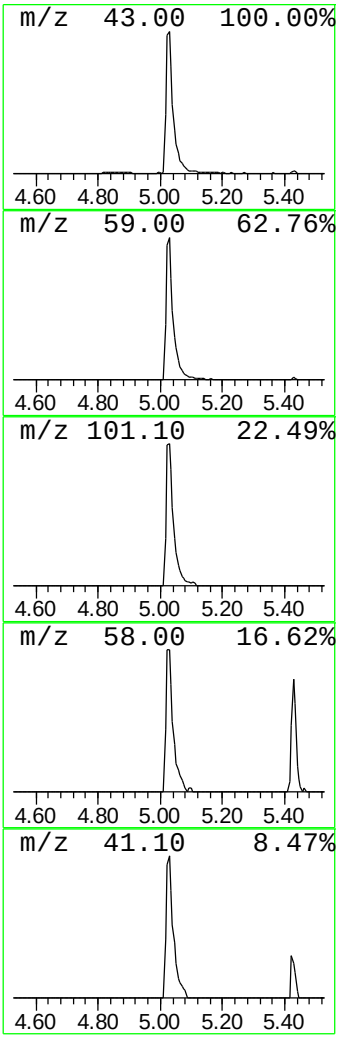
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	12.81 ng	313632	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF099797.D
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Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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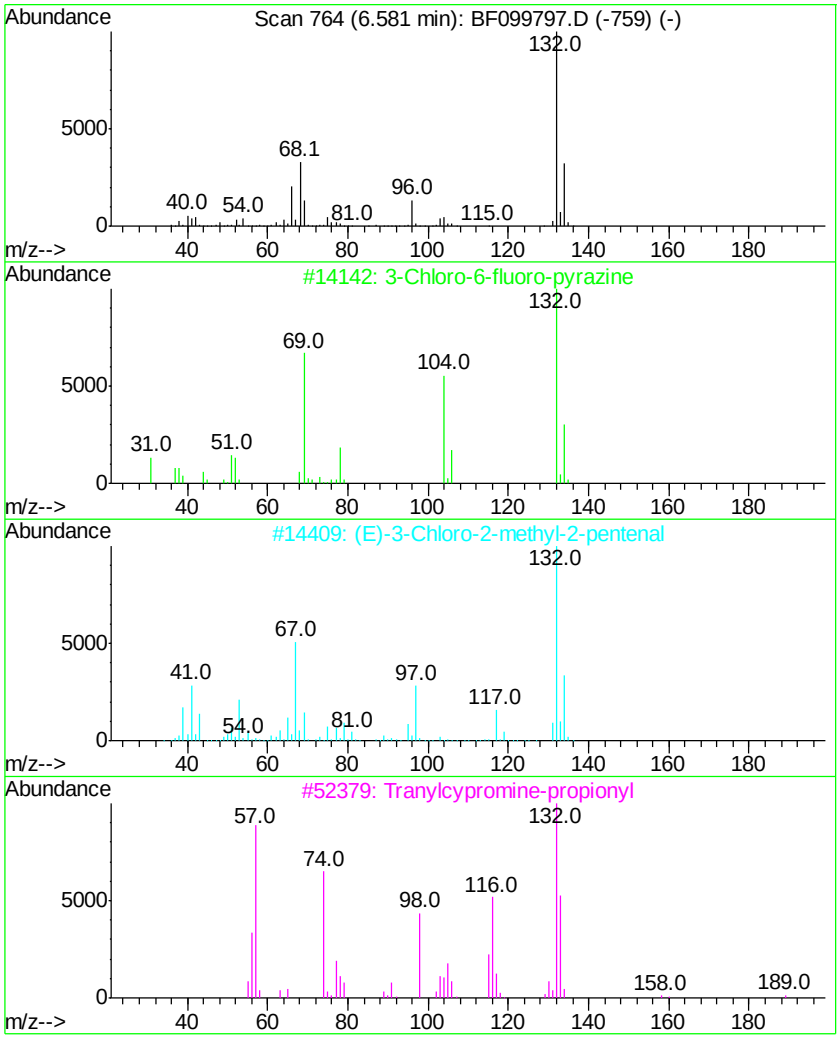
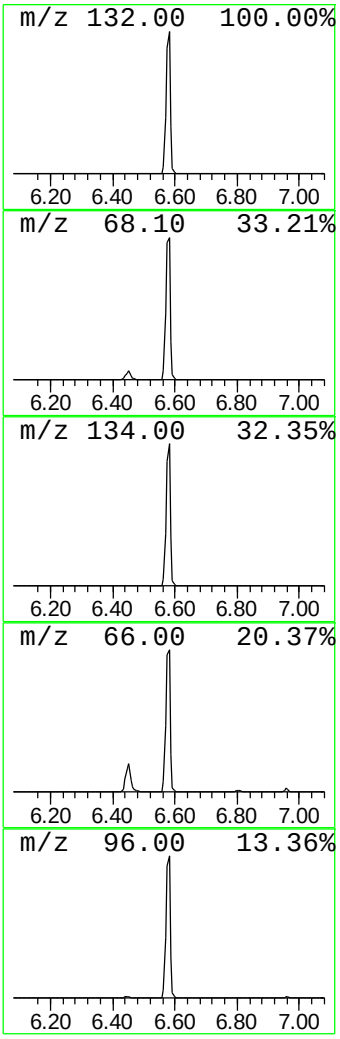
Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	81.40 ng	1993360	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099797.D
Acq On : 24 Oct 2017 19:28
Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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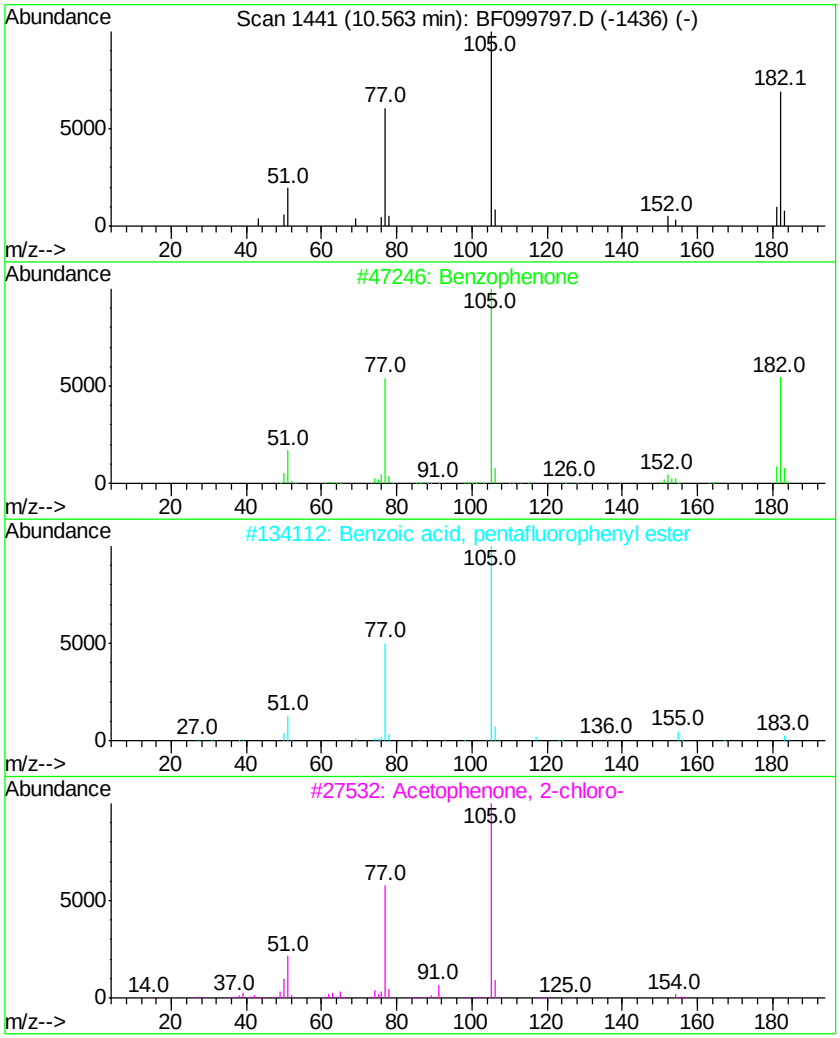
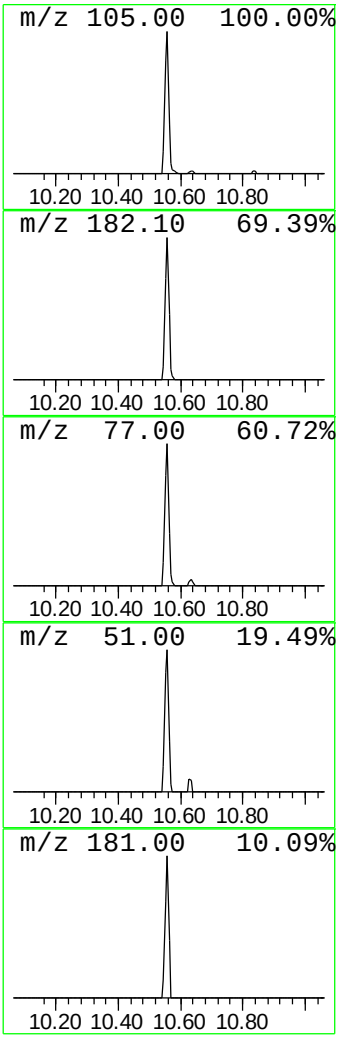
Peak Number 4 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.08 ng	67903	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4	Vinyl benzoate	148	C9H8O2	000769-78-8	43
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
Data File : BF099797.D
Acq On : 24 Oct 2017 19:28
Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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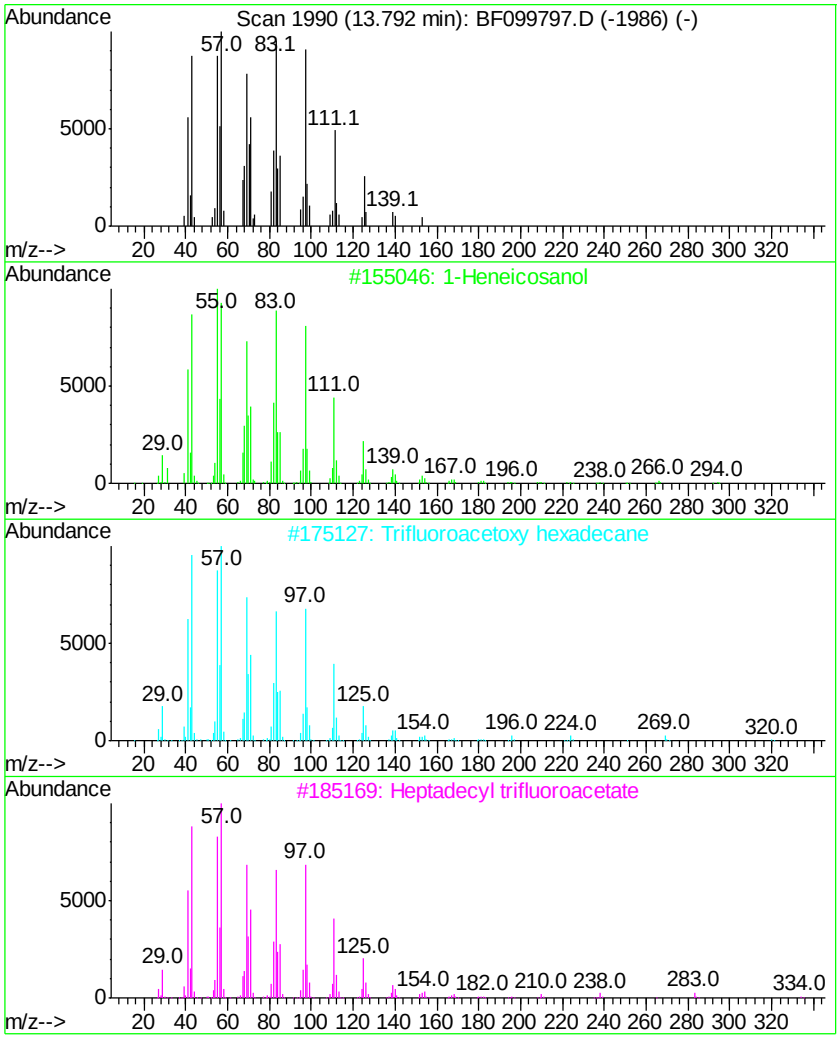
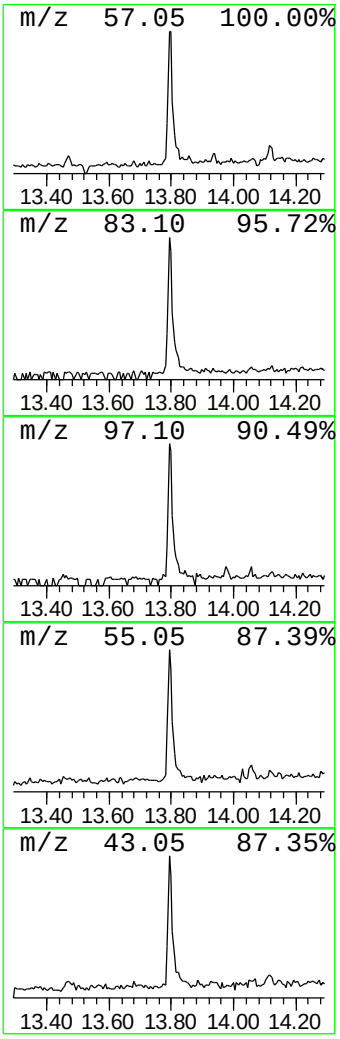
Peak Number 5 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	5.06 ng	111621	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	92
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102417\
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Acq On : 24 Oct 2017 19:28
Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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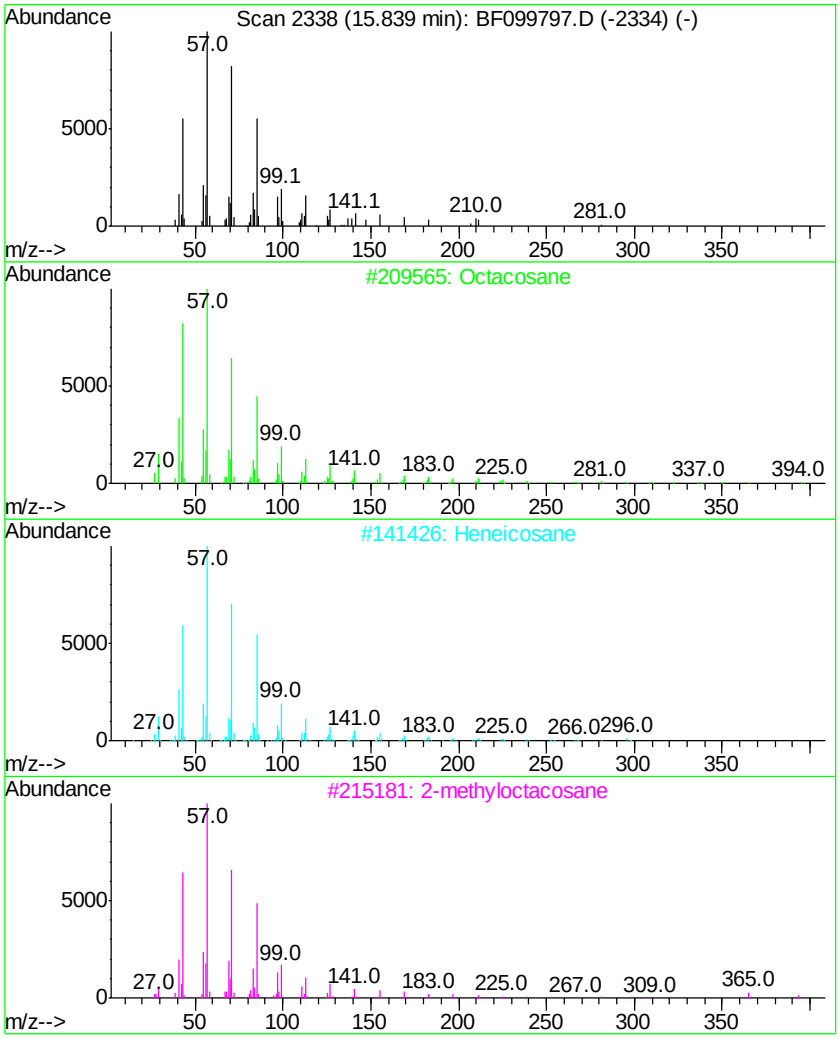
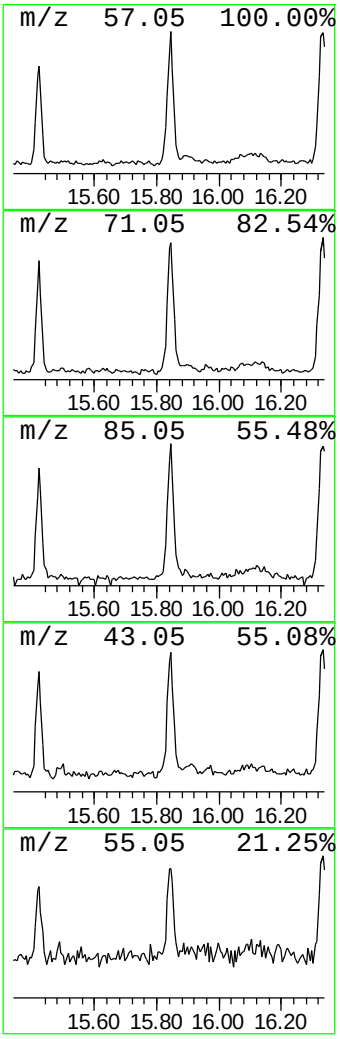
Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	4.27 ng	93240	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Triacontane	422	C30H62	000638-68-6	91





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Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

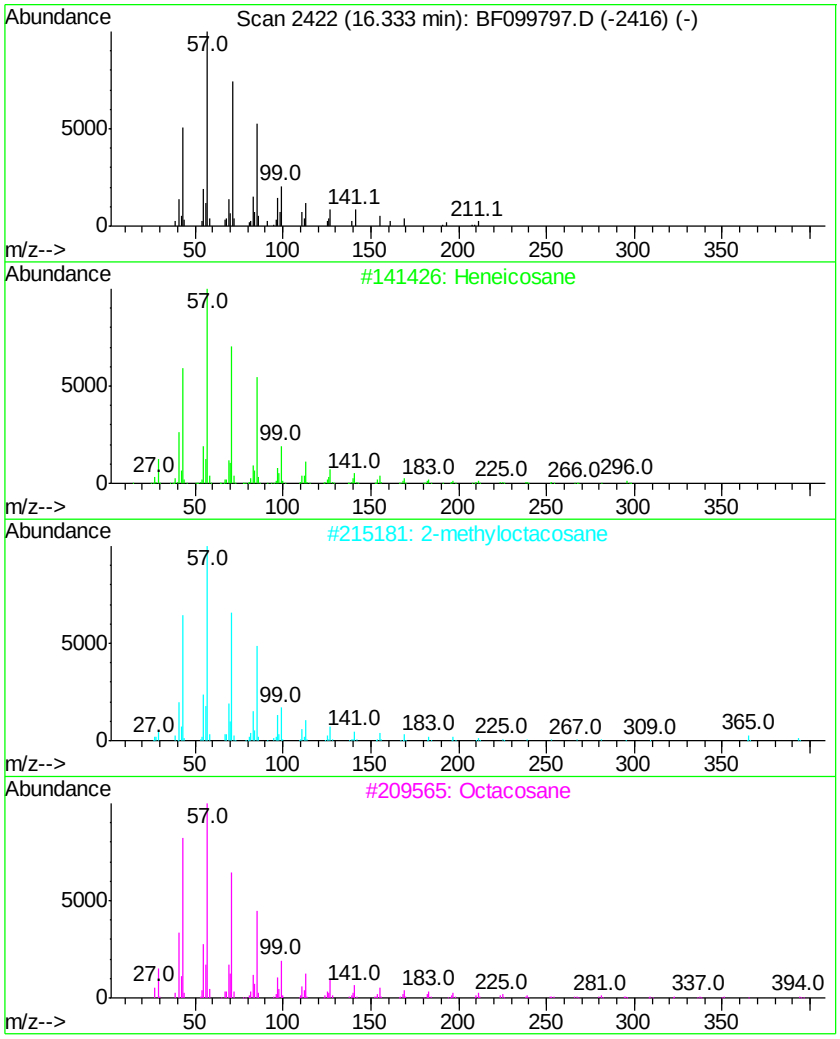
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

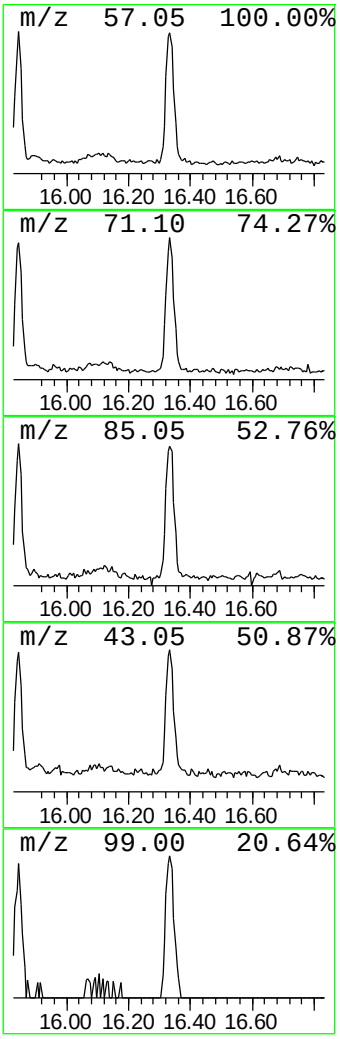
****

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	6.12 ng	133590	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

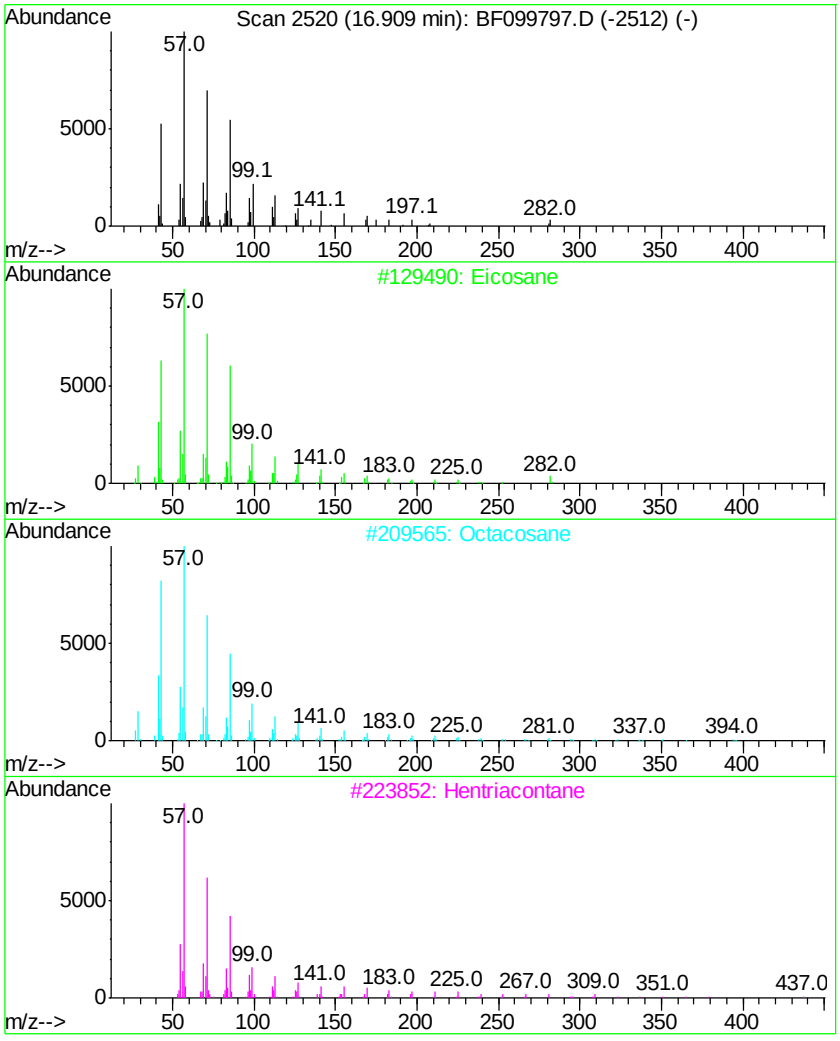
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

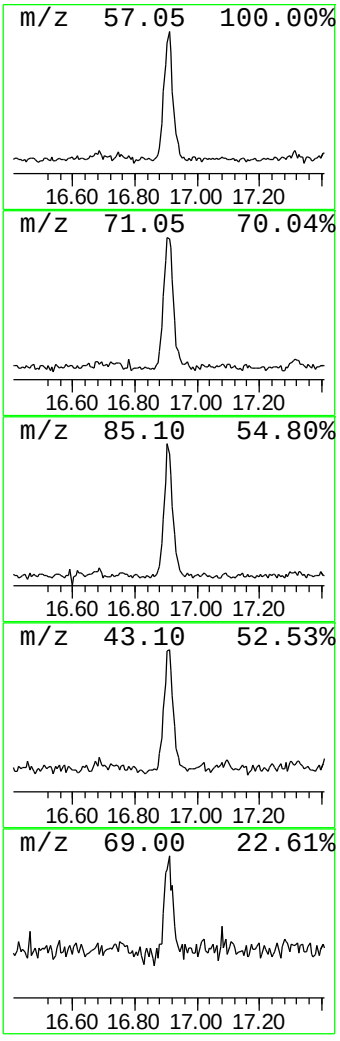
****

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.91	5.83 ng	127131	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Octacosane	394	C28H58	000630-02-4	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Sample : I5956-01
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Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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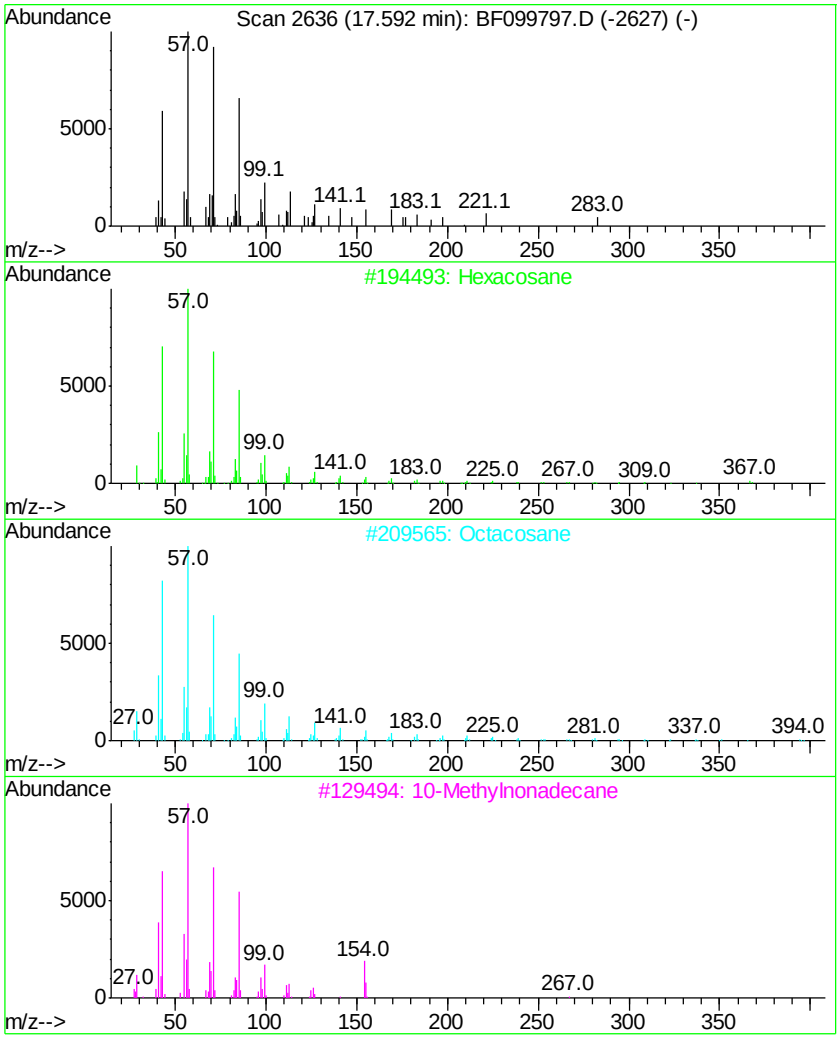
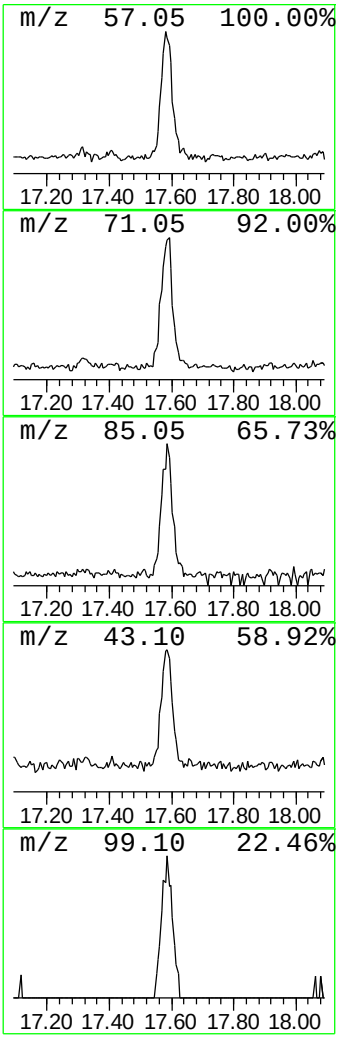
Peak Number 9 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.59	5.27 ng	114918	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	10-Methylnonadecane	282	C20H42	056862-62-5	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Triacontane	422	C30H62	000638-68-6	90





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Acq On : 24 Oct 2017 19:28
Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

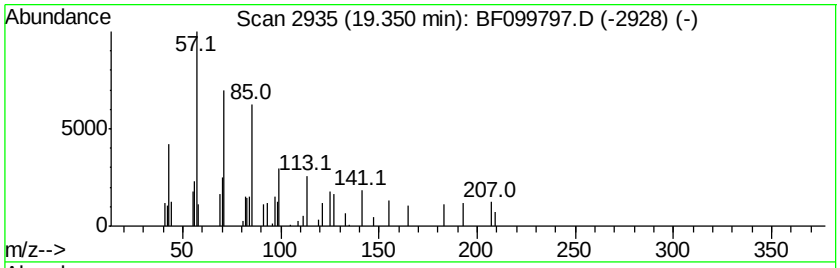
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

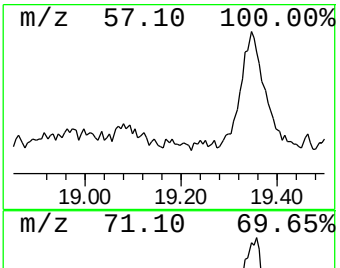
****

Peak Number 11 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	2.55 ng	55667	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	53
2	Tetradecane, 3-methyl-	212	C15H32	018435-22-8	50
3	Hexacosane	366	C26H54	000630-01-3	49
4	Heptadecane	240	C17H36	000629-78-7	47
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102417\
Data File : BF099797.D
Acq On : 24 Oct 2017 19:28
Operator : SJ/JU
Sample : I5956-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-M-6(50-52)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	12.8	ng	313632	1	6.80	489776	20.0
unknown6.58	6.58	81.4	ng	1993360	1	6.80	489776	20.0
Benzophenone	10.56	2.1	ng	67903	3	9.84	652241	20.0
1-Heneicosanol	13.79	5.1	ng	111621	5	13.98	441464	20.0
Octacosane	15.84	4.3	ng	93240	6	15.45	436259	20.0
Heneicosane	16.33	6.1	ng	133590	6	15.45	436259	20.0
Eicosane	16.91	5.8	ng	127131	6	15.45	436259	20.0
Hexacosane	17.59	5.3	ng	114918	6	15.45	436259	20.0
Octadecane	19.35	2.5	ng	55667	6	15.45	436259	20.0