LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100186.D
Acq On : 4 Nov 2017 18:44
Operator : SJ/JU
Sample : I6099-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ERM-P-2

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	4.987	490	493	514	rBV	167105	315316	14.53%	1.680%
2	5.398	560	563	591	rBV	1451338	2061563	95.00%	10.985%
3	6.422	733	737	754	rBV	1836632	2109490	97.21%	11.241%
4	6.539	754	757	776	rVB	2106563	2170004	100.00%	11.563%
5	6.763	792	795	805	rVB	518346	464336	21.40%	2.474%
6	6.916	818	821	847	rVB	1543034	1468775	67.69%	7.827%
7	7.334	889	892	909	rBV	1120183	1234282	56.88%	6.577%
8	8.045	1010	1013	1026	rBV	697849	659174	30.38%	3.513%
9	8.610	1106	1109	1120	rBB	67286	70912	3.27%	0.378%
10	9.116	1191	1195	1198	rBV	2132265	1760911	81.15%	9.383%
11	9.516	1260	1263	1273	rVB	408110	328885	15.16%	1.753%
12	9.798	1307	1311	1319	rVB	805097	743213	34.25%	3.960%
13	10.510	1429	1432	1437	rBV	313148	248303	11.44%	1.323%
14	10.598	1443	1447	1458	rBV	1233166	1311675	60.45%	6.990%
15	11.286	1561	1564	1573	rBV	776198	739671	34.09%	3.941%
16	11.804	1648	1652	1656	rBV	56118	61053	2.81%	0.325%
17	12.868	1829	1833	1836	rBV	1536563	1379942	63.59%	7.353%
18	13.739	1977	1981	1987	rBV3	46768	60239	2.78%	0.321%
19	13.939	2012	2015	2025	rBV	515925	504392	23.24%	2.688%
20	14.368	2084	2088	2092	rBV2	21263	27530	1.27%	0.147%
21	14.539	2111	2117	2122	rBV9	15215	37219	1.72%	0.198%
22	14.604	2124	2128	2129	rBV2	19152	23113	1.07%	0.123%
23	14.662	2136	2138	2145	rVB2	24832	26206	1.21%	0.140%
24	14.980	2189	2192	2196	rBV	42066	42065	1.94%	0.224%
25	15.339	2249	2253	2258	rVV2	52036	65597	3.02%	0.350%
26	15.398	2259	2263	2277	rVB	300192	425001	19.59%	2.265%
27	15.751	2319	2323	2329	rVB	57880	80931	3.73%	0.431%
28	16.227	2399	2404	2410	rBV2	60162	106517	4.91%	0.568%
29	16.786	2493	2499	2507	rVB4	48205	100809	4.65%	0.537%
30	17.439	2604	2610	2618	rBV4	32801	74881	3.45%	0.399%
31	18.215	2736	2742	2753	rVB5	24540	64278	2.96%	0.343%

Sum of corrected areas: 18766283

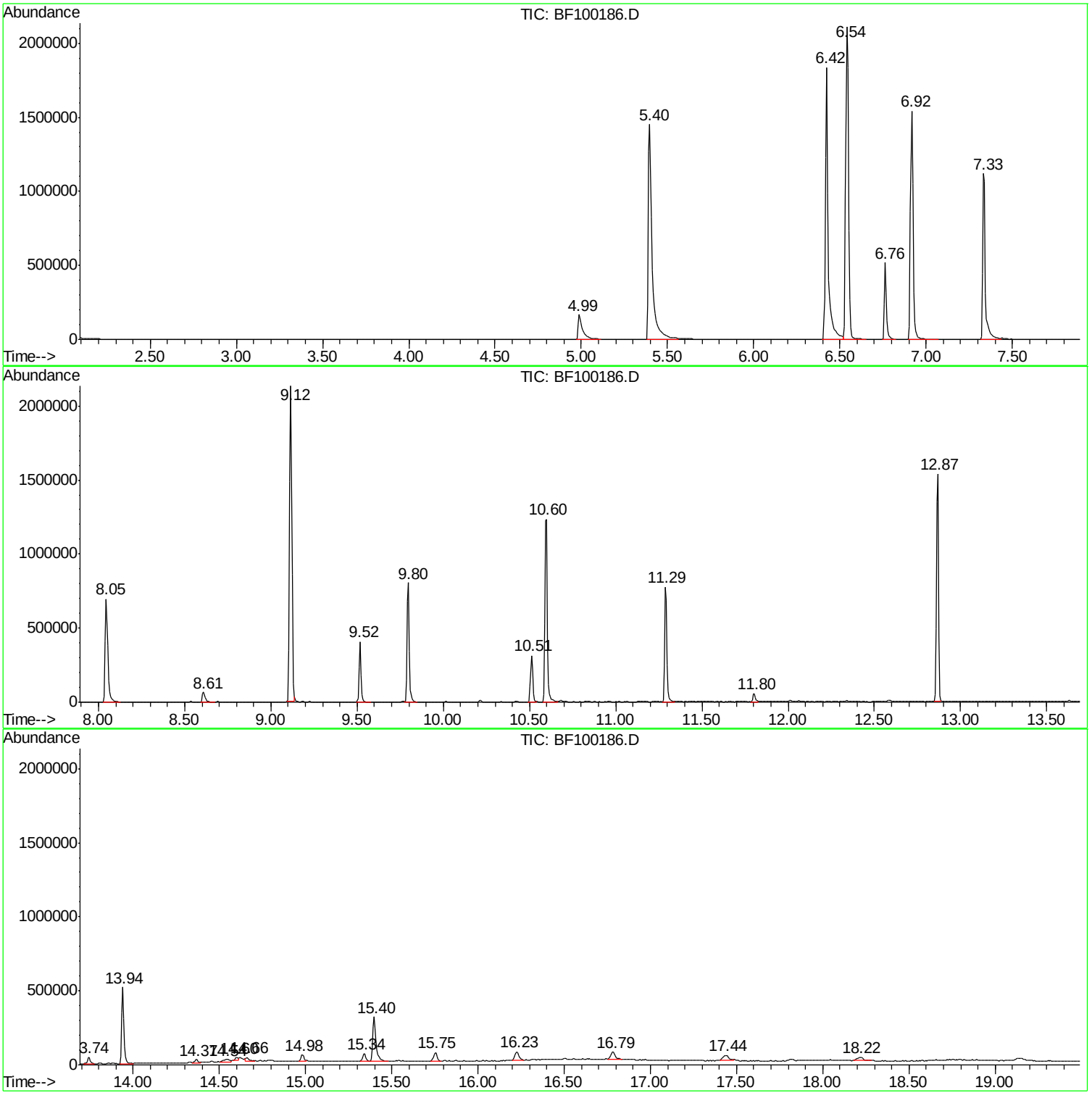
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100186.D
Acq On : 4 Nov 2017 18:44
Operator : SJ/JU
Sample : I6099-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ERM-P-2

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



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110417\
Data File : BF100186.D
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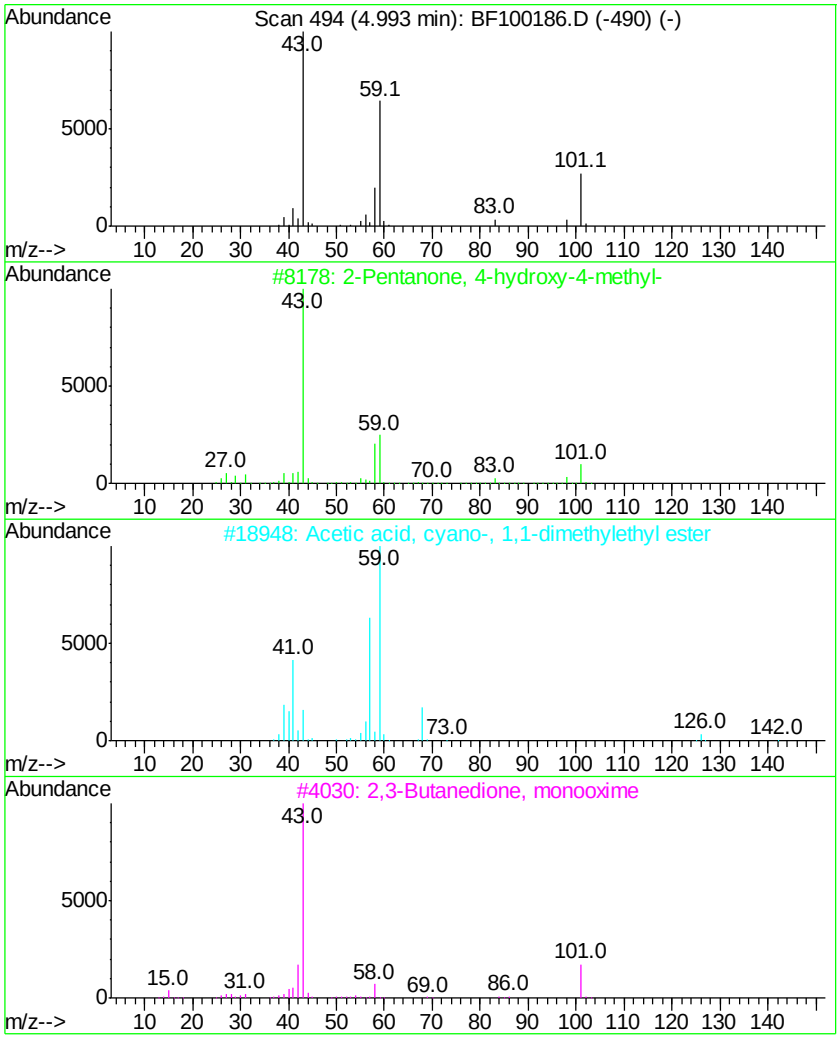
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

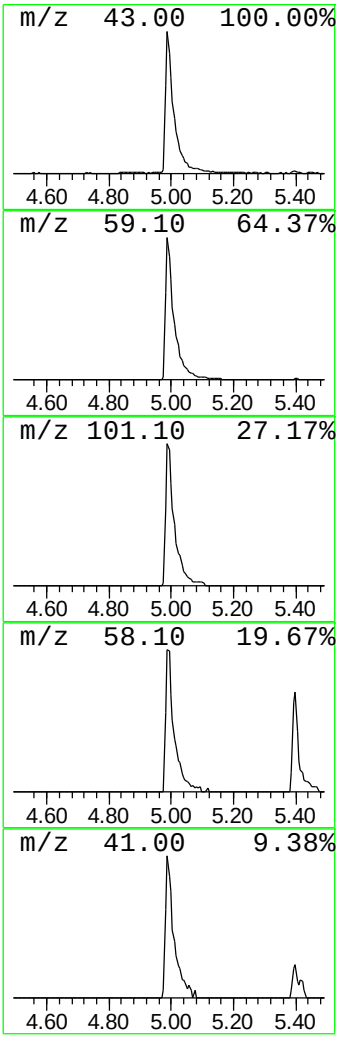
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	13.58 ng	315316	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : ERM-P-2

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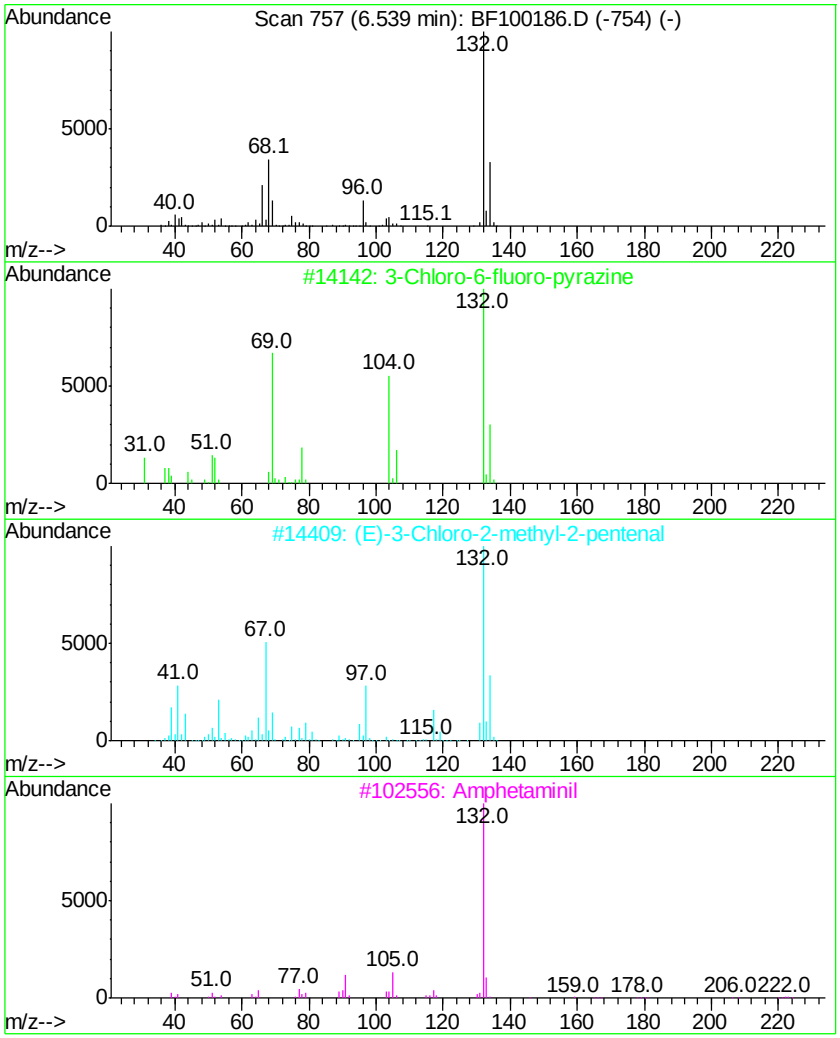
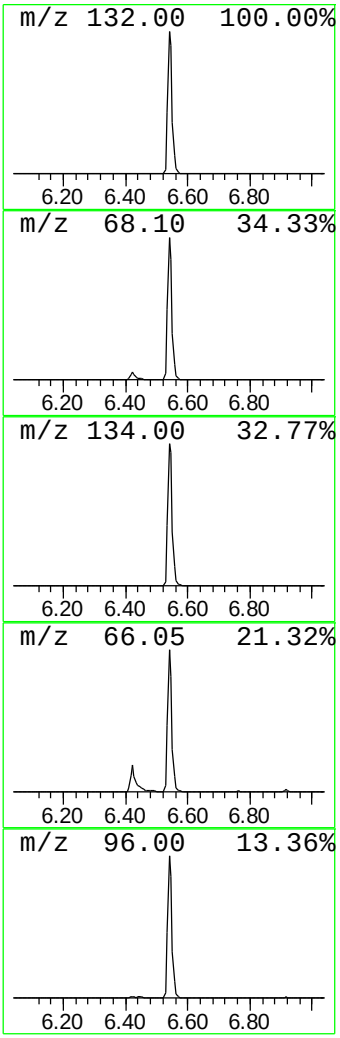
****

Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	93.47 ng	2170000	1,4-Dichlorobenzene-d4	6.76

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	17
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5	1-Aminoindan	133	C9H11N	034698-41-4	9





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ERM-P-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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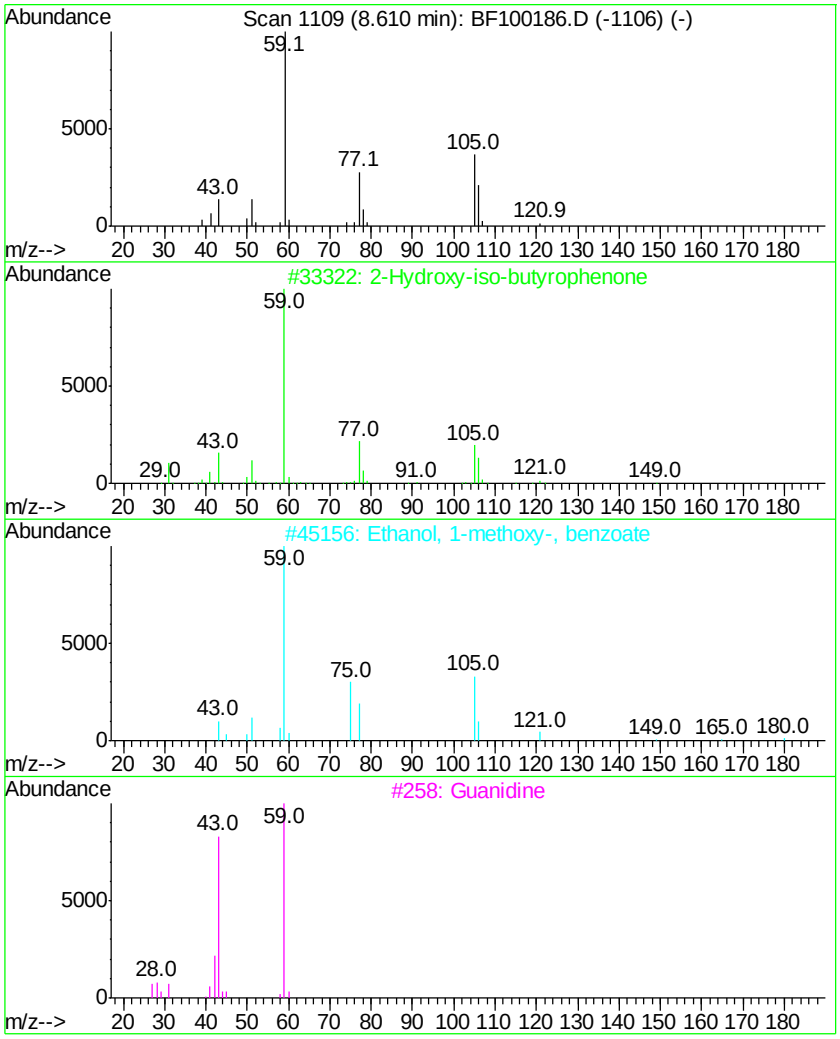
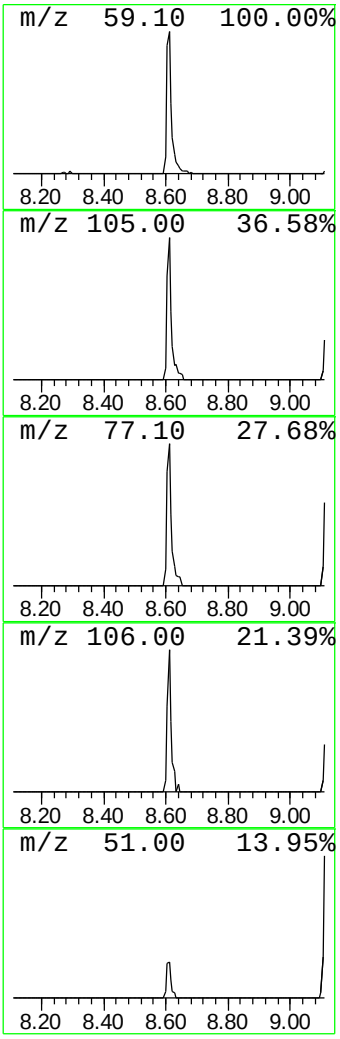
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.61	2.15 ng	70912	Naphthalene-d8	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	45
3	Guanidine	59	CH5N3	000113-00-8	7
4	.alpha.-(Methylthio)acetamide	105	C3H7NOS	022551-24-2	7
5	Acetamide	59	C2H5NO	000060-35-5	5





Library Search Compound Report

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Data File : BF100186.D
Acq On : 4 Nov 2017 18:44
Operator : SJ/JU
Sample : I6099-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ERM-P-2

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

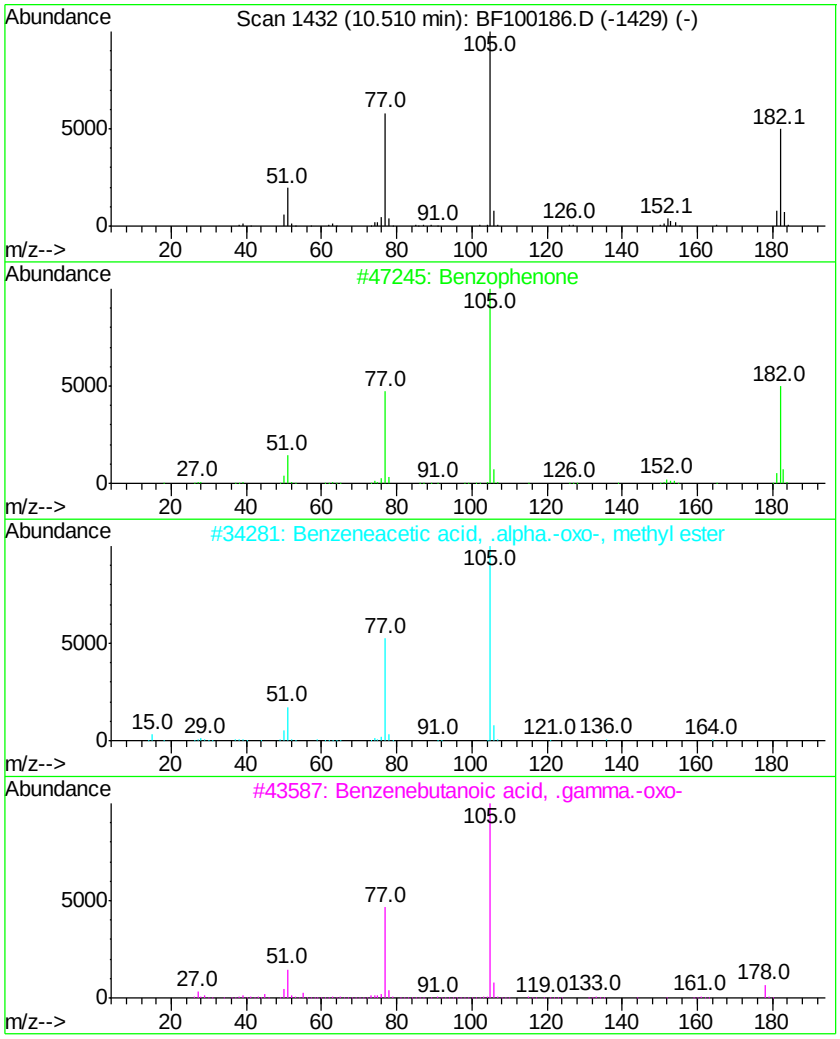
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

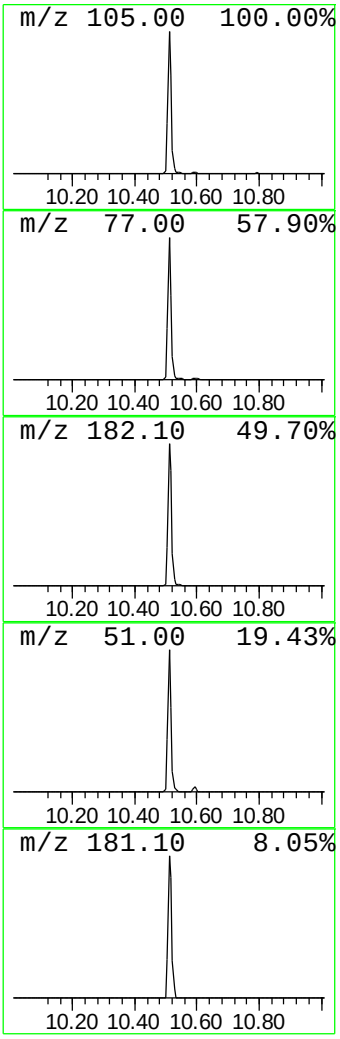
****

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	6.68 ng	248303	Acenaphthene-d10	9.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
3	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
5	Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47





Library Search Compound Report

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Operator : SJ/JU
Sample : I6099-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ERM-P-2

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

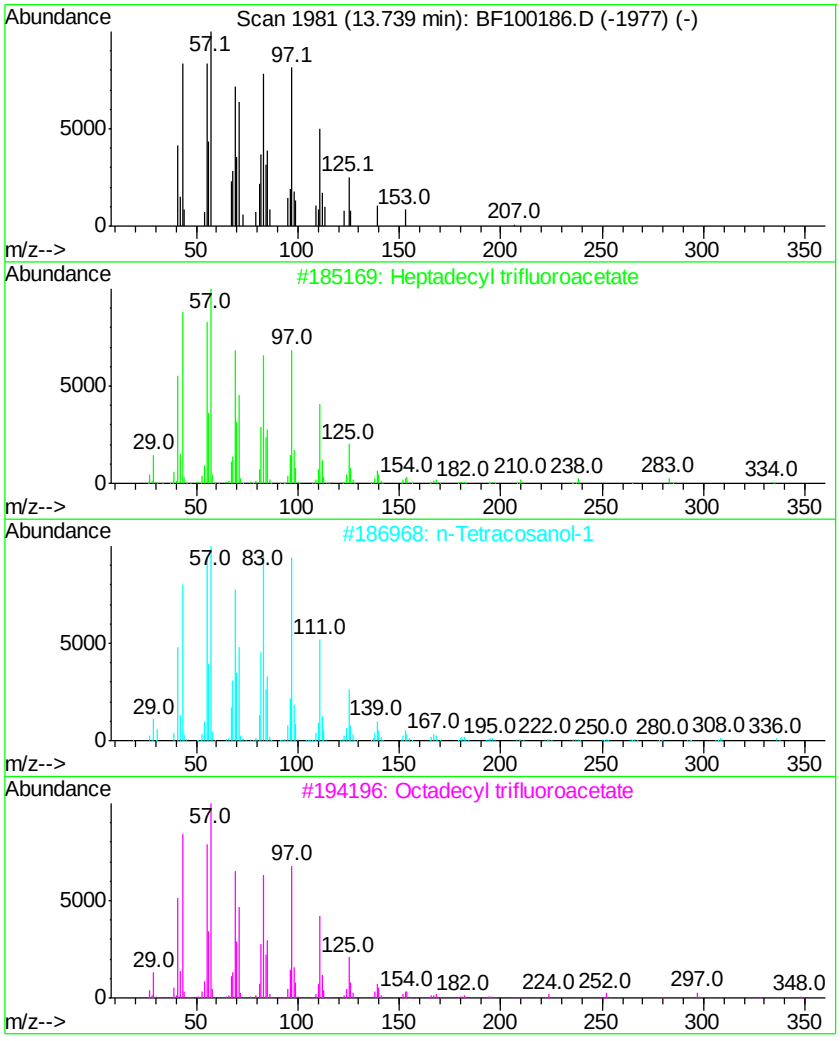
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

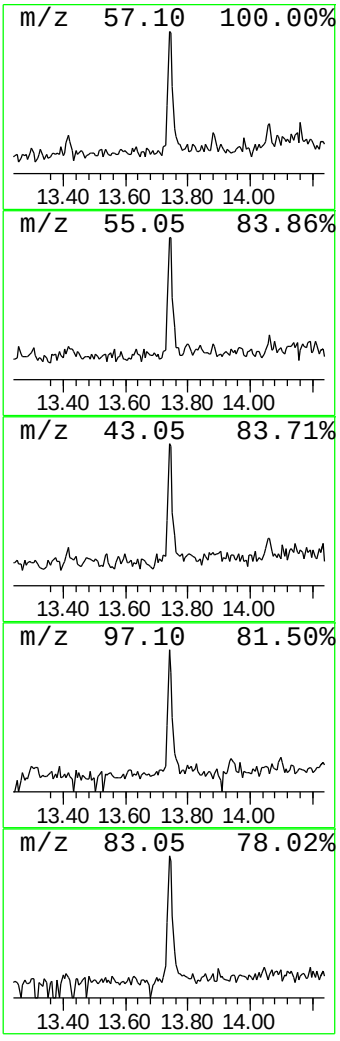
****

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.39 ng	60239	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
4	Octacosanol	410	C28H58O	000557-61-9	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	93





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Operator : SJ/JU
Sample : I6099-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ERM-P-2

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

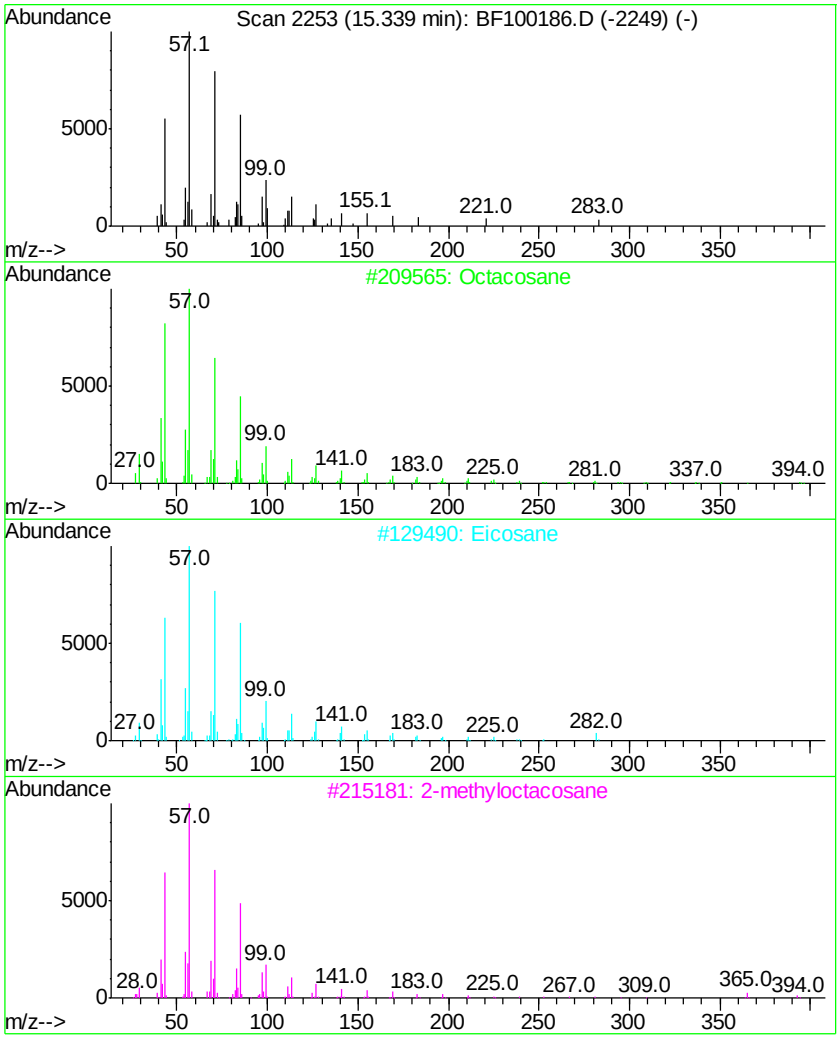
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

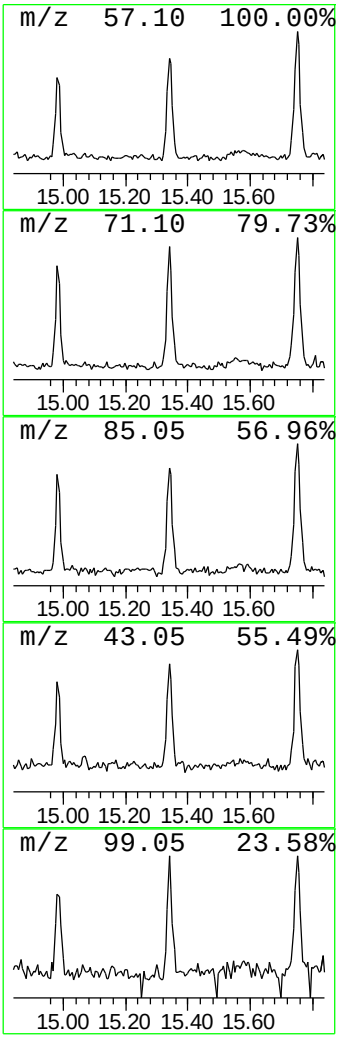
****

Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	3.09 ng	65597	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Eicosane	282	C20H42	000112-95-8	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Hexacosane	366	C26H54	000630-01-3	86





Library Search Compound Report

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Acq On : 4 Nov 2017 18:44
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Misc :
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Instrument : BNA_F
ClientSampleId : ERM-P-2

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

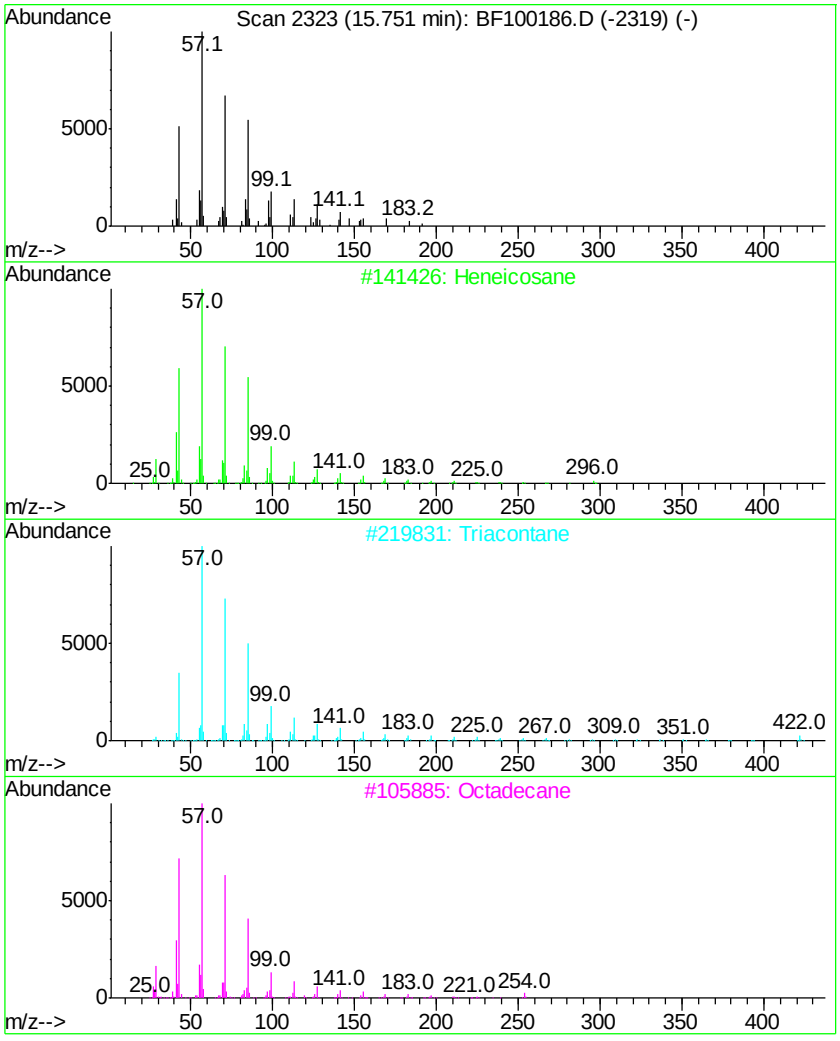
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

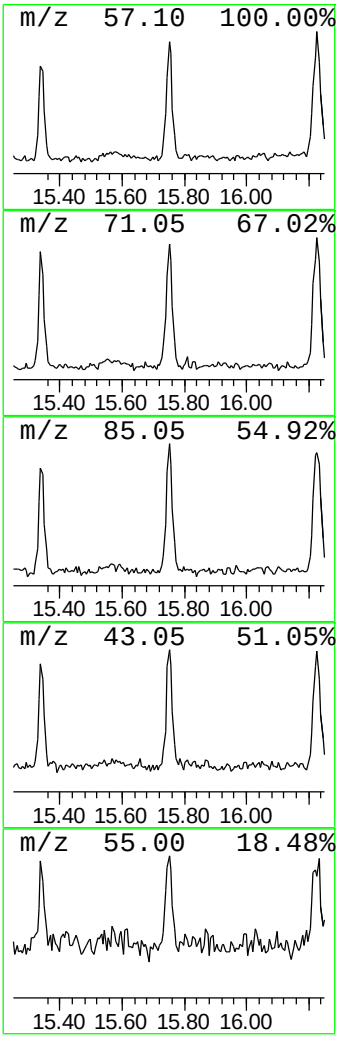
****

Peak Number 8 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	3.81 ng	80931	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Triacontane	422	C30H62	000638-68-6	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptadecane	240	C17H36	000629-78-7	86





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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
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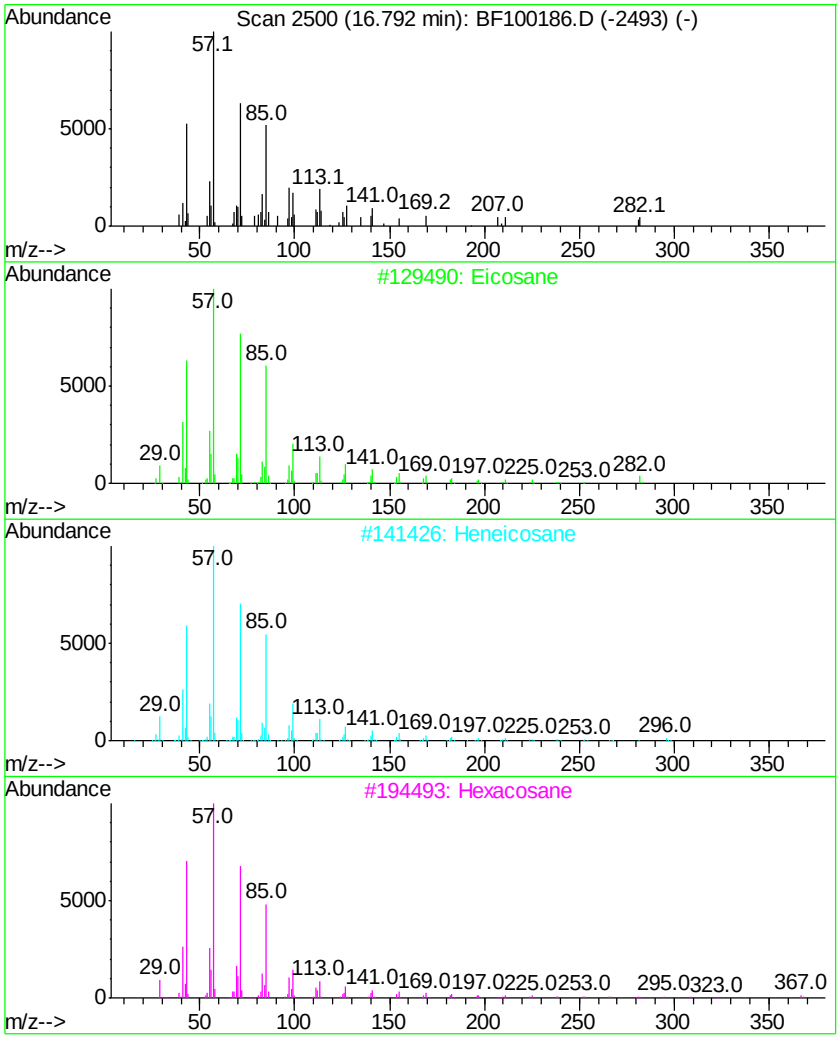
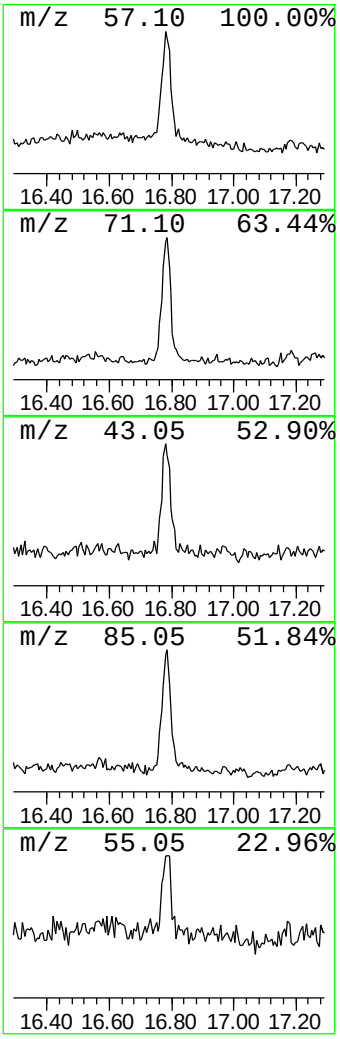
Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.79	4.74 ng	100809	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heneicosane	296	C21H44	000629-94-7	83
3	Hexacosane	366	C26H54	000630-01-3	78
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	78
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	72





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Sample : I6099-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ERM-P-2

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

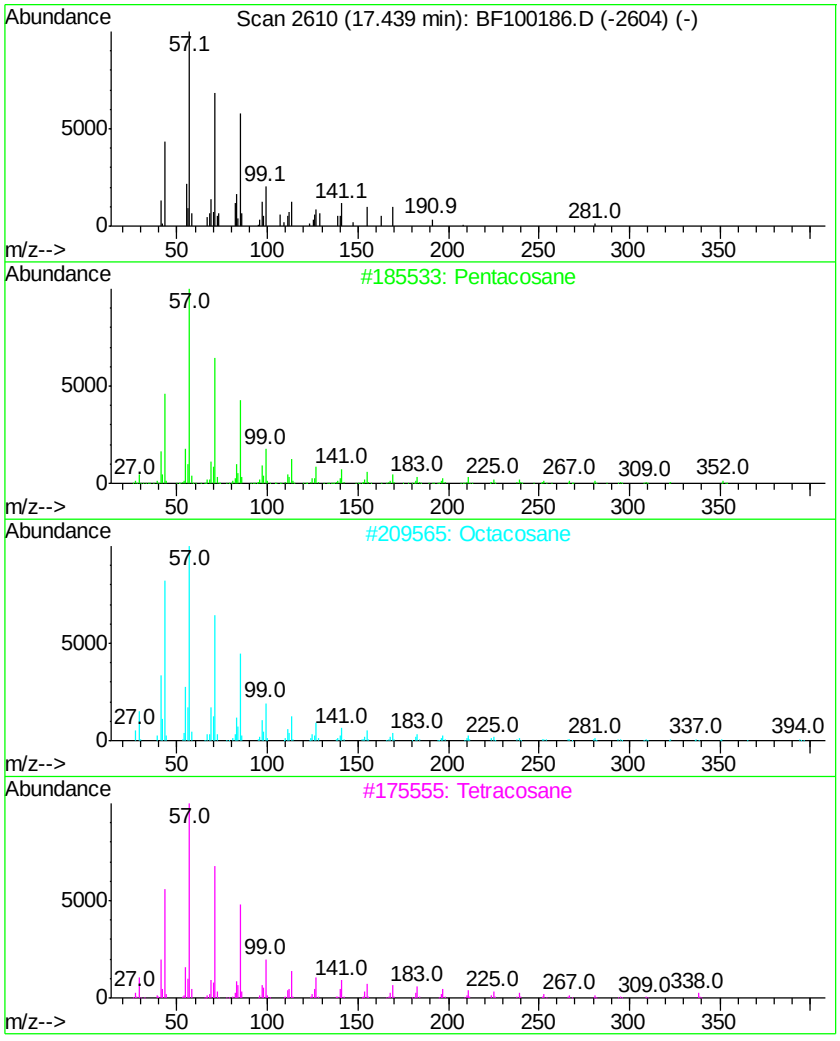
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

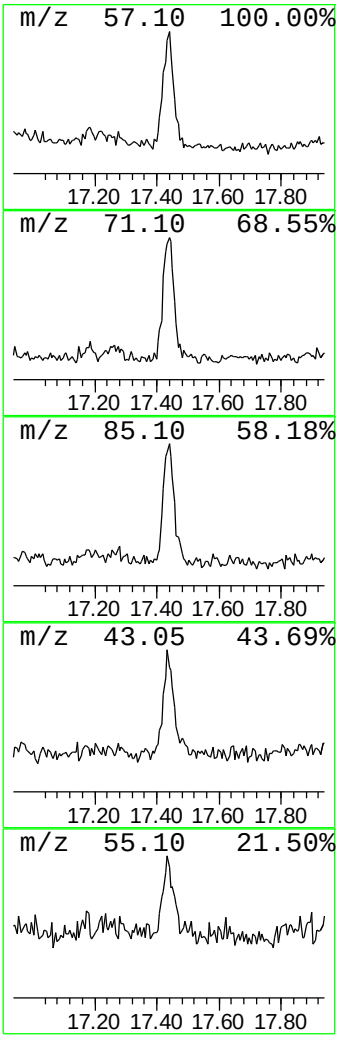
****

Peak Number 11 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	3.52 ng	74881	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Triacontane	422	C30H62	000638-68-6	90
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86





Tentatively Identified Compound (LSC) summary

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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...	4.99	13.6	ng	315316	1	6.76	464336	20.0
unknown6.54	6.54	93.5	ng	2170000	1	6.76	464336	20.0
2-Hydroxy-iso-but...	8.61	2.1	ng	70912	2	8.05	659174	20.0
Benzophenone	10.51	6.7	ng	248303	3	9.80	743213	20.0
Heptadecyl triflu...	13.74	2.4	ng	60239	5	13.94	504392	20.0
Octacosane	15.34	3.1	ng	65597	6	15.40	425001	20.0
Heneicosane	15.75	3.8	ng	80931	6	15.40	425001	20.0
Eicosane	16.79	4.7	ng	100809	6	15.40	425001	20.0
Pentacosane	17.44	3.5	ng	74881	6	15.40	425001	20.0