LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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	4.981	489	492	514	rBV	133896	233032	16.12%	1.788%
2	5.393	560	562	599	rBV	749363	1332233	92.13%	10.220%
3	6.416	733	736	754	rBV	935164	1290142	89.22%	9.897%
4	6.540	754	757	774	rVB	1370757	1445982	100.00%	11.092%
5	6.763	792	795	808	rBV	485375	456548	31.57%	3.502%
6	6.916	818	821	841	rBV	1193929	1089902	75.37%	8.361%
7	7.334	889	892	917	rBV	676499	772577	53.43%	5.926%
8	8.045	1010	1013	1032	rBV	593342	596228	41.23%	4.574%
9	9.116	1191	1195	1205	rBV	1491018	1337556	92.50%	10.260%
10	9.522	1261	1264	1273	rBV	48748	52479	3.63%	0.403%
11	9.792	1307	1310	1324	rBB	562183	544319	37.64%	4.175%
12	10.592	1443	1446	1458	rBV	573335	563761	38.99%	4.325%
13	11.286	1561	1564	1576	rBV	464633	434124	30.02%	3.330%
14	11.798	1648	1651	1664	rVB2	71117	72324	5.00%	0.555%
15	12.245	1723	1727	1736	rVB	65558	63062	4.36%	0.484%
16	12.345	1741	1744	1748	rVV	25584	24634	1.70%	0.189%
17	12.863	1828	1832	1836	rBV	1135288	934539	64.63%	7.169%
18	13.004	1852	1856	1862	rBV	137664	117269	8.11%	0.900%
19	13.098	1869	1872	1875	rVB	23715	24709	1.71%	0.190%
20	13.710	1971	1976	1978	rBV2	14257	16649	1.15%	0.128%
21	13.739	1978	1981	1988	rVB	88994	100040	6.92%	0.767%
22	13.939	2011	2015	2022	rBV	478726	463706	32.07%	3.557%
23	14.363	2083	2087	2093	rBV4	16144	29260	2.02%	0.224%
24	14.657	2133	2137	2145	rVB2	35977	48463	3.35%	0.372%
25	14.980	2188	2192	2195	rBV	46331	51366	3.55%	0.394%
26	15.339	2248	2253	2258	rBV	53778	68260	4.72%	0.524%
27	15.398	2258	2263	2276	rVB	293248	420438	29.08%	3.225%
28	15.745	2317	2322	2327	rBV	66207	91136	6.30%	0.699%
29	15.798	2328	2331	2339	rVV7	17124	30166	2.09%	0.231%
30	16.221	2398	2403	2413	rVB2	48380	85433	5.91%	0.655%
31	16.498	2443	2450	2456	rBV5	25361	51321	3.55%	0.394%
32	16.774	2492	2497	2505	rVB3	38563	77125	5.33%	0.592%
33	17.280	2579	2583	2591	rVB10	17601	36261	2.51%	0.278%
34	17.427	2603	2608	2616	rVB4	24898	54806	3.79%	0.420%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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

35	18.198	2735	2739	2746	rBV6	10472	26282	1.82%	0.202%

Sum of corrected areas: 13036132

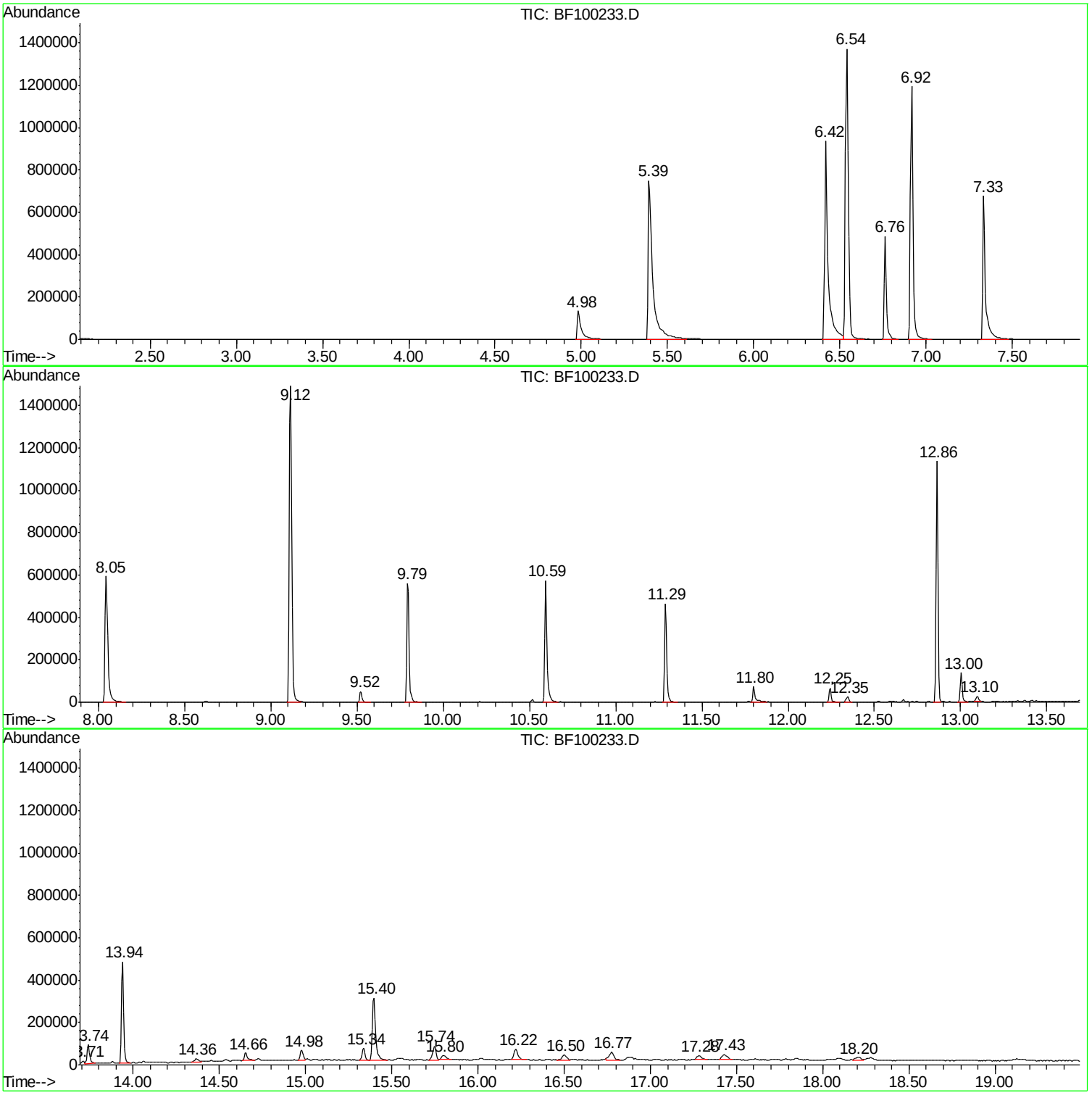
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P002-S001-0001-02

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\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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

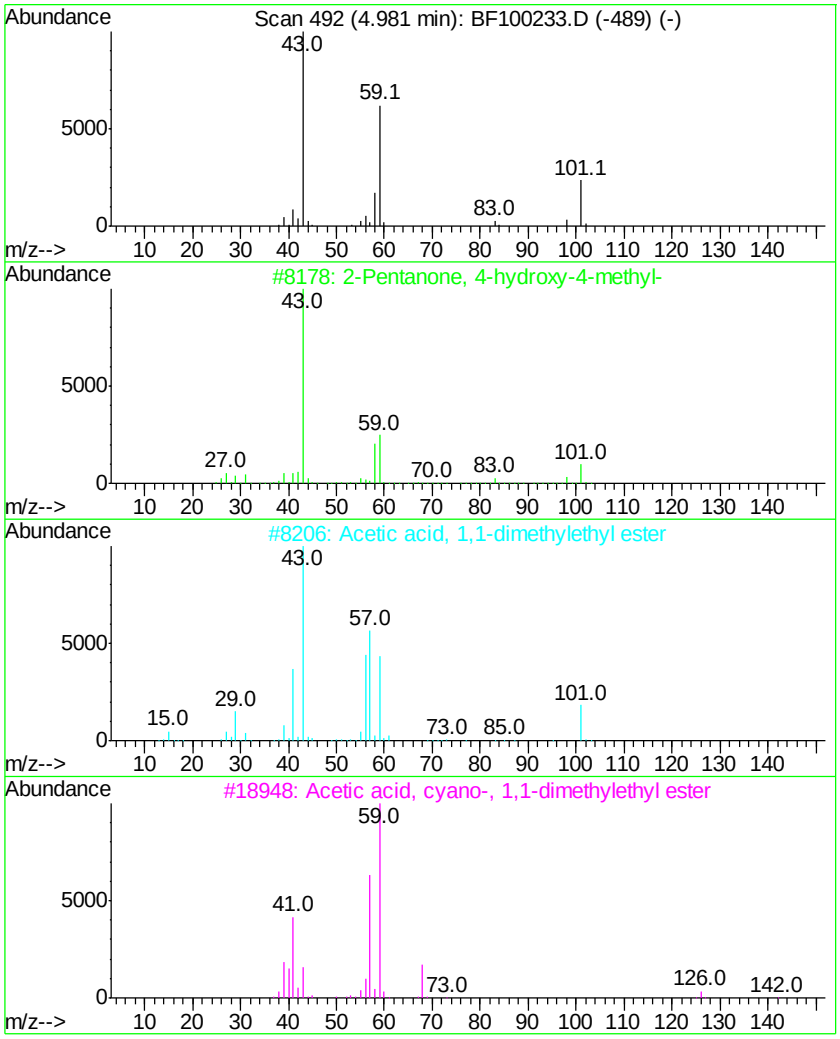
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

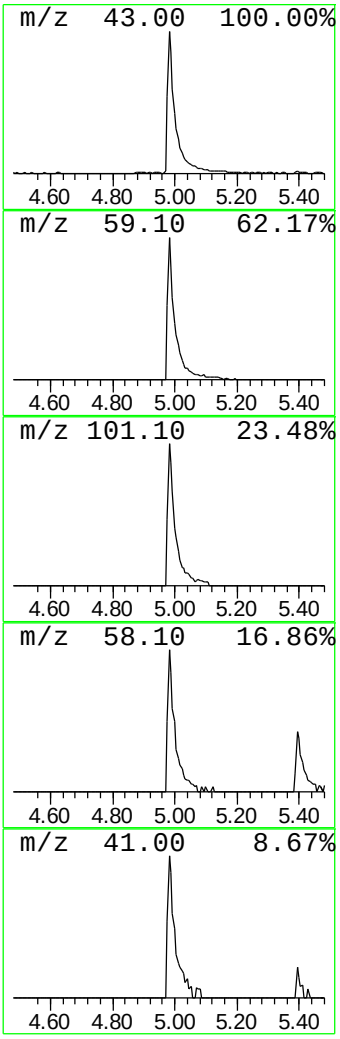
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	10.21 ng	233032	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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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

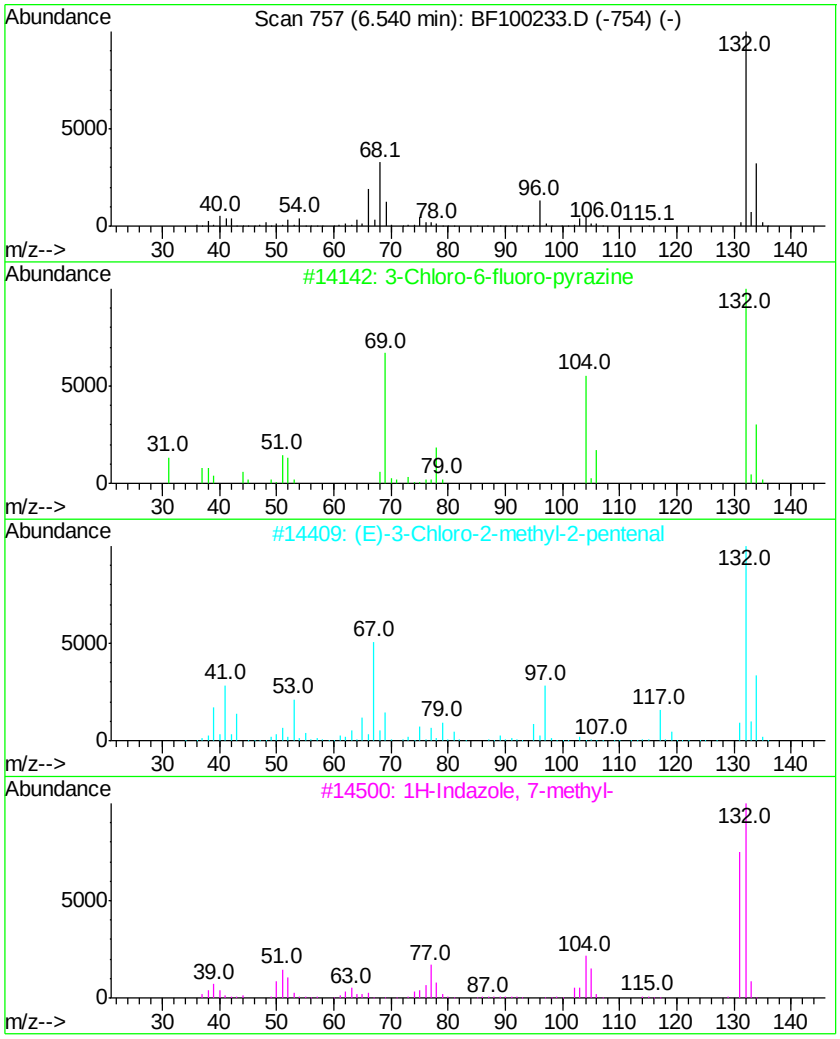
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

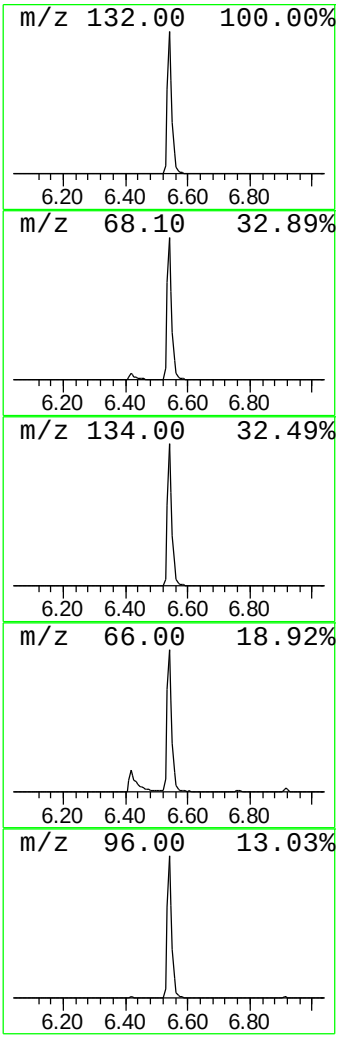
****

Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	63.34 ng	1445980	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	52
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	38
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	25
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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

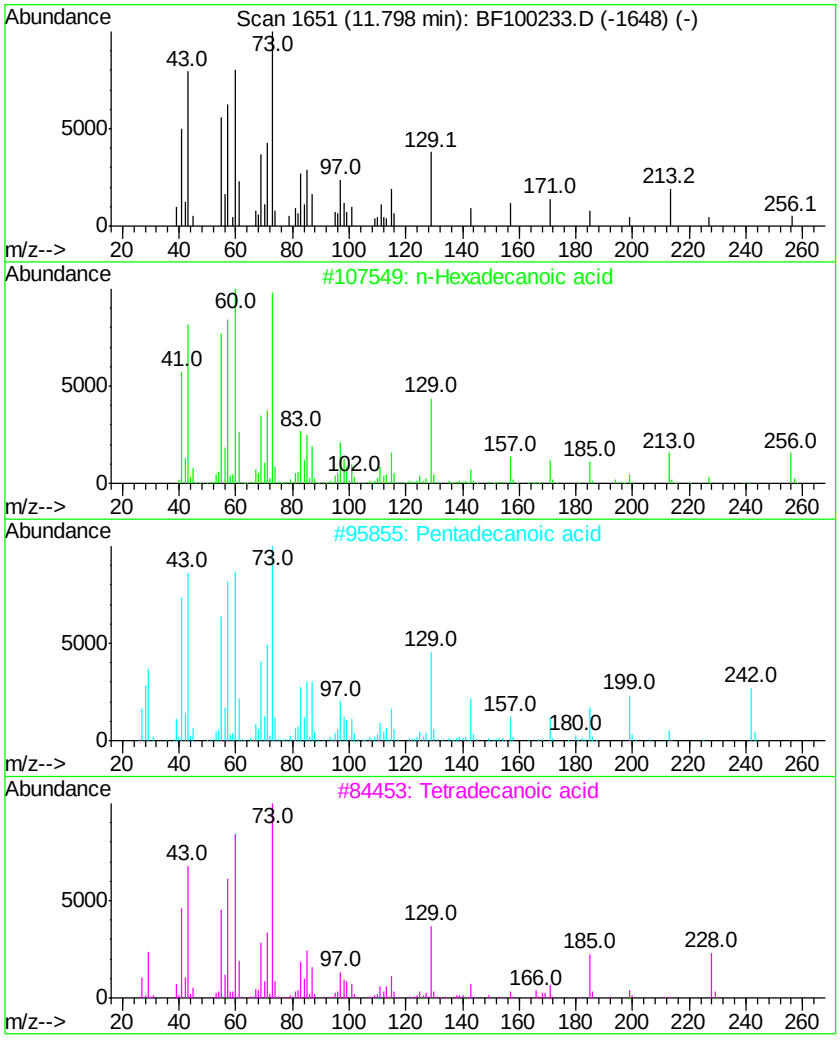
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

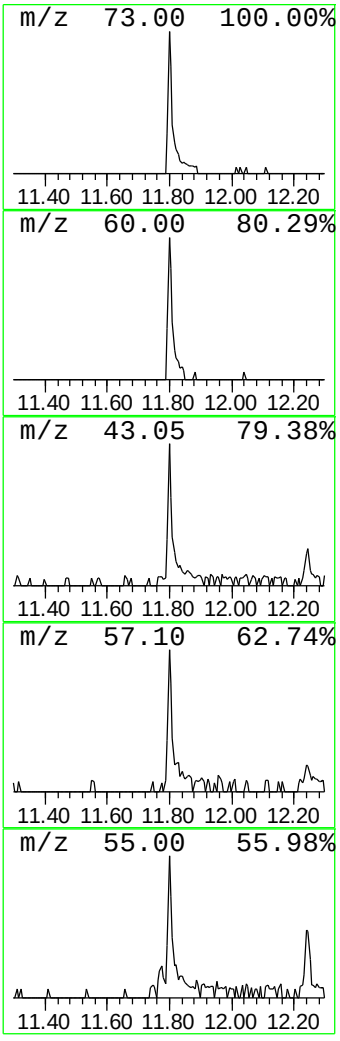
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	3.33 ng	72324	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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

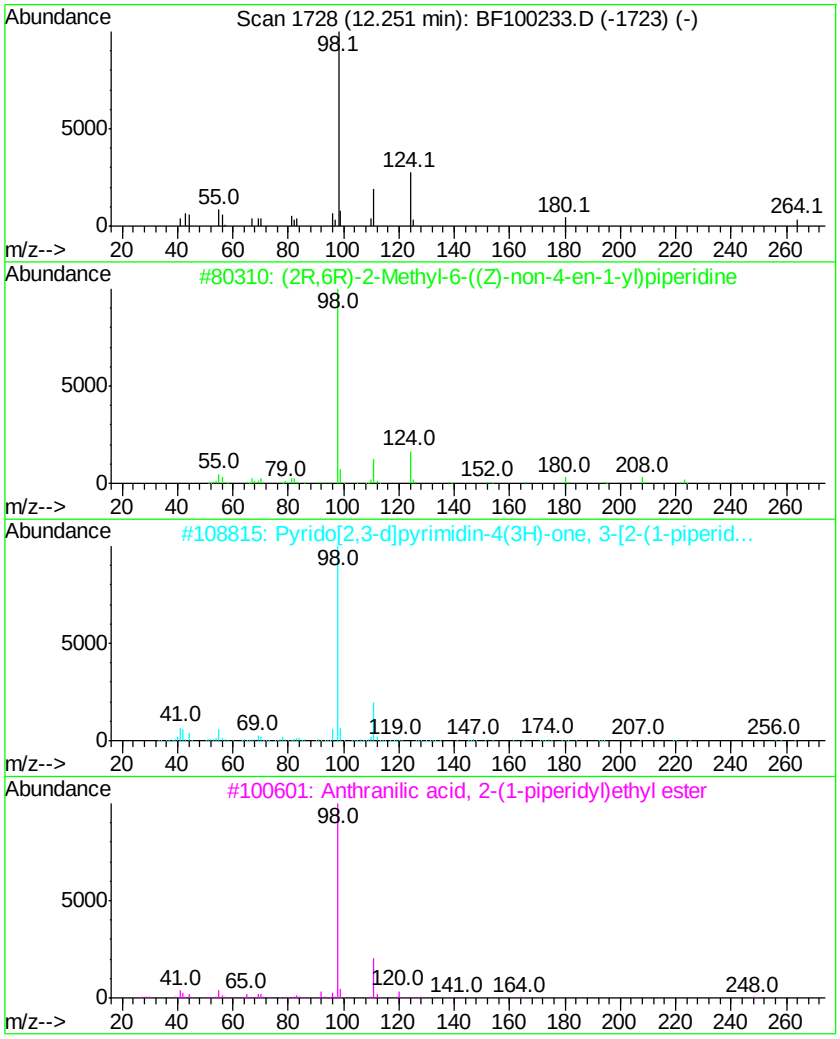
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

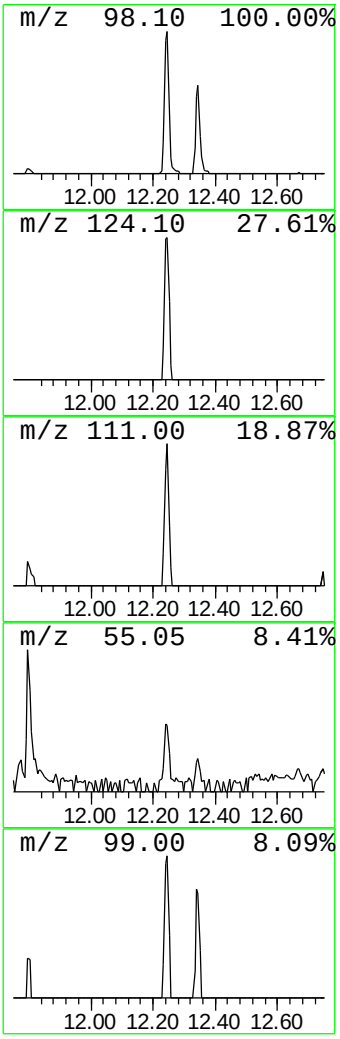
****

Peak Number 5 (2R,6R)-2-Methyl-6-((Z)-non... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.25	2.91 ng	63062	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2R,6R)-2-Methyl-6-((Z)-non-4-en...	223	C15H29N	181221-89-6	86
2	Pyrido[2,3-d]pyrimidin-4(3H)-one...	258	C14H18N4O	161562-65-8	53
3	Anthranilic acid, 2-(1-piperidyl...	248	C14H20N2O2	088562-51-0	53
4	(2S,6R)-2-Methyl-6-((Z)-non-4-en...	223	C15H29N	181378-96-1	52
5	Pentan-1-one, 1-phenyl-5-(1-pipe...	245	C16H23NO	116849-53-7	50





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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

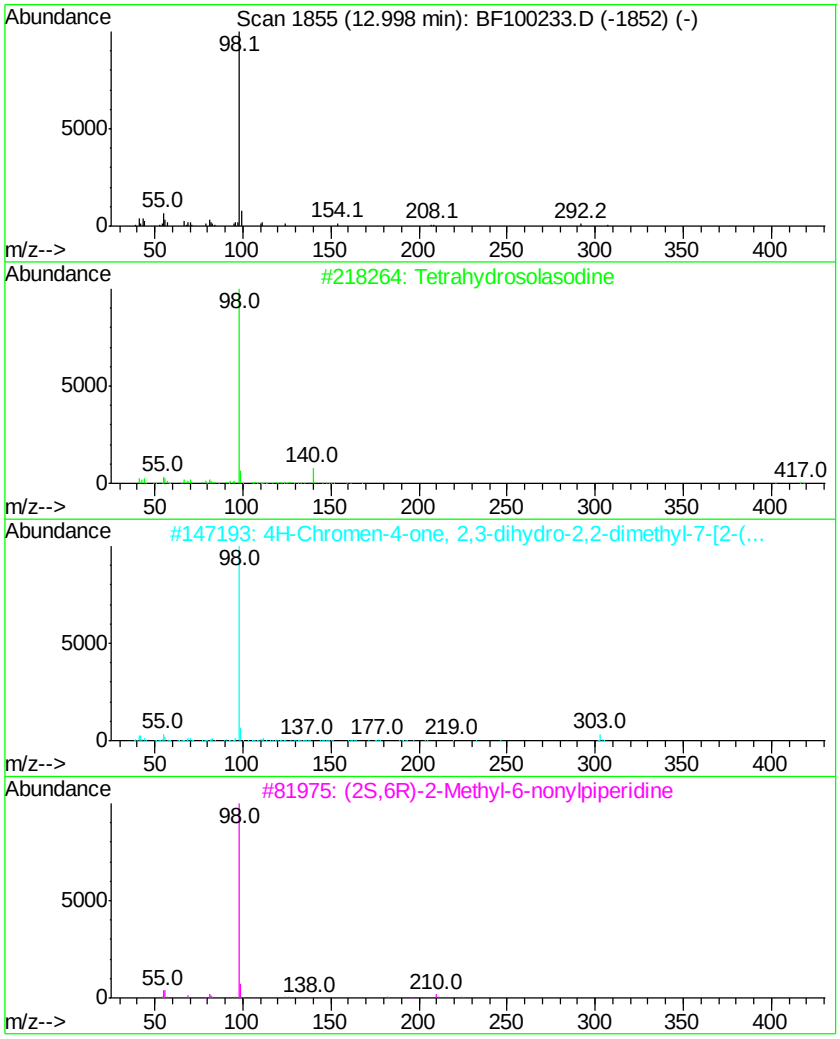
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

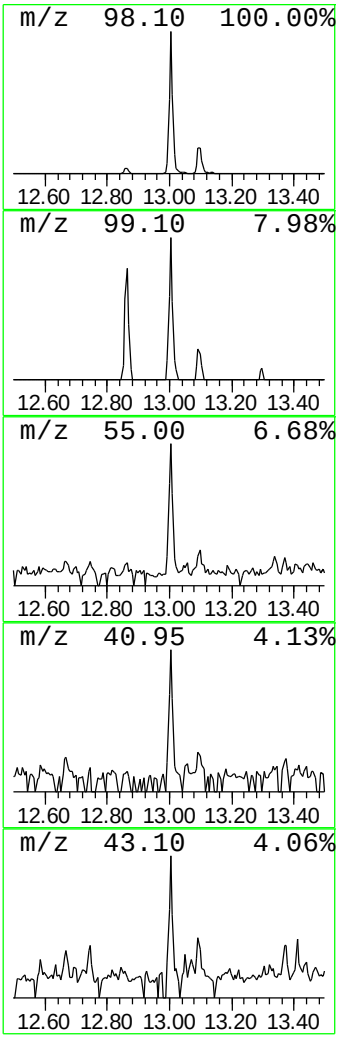
****

Peak Number 6 Tetrahydrosolasodine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.00	5.06 ng	117269	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrahydrosolasodine	417	C27H47NO2	071473-03-5	64
2	4H-Chromen-4-one, 2,3-dihydro-2,...	303	C18H25NO3	128890-42-6	64
3	(2S,6R)-2-Methyl-6-nonylpiperidine	225	C15H31N	848415-28-1	64
4	2-Piperidinoethyl 3,5-dichlorobe...	301	C14H17Cl2NO2	1000240-19-9	64
5	16-Epi-dihydro-solasodine	415	C27H45NO2	1000256-11-6	64





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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

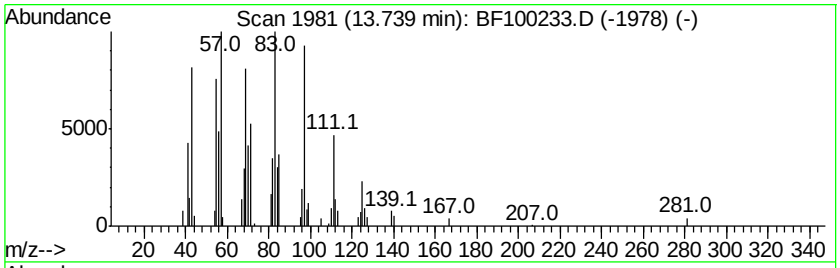
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

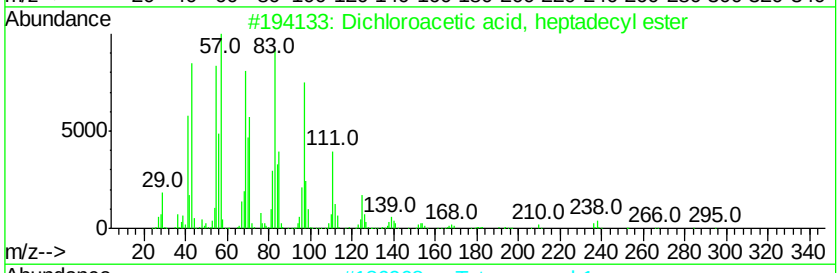
****

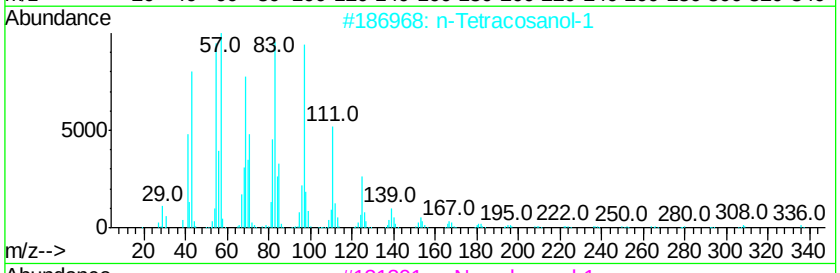
Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 6

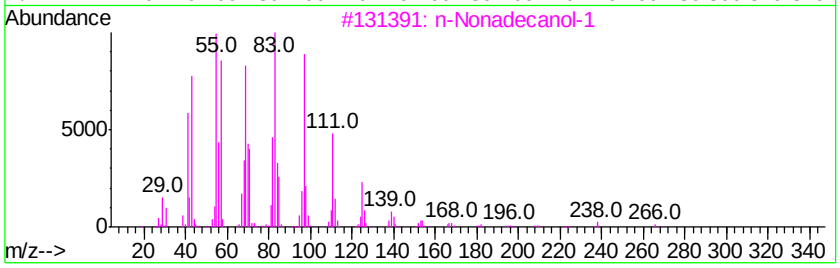
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	4.31 ng	100040	Chrysene-d12	13.94

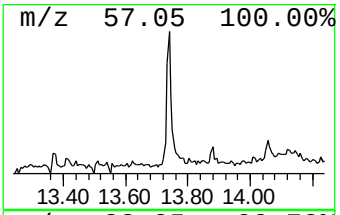
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91

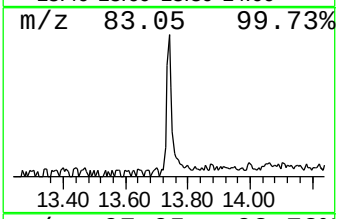


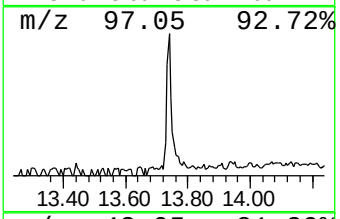


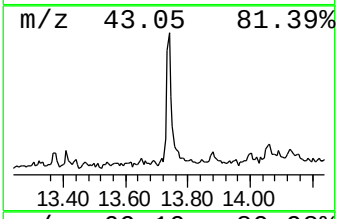


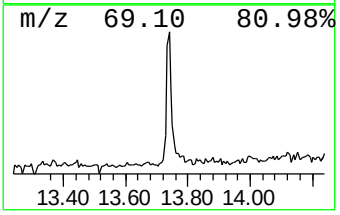












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Data File : BF100233.D
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Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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

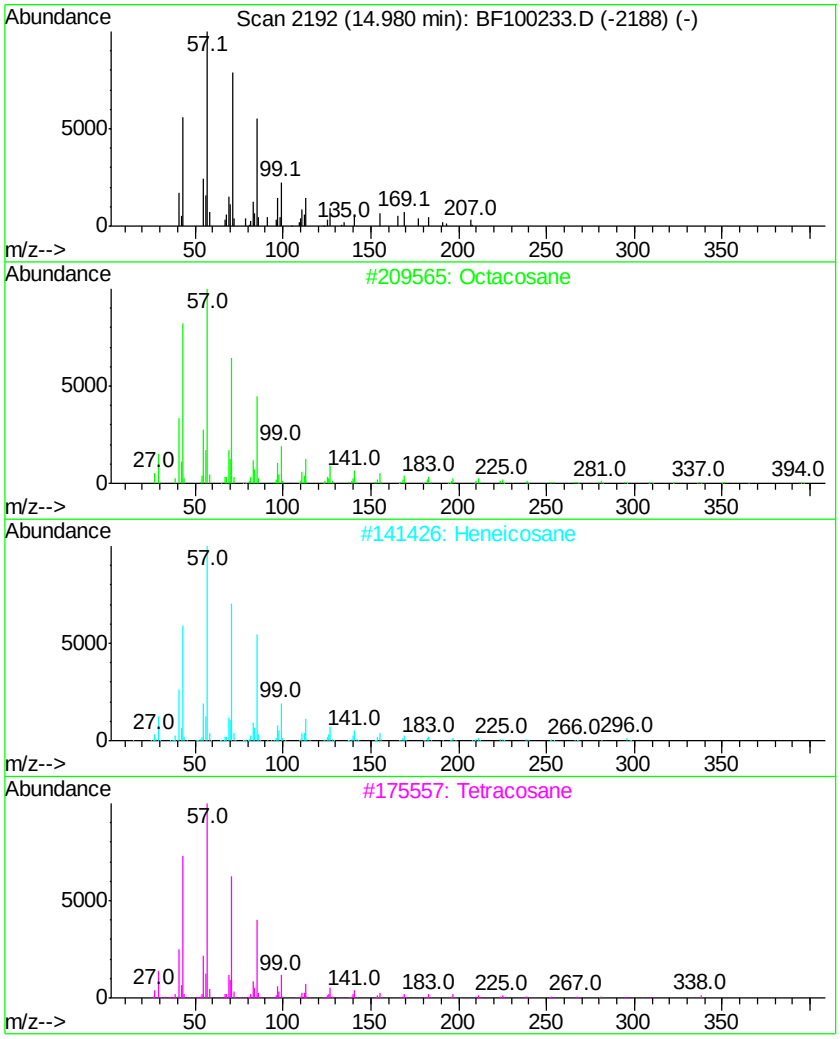
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

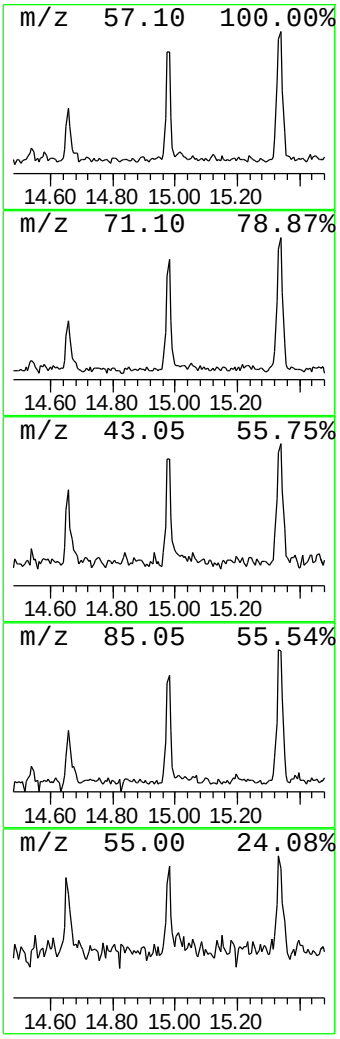
****

Peak Number 9 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.44 ng	51366	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Hexacosane	366	C26H54	000630-01-3	87





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Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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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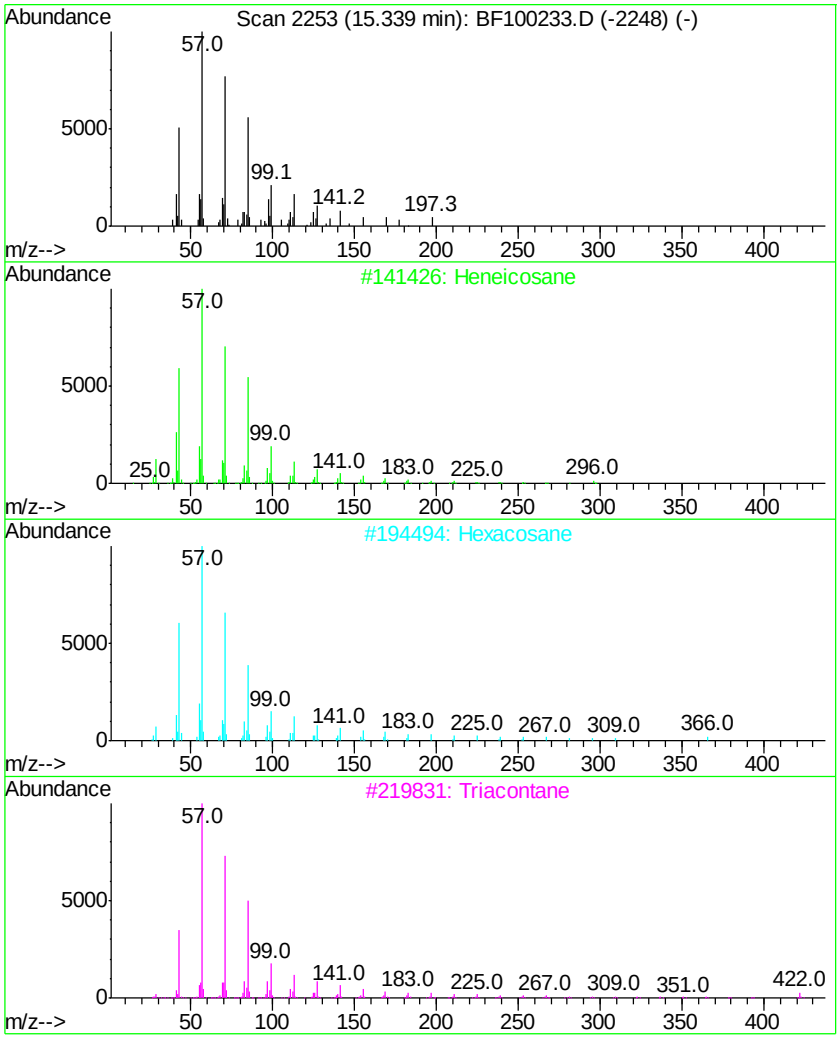
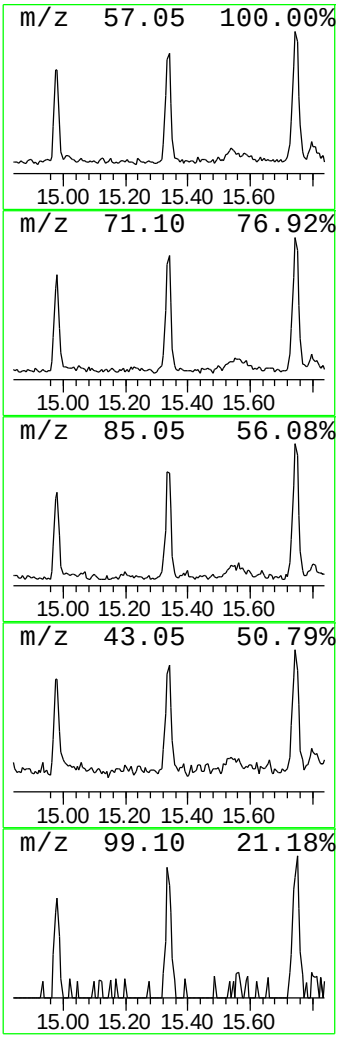
Peak Number 10 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	3.25 ng	68260	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Octacosane	394	C28H58	000630-02-4	90
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	90





Library Search Compound Report

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Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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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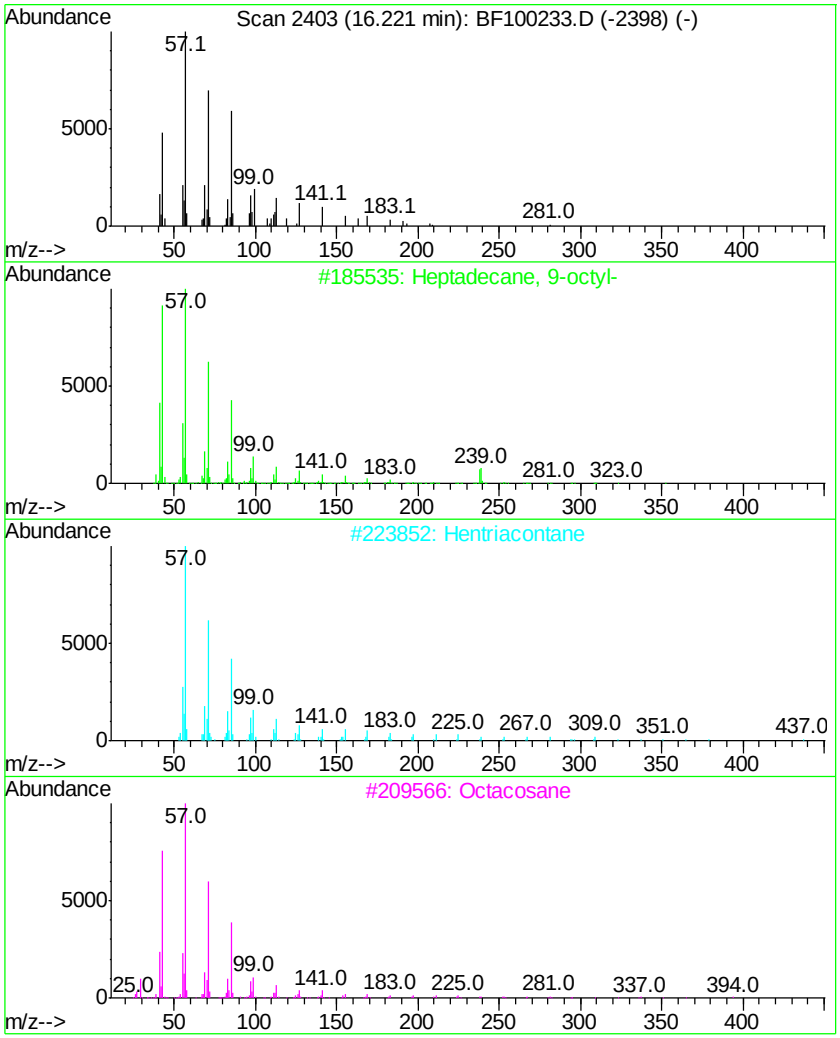
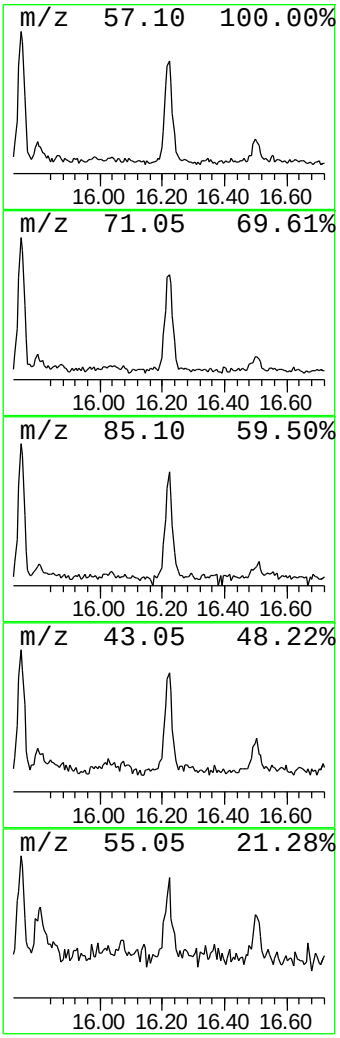
Peak Number 12 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	4.06 ng	85433	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Octacosane	394	C28H58	000630-02-4	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Heneicosane	296	C21H44	000629-94-7	87





Library Search Compound Report

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Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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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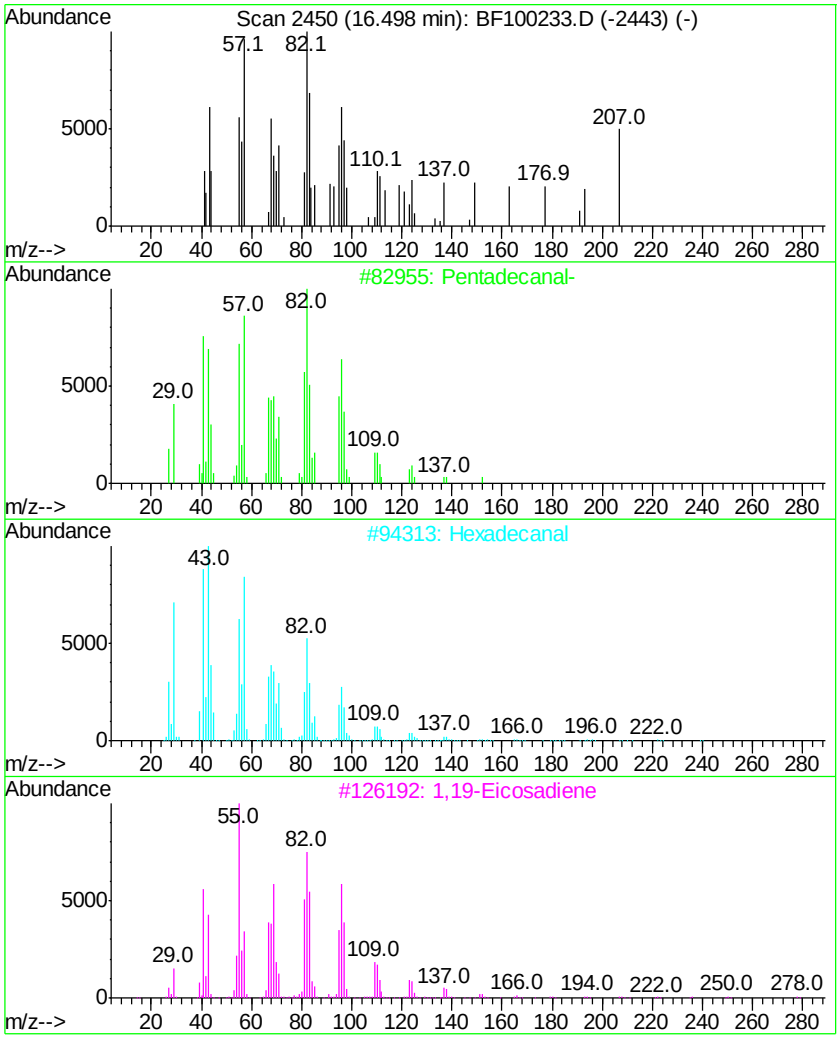
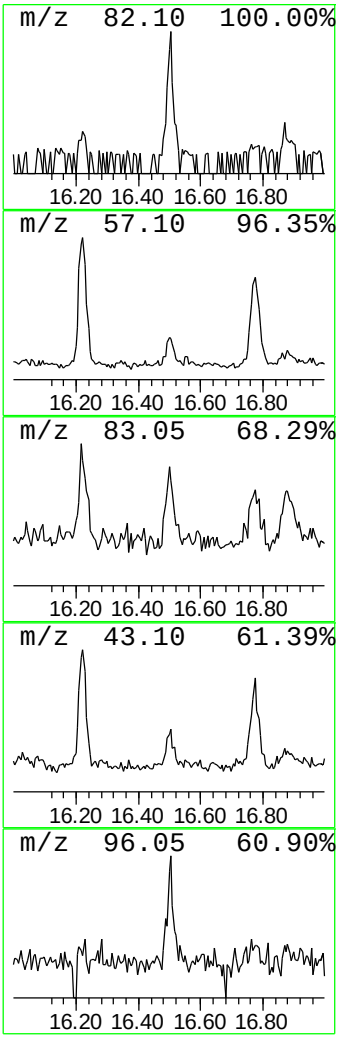
Peak Number 13 unknown16.50 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	2.44 ng	51321	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanal-	226	C15H30O	002765-11-9	49
2	Hexadecanal	240	C16H32O	000629-80-1	49
3	1,19-Eicosadiene	278	C20H38	014811-95-1	47
4	Tetradecanal	212	C14H28O	000124-25-4	43
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	43





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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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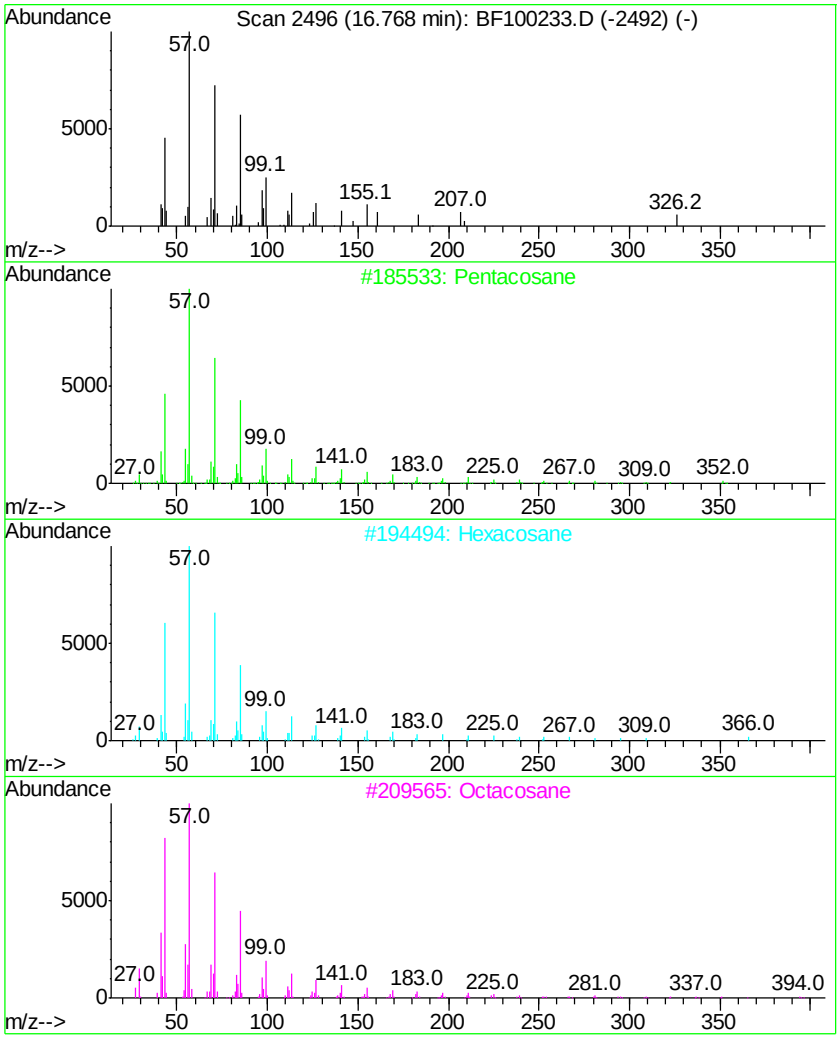
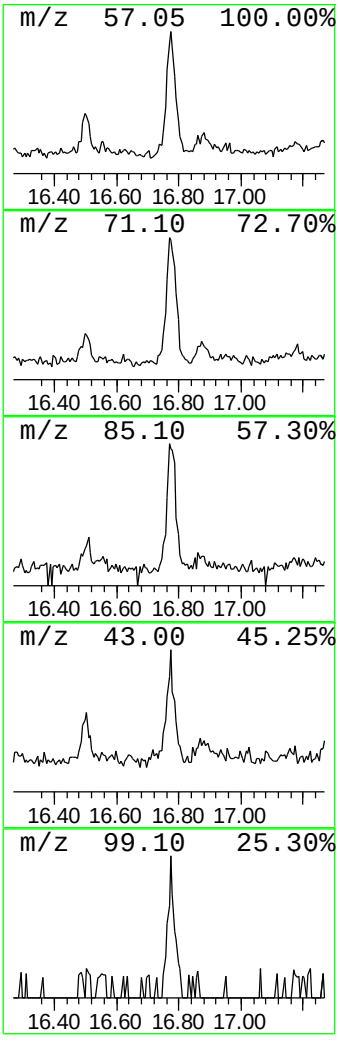
Peak Number 14 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	3.67 ng	77125	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	80
2	Hexacosane	366	C26H54	000630-01-3	80
3	Octacosane	394	C28H58	000630-02-4	72
4	Hentriacontane	437	C31H64	000630-04-6	68
5	Heneicosane	296	C21H44	000629-94-7	64





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF110517\
Data File : BF100233.D
Acq On : 5 Nov 2017 19:26
Operator : SJ/JU
Sample : I6285-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P002-S001-0001-02

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...	4.98	10.2	ng	233032	1	6.76	456548	20.0
3-Chloro-6-fluoro...	6.54	63.3	ng	1445980	1	6.76	456548	20.0
n-Hexadecanoic acid	11.80	3.3	ng	72324	4	11.29	434124	20.0
(2R,6R)-2-Methyl-...	12.25	2.9	ng	63062	4	11.29	434124	20.0
Tetrahydrosolasodine	13.00	5.1	ng	117269	5	13.94	463706	20.0
Dichloroacetic ac...	13.74	4.3	ng	100040	5	13.94	463706	20.0
Octacosane	14.98	2.4	ng	51366	6	15.40	420438	20.0
Heneicosane	15.34	3.3	ng	68260	6	15.40	420438	20.0
Heptadecane, 9-oc...	16.22	4.1	ng	85433	6	15.40	420438	20.0
unknown16.50	16.50	2.4	ng	51321	6	15.40	420438	20.0
Pentacosane	16.77	3.7	ng	77125	6	15.40	420438	20.0