LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100222.D
Acq On : 5 Nov 2017 14:31
Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-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	4.987	490	493	519	rBV	142612	278640	13.71%	1.599%
2	5.392	559	562	596	rBV	1293023	1799200	88.54%	10.322%
3	6.416	733	736	754	rBV	1463610	1797454	88.46%	10.312%
4	6.539	754	757	772	rVB	1955748	1936110	95.28%	11.107%
5	6.763	792	795	806	rBV	517595	476533	23.45%	2.734%
6	6.916	818	821	835	rBV	1627445	1492991	73.47%	8.565%
7	7.333	889	892	916	rBV	963300	1117186	54.98%	6.409%
8	8.045	1010	1013	1037	rBV	665040	642981	31.64%	3.689%
9	9.116	1191	1195	1198	rBV	2399651	2032001	100.00%	11.657%
10	9.516	1260	1263	1272	rBV	141423	126467	6.22%	0.726%
11	9.798	1307	1311	1321	rBV	653184	648205	31.90%	3.719%
12	10.510	1429	1432	1441	rBB	72408	61960	3.05%	0.355%
13	10.592	1442	1446	1459	rBV	1014652	992738	48.86%	5.695%
14	11.286	1561	1564	1575	rBV	580264	545215	26.83%	3.128%
15	11.798	1648	1651	1656	rBV	80214	82771	4.07%	0.475%
16	12.580	1781	1784	1789	rBV	41608	44642	2.20%	0.256%
17	12.868	1829	1833	1836	rBV	1413651	1349643	66.42%	7.743%
18	13.710	1971	1976	1979	rBV	218087	201548	9.92%	1.156%
19	13.739	1979	1981	1986	rVB	53846	57103	2.81%	0.328%
20	13.880	2003	2005	2012	rVB	34927	35925	1.77%	0.206%
21	13.939	2012	2015	2022	rBV	487161	473403	23.30%	2.716%
22	14.039	2029	2032	2036	rBV	101990	101011	4.97%	0.579%
23	14.080	2036	2039	2041	rVV	165182	154084	7.58%	0.884%
24	14.104	2041	2043	2045	rVV	53132	49593	2.44%	0.285%
25	14.127	2045	2047	2051	rVB	63464	58488	2.88%	0.336%
26	14.362	2084	2087	2092	rBV4	32282	43205	2.13%	0.248%
27	14.980	2189	2192	2195	rVB	45285	43214	2.13%	0.248%
28	15.398	2259	2263	2270	rVB	361310	495574	24.39%	2.843%
29	15.751	2319	2323	2326	rVB	47127	63600	3.13%	0.365%
30	16.503	2447	2451	2460	rVB4	51149	99841	4.91%	0.573%
31	17.280	2578	2583	2593	rBV7	57645	129584	6.38%	0.743%

Sum of corrected areas: 17430910

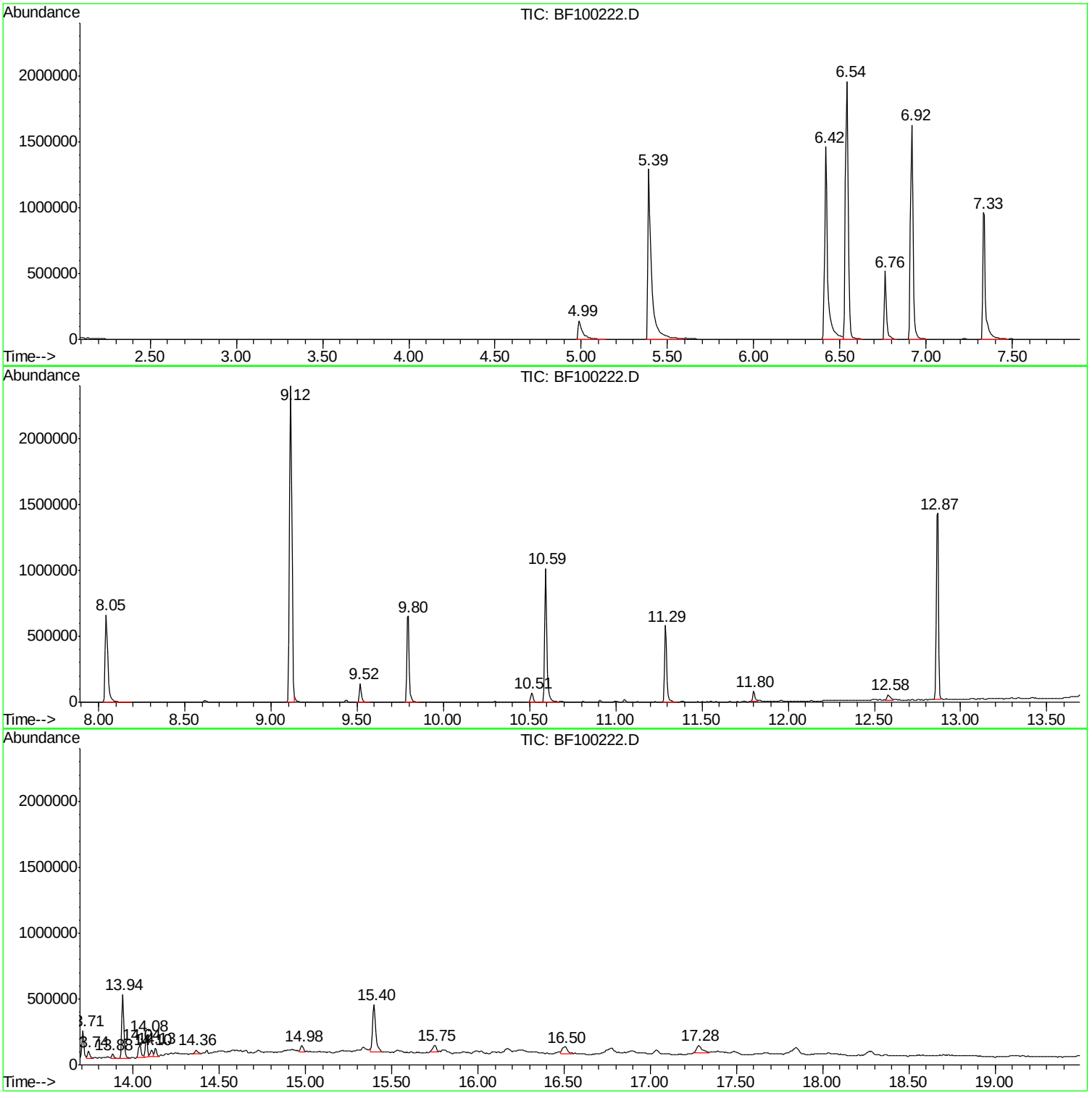
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100222.D
Acq On : 5 Nov 2017 14:31
Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
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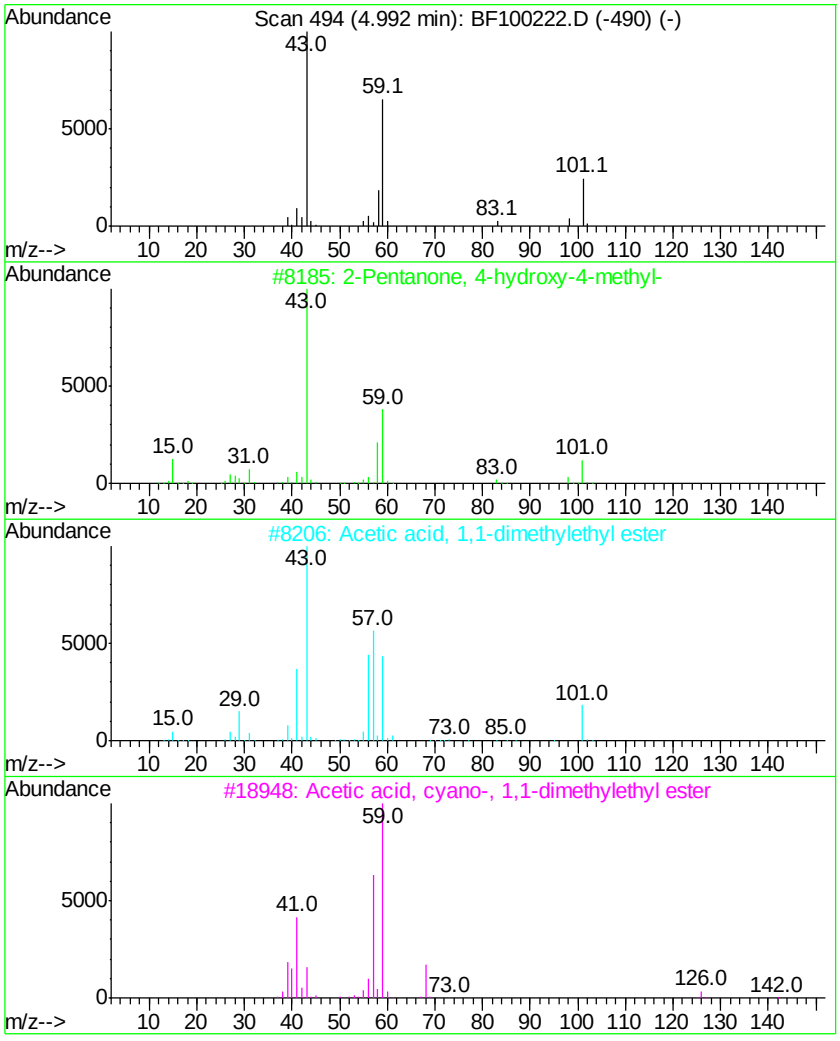
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

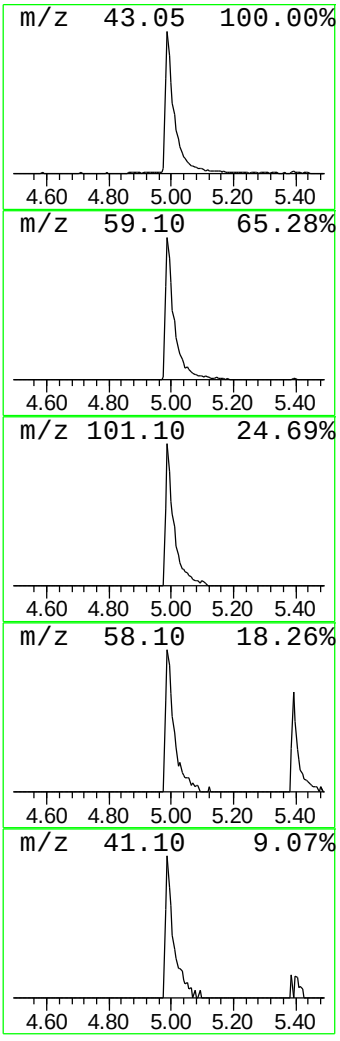
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	11.69 ng	278640	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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100222.D
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Operator : SJ/JU
Sample : I6267-02
Misc :
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Instrument : BNA_F
ClientSampleId : P001-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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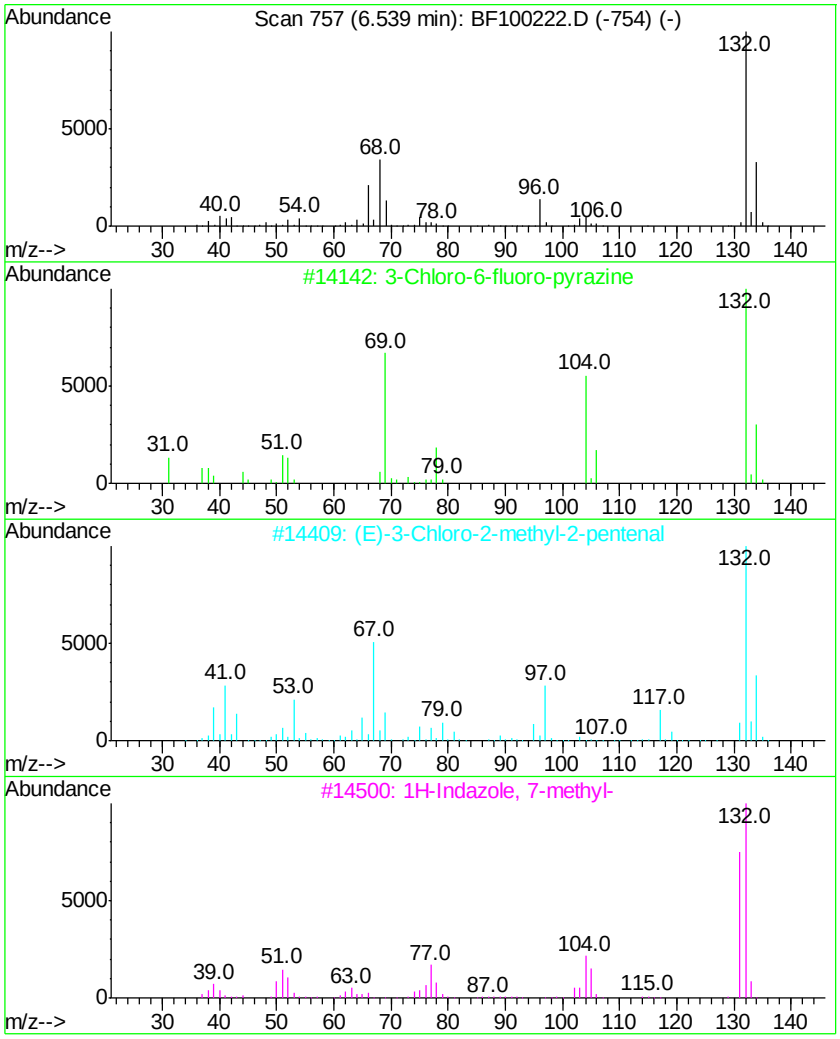
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

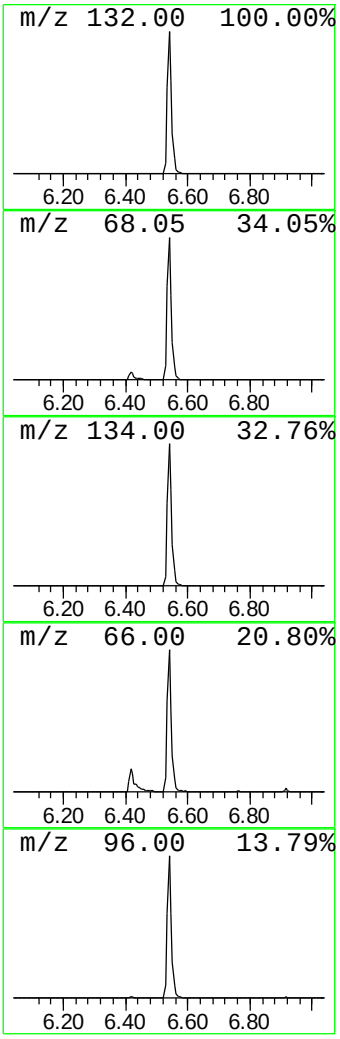
****

Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	81.26 ng	1936110	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	25
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Data File : BF100222.D
Acq On : 5 Nov 2017 14:31
Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-S001-0001-02

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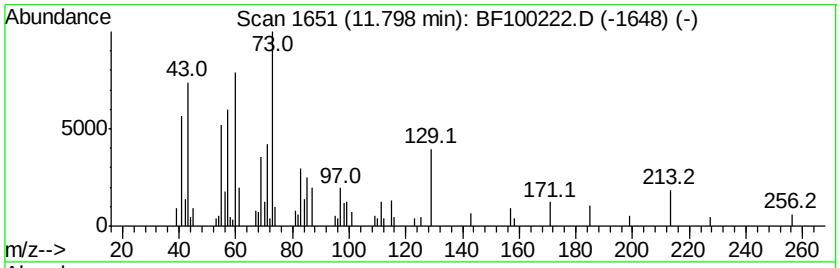
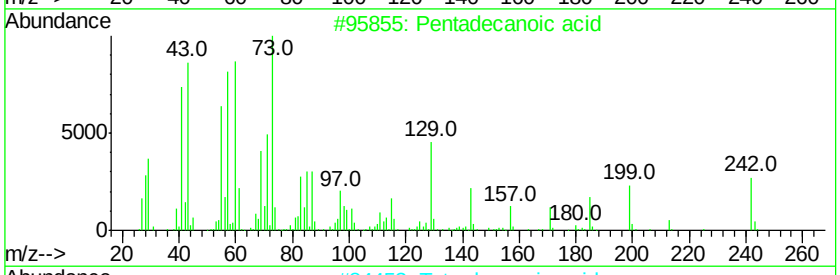
****

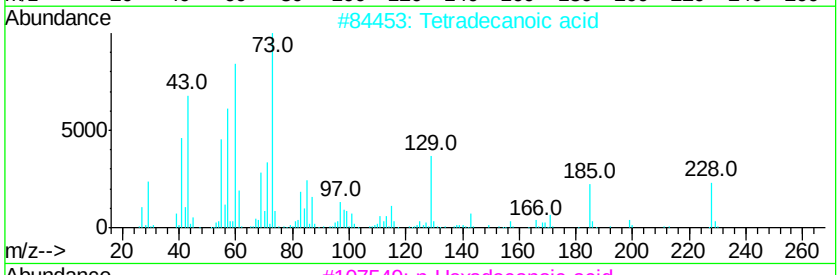
Peak Number 4 Pentadecanoic acid Concentration Rank 9

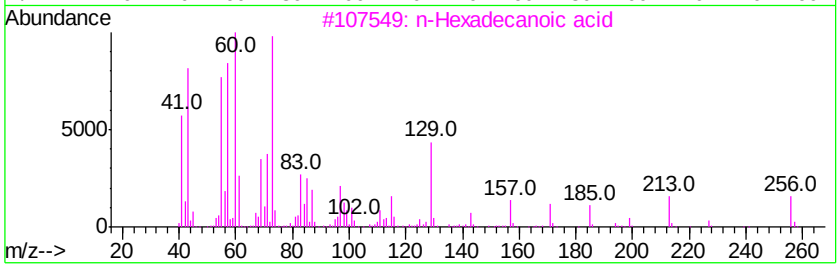
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	3.04 ng	82771	Phenanthrene-d10	11.29

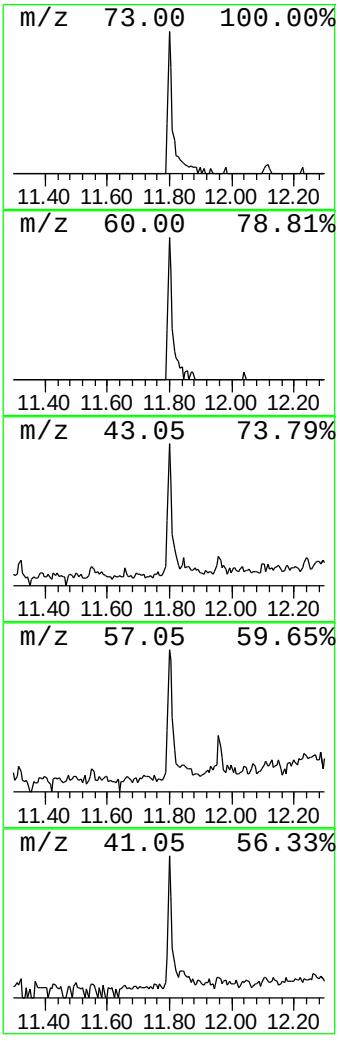
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	15











Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110517\
Data File : BF100222.D
Acq On : 5 Nov 2017 14:31
Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-S001-0001-02

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

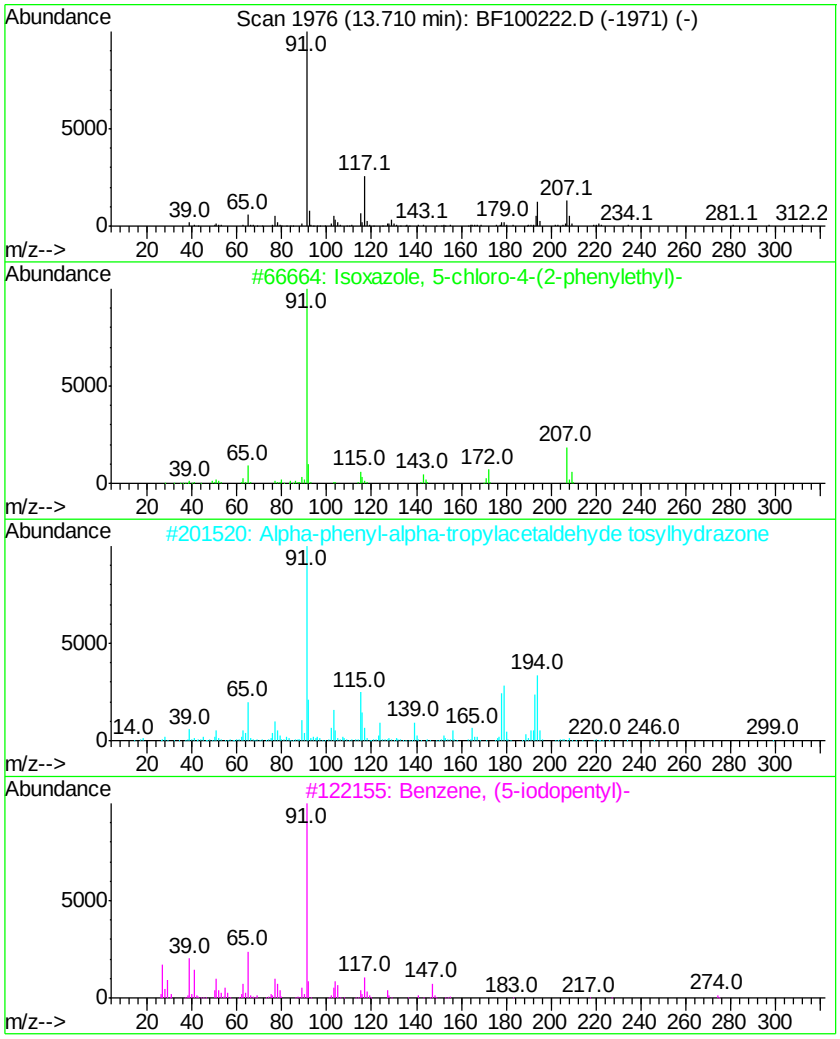
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

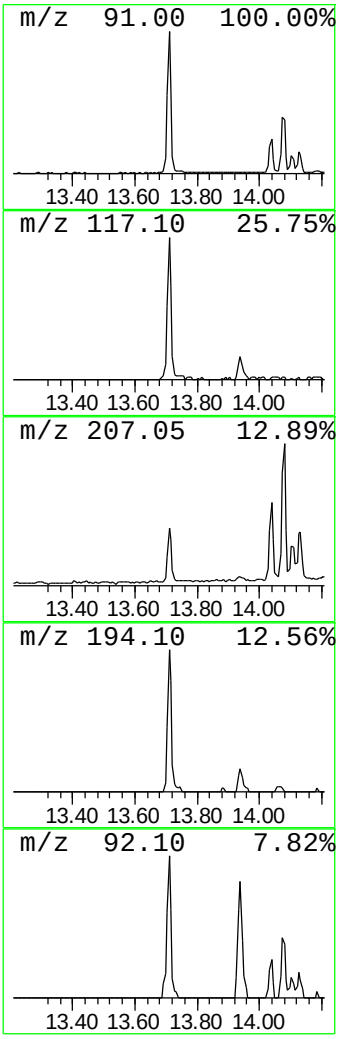
****

Peak Number 5 unknown13.71 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	8.51 ng	201548	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 5-chloro-4-(2-phenyle...	207	C11H10ClNO	1000362-09-0	25
2	Alpha-phenyl-alpha-tropylacetald...	378	C22H22N2O2S	022532-16-7	17
3	Benzene, (5-iodopentyl)-	274	C11H15I	099858-37-4	17
4	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	12
5	1,2-Propanediol, 3-benzyloxy-1,2...	266	C14H18O5	013754-10-4	12





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Acq On : 5 Nov 2017 14:31
Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-S001-0001-02

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

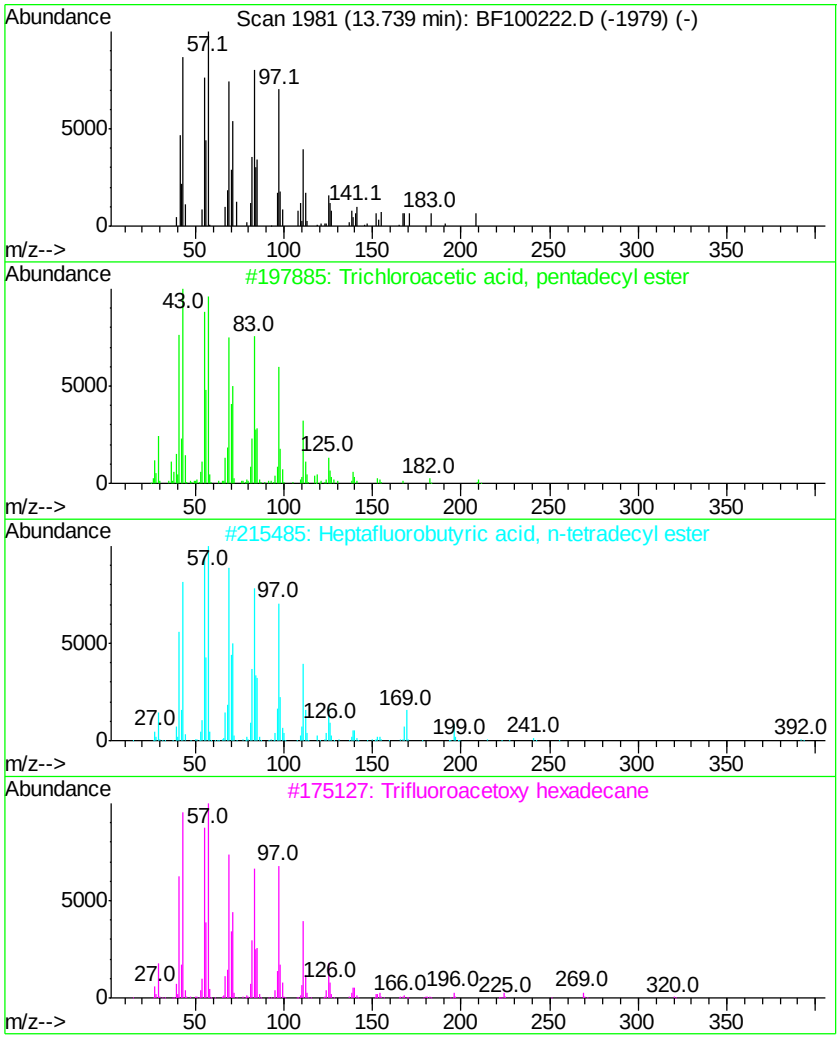
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

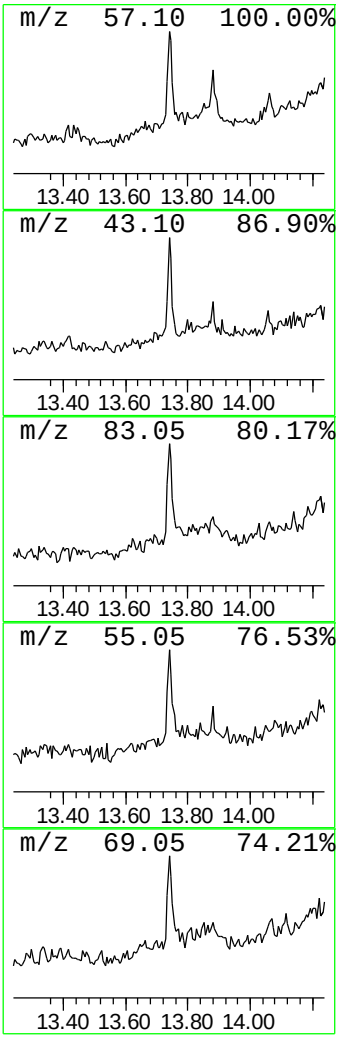
****

Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.41 ng	57103	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	76





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Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-S001-0001-02

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

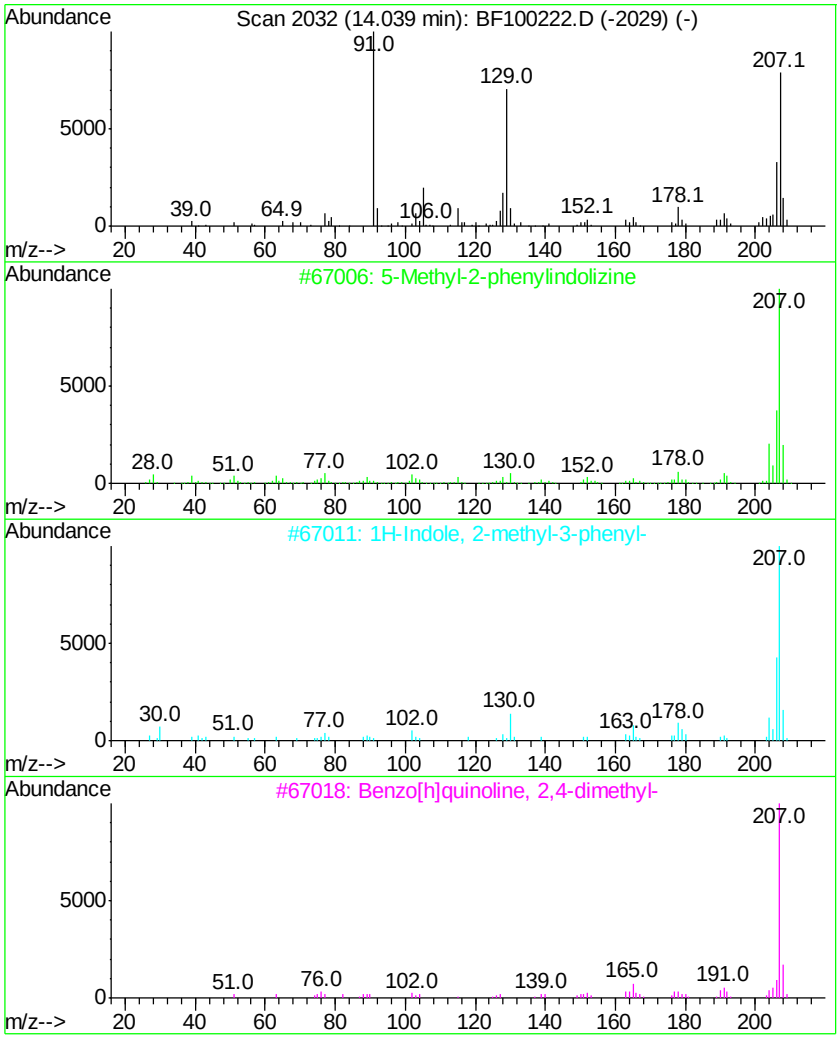
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

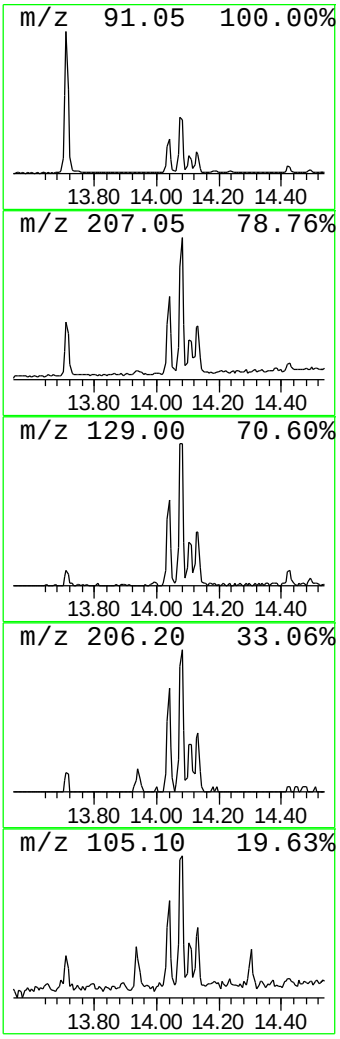
****

Peak Number 7 5-Methyl-2-phenylindolizine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	4.27 ng	101011	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	55
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	46
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	46
4	Indolizine, 2-(4-methylphenyl)-	207	C15H13N	007496-81-3	41
5	Hexahydropyridine, 1-methyl-4-[4...	207	C12H17NO2	094427-47-1	38





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TIC Library : C:\DATABASE\NIST11.L
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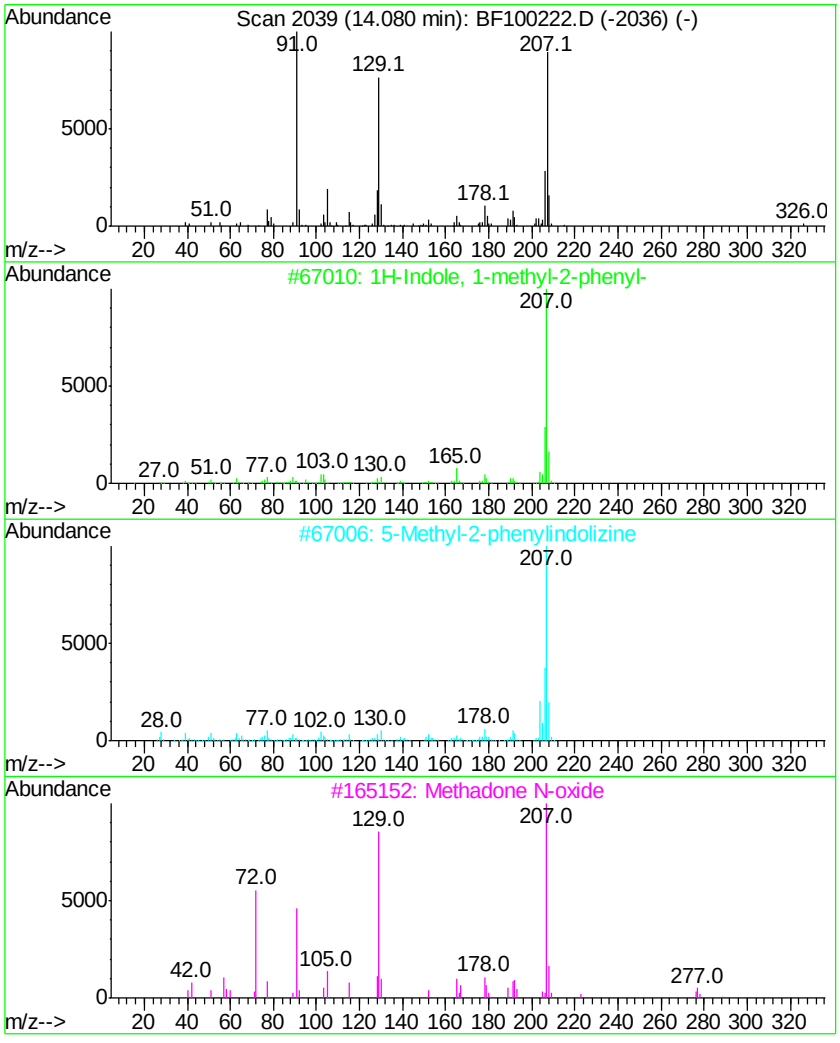
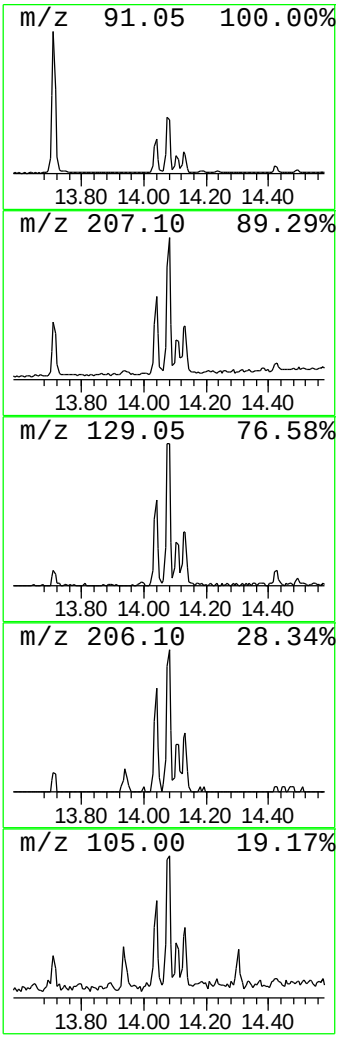
****

Peak Number 8 unknown14.08 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	6.51 ng	154084	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	46
2	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	45
3	Methadone N-oxide	325	C21H27NO2	1000120-80-7	45
4	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	43
5	3-Methyl-2-phenylindole	207	C15H13N	010257-92-8	42





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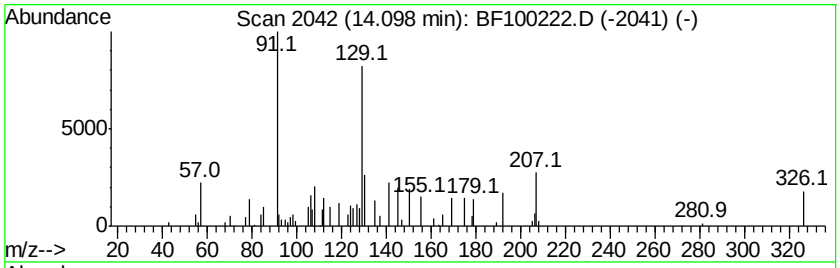
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

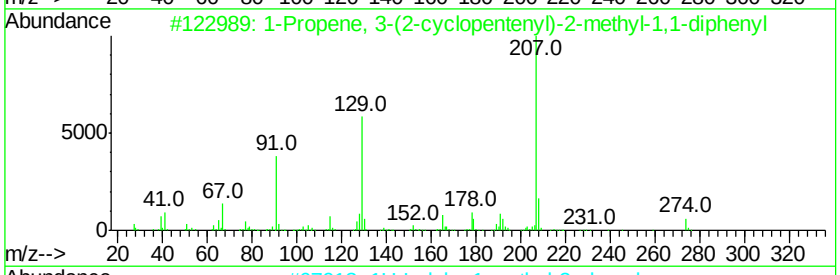
****

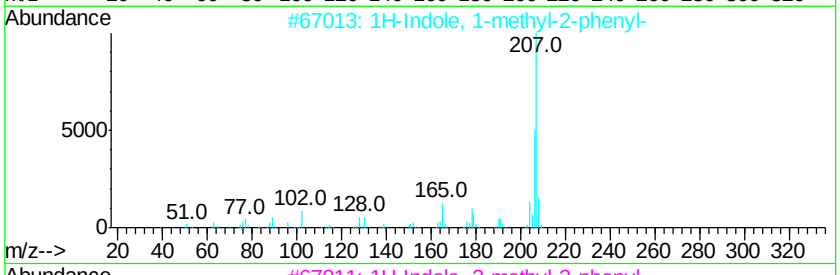
Peak Number 9 1-Propene, 3-(2-cyclopenten... Concentration Rank 13

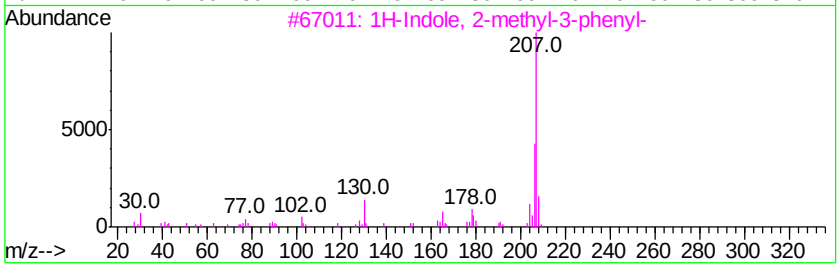
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	2.10 ng	49593	Chrysene-d12	13.94

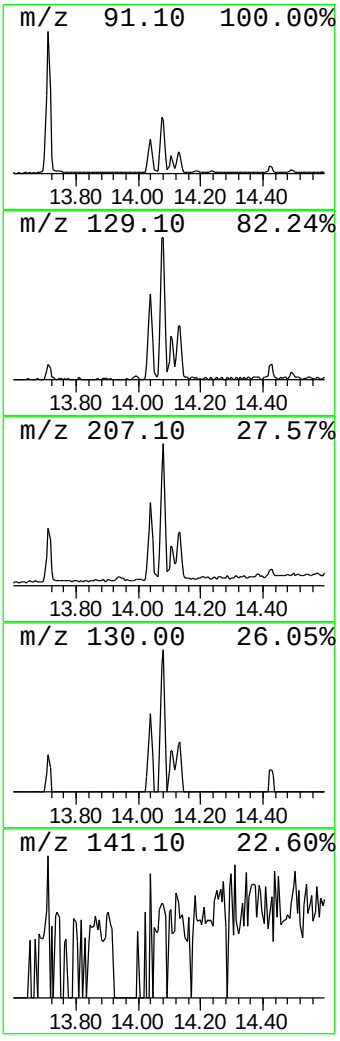
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	50
2	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	42
3	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	42
4	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	32
5	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	30











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Acq On : 5 Nov 2017 14:31
Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-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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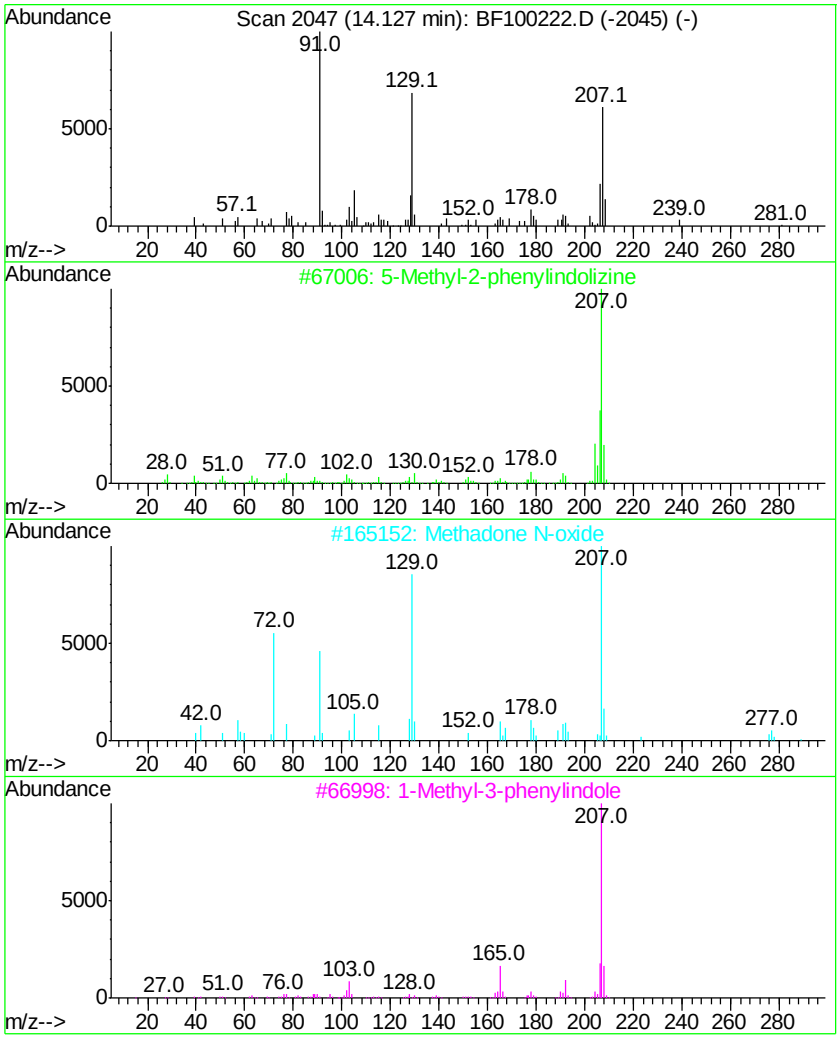
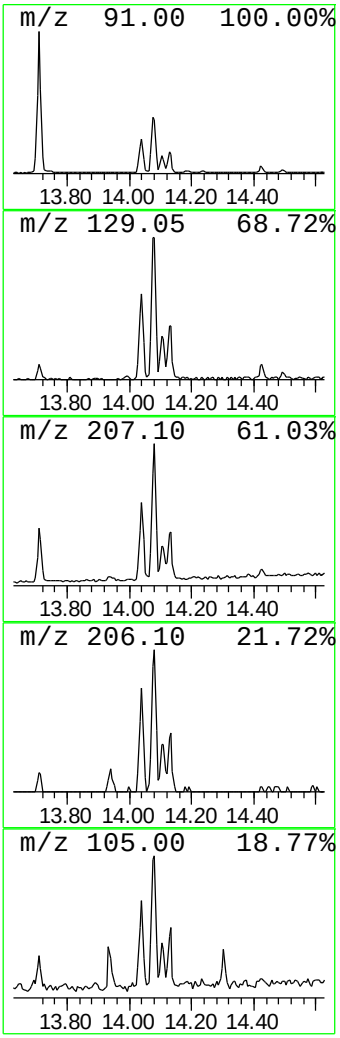
Peak Number 10 unknown14.13 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	2.47 ng	58488	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	46
2	Methadone N-oxide	325	C21H27NO2	1000120-80-7	43
3	1-Methyl-3-phenylindole	207	C15H13N	030020-98-5	38
4	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	38
5	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	37





Library Search Compound Report

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Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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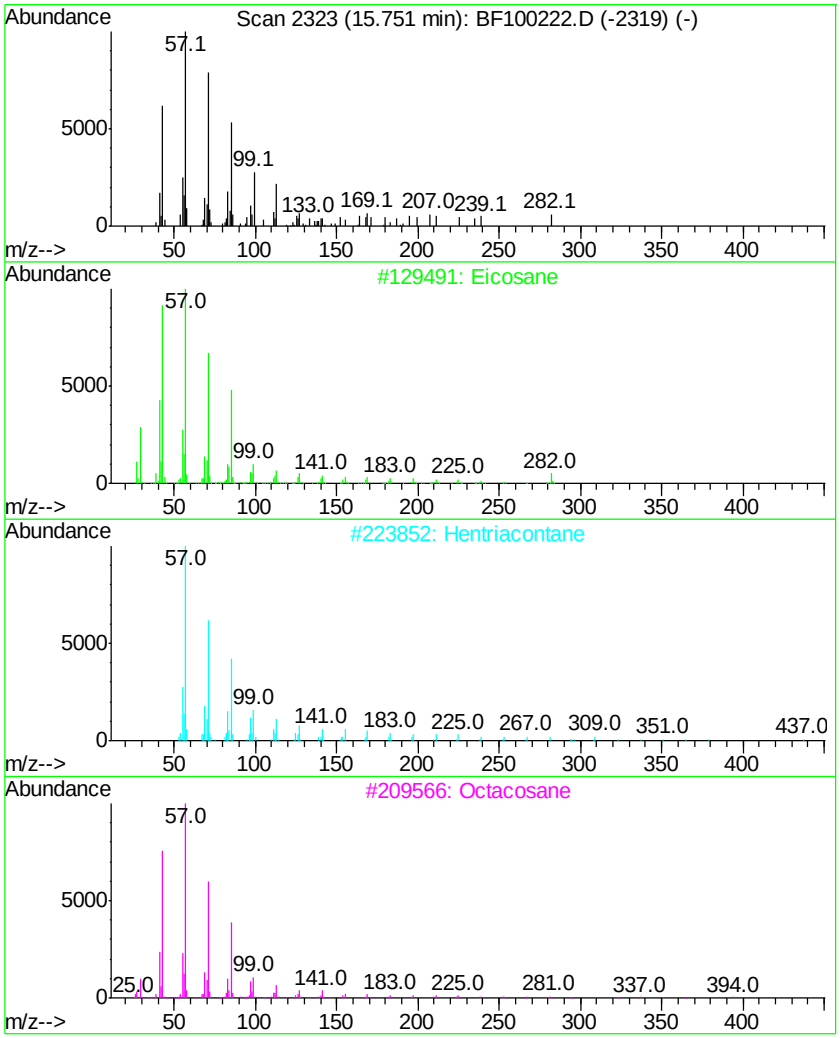
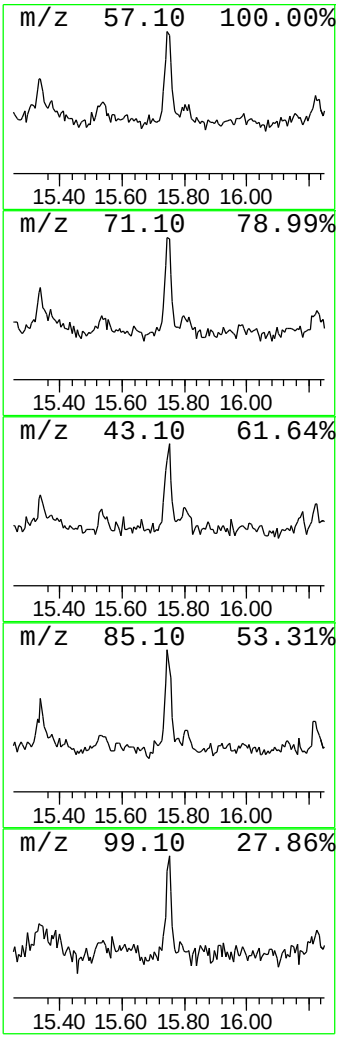
Peak Number 11 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	2.57 ng	63600	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hentriacontane	437	C31H64	000630-04-6	72
3	Octacosane	394	C28H58	000630-02-4	72
4	Heneicosane	296	C21H44	000629-94-7	72
5	Hexacosane	366	C26H54	000630-01-3	68





Library Search Compound Report

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Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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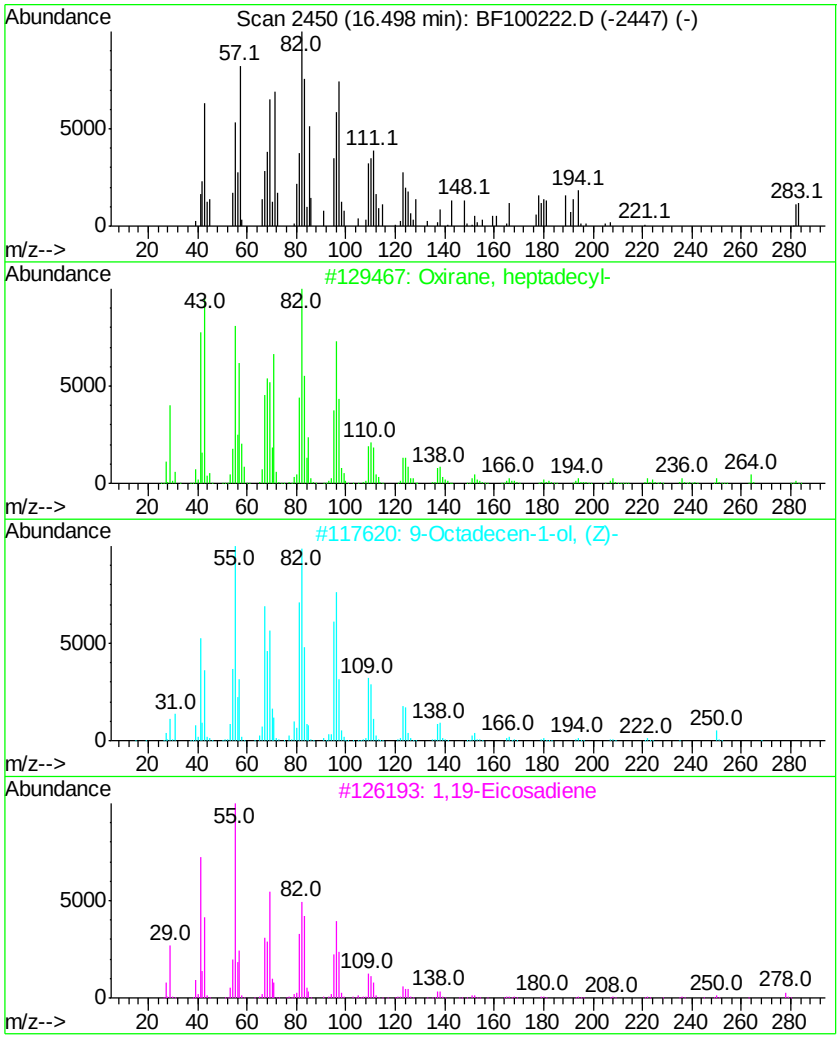
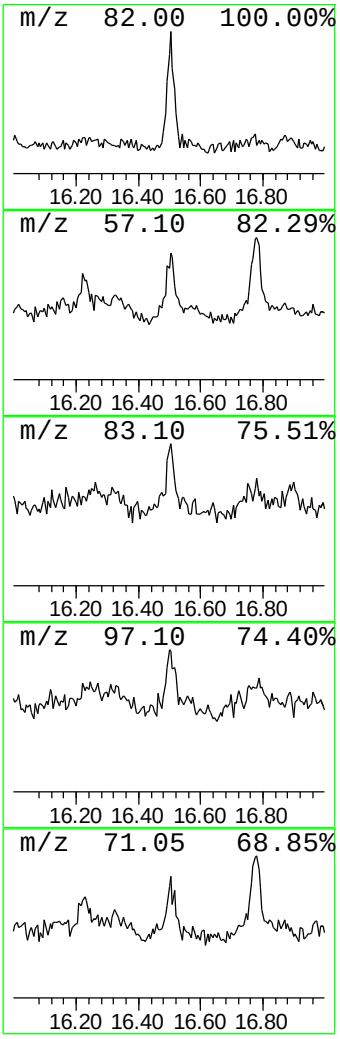
Peak Number 12 Oxirane, heptadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.50	4.03 ng	99841	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	72
2	9-Octadecen-1-ol, (Z)-	268	C18H36O	000143-28-2	50
3	1,19-Eicosadiene	278	C20H38	014811-95-1	49
4	Dodecane, 2-cyclohexyl-	252	C18H36	013151-82-1	35
5	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	25





Library Search Compound Report

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Data File : BF100222.D
Acq On : 5 Nov 2017 14:31
Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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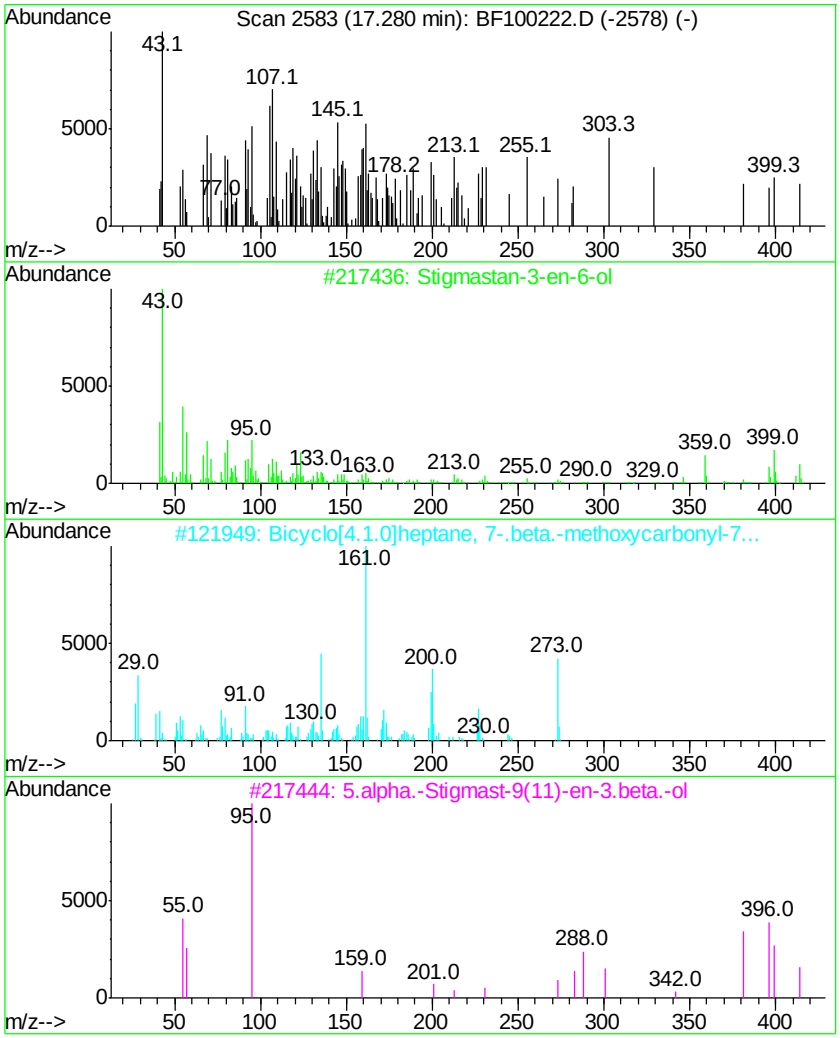
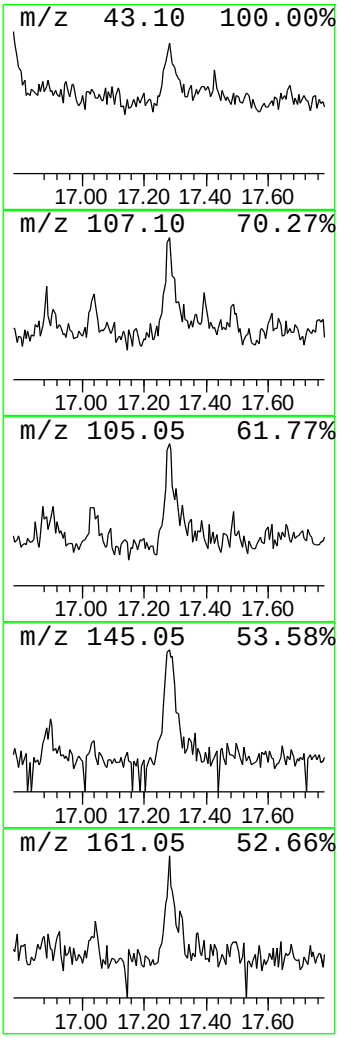
Peak Number 13 unknown17.28 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	5.23 ng	129584	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	9
2	Bicyclo[4.1.0]heptane, 7-.beta.-...	273	C16H19NO3	1000160-35-1	9
3	5.alpha.-Stigmast-9(11)-en-3.bet...	414	C29H50O	077794-81-1	7
4	4-Penten-3-one, 2-methyl-5-(1,3,...	273	C14H19N5O	312311-98-1	7
5	N-(4-Methyl-benzyl)-2-(5-trifluo...	396	C18H15F3N2OS2	1000275-06-6	4





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF110517\
Data File : BF100222.D
Acq On : 5 Nov 2017 14:31
Operator : SJ/JU
Sample : I6267-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P001-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...	4.99	11.7	ng	278640	1	6.76	476533	20.0
unknown6.54	6.54	81.3	ng	1936110	1	6.76	476533	20.0
Pentadecanoic acid	11.80	3.0	ng	82771	4	11.29	545215	20.0
unknown13.71	13.71	8.5	ng	201548	5	13.94	473403	20.0
Trichloroacetic a...	13.74	2.4	ng	57103	5	13.94	473403	20.0
5-Methyl-2-phenyl...	14.04	4.3	ng	101011	5	13.94	473403	20.0
unknown14.08	14.08	6.5	ng	154084	5	13.94	473403	20.0
1-Propene, 3-(2-c...	14.10	2.1	ng	49593	5	13.94	473403	20.0
unknown14.13	14.13	2.5	ng	58488	5	13.94	473403	20.0
Eicosane	15.75	2.6	ng	63600	6	15.40	495574	20.0
Oxirane, heptadecyl-	16.50	4.0	ng	99841	6	15.40	495574	20.0
unknown17.28	17.28	5.2	ng	129584	6	15.40	495574	20.0