LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024712.D
Acq On : 5 Nov 2016 14:38
Operator : UM/SJ
Sample : H5527-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-99-7.95-15.0

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_G\METHODS\8270-BG102516.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	3.599	124	129	144	rVB2	216449	402129	4.45%	0.909%
2	4.716	314	319	328	rVB	244527	383362	4.24%	0.867%
3	5.327	417	423	430	rBV	263671	416141	4.60%	0.941%
4	5.797	495	503	516	rBV	1184354	1993803	22.05%	4.508%
5	7.401	768	776	791	rVB2	844009	1767549	19.55%	3.996%
6	7.788	834	842	856	rBV	1656871	3052738	33.77%	6.902%
7	8.264	916	923	930	rBV	360247	649409	7.18%	1.468%
8	8.593	972	979	989	rVB	1406955	2534985	28.04%	5.732%
9	9.439	1115	1123	1132	rBV	1274160	2335158	25.83%	5.280%
10	11.090	1396	1404	1411	rBV	460933	878003	9.71%	1.985%
11	11.843	1526	1532	1539	rBV2	80632	144605	1.60%	0.327%
12	13.505	1807	1815	1824	rBV	3234386	5075920	56.14%	11.477%
13	14.322	1948	1954	1959	rBV	338020	519179	5.74%	1.174%
14	14.880	2039	2049	2056	rBV	793010	1279496	14.15%	2.893%
15	15.280	2113	2117	2123	rVB	60660	100907	1.12%	0.228%
16	15.679	2181	2185	2189	rVB	77580	102440	1.13%	0.232%
17	16.085	2238	2254	2257	rBV9	32704	95786	1.06%	0.217%
18	16.367	2294	2302	2310	rBV	3240236	5186438	57.37%	11.727%
19	16.537	2326	2331	2337	rBV	100824	162489	1.80%	0.367%
20	17.277	2450	2457	2462	rBV2	125254	211806	2.34%	0.479%
21	17.624	2509	2516	2520	rBV	1111304	1778937	19.68%	4.022%
22	17.665	2520	2523	2529	rVB	226252	329577	3.65%	0.745%
23	18.464	2654	2659	2667	rBV4	167854	270051	2.99%	0.611%
24	19.028	2750	2755	2761	rVB4	60233	98565	1.09%	0.223%
25	19.657	2857	2862	2867	rVB	130952	205792	2.28%	0.465%
26	20.021	2920	2924	2929	rVB	89298	133724	1.48%	0.302%
27	20.203	2948	2955	2963	rBV	6622696	9040899	100.00%	20.442%
28	21.496	3170	3175	3184	rBV4	183011	351563	3.89%	0.795%
29	21.919	3239	3247	3253	rBV	1347506	2390612	26.44%	5.405%
30	25.344	3819	3830	3845	rVB2	741390	2335579	25.83%	5.281%

Sum of corrected areas: 44227642

LSC Report - Integrated Chromatogram

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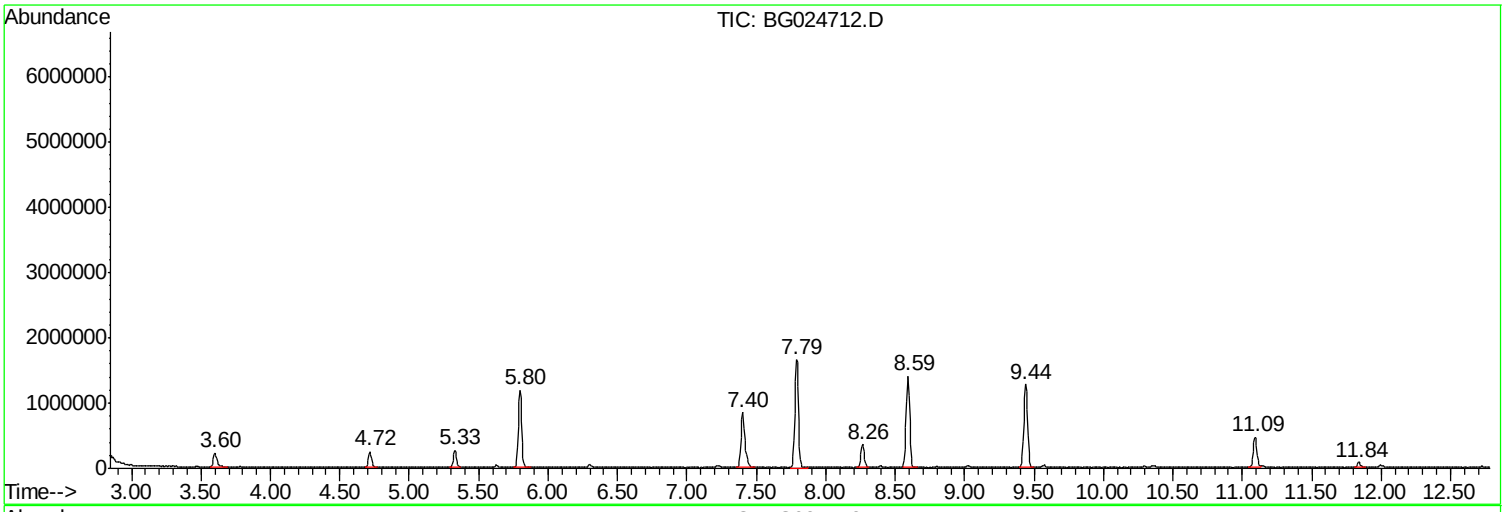
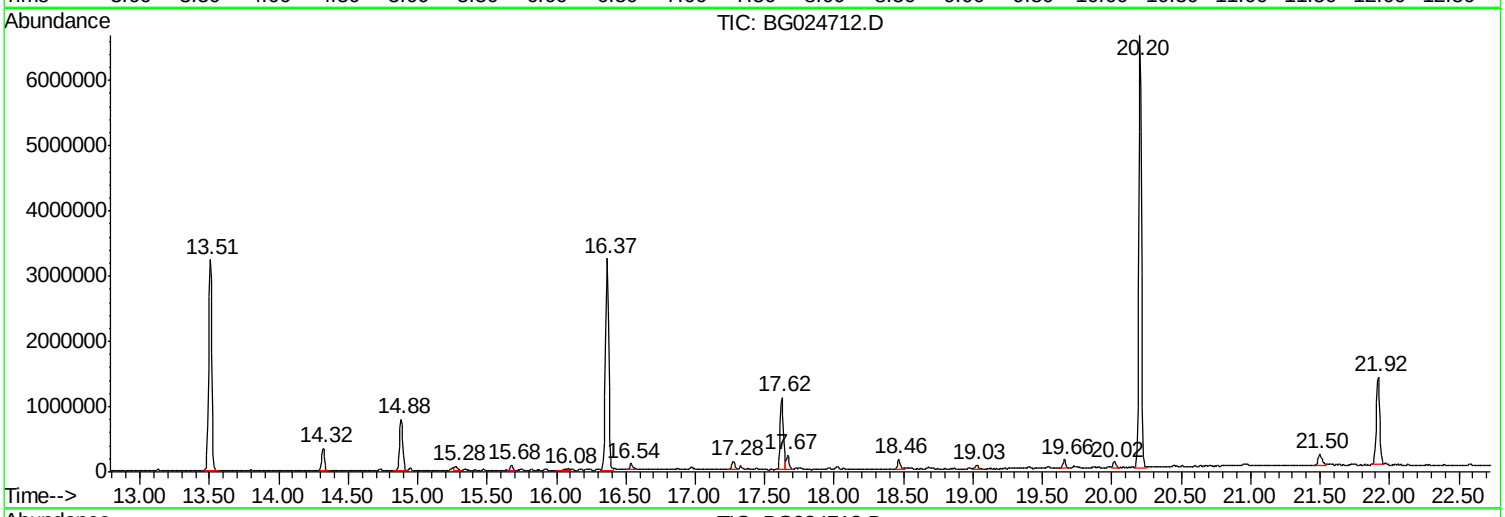
Data File : BG024712.D
Acq On : 5 Nov 2016 14:38
Operator : UM/SJ
Sample : H5527-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

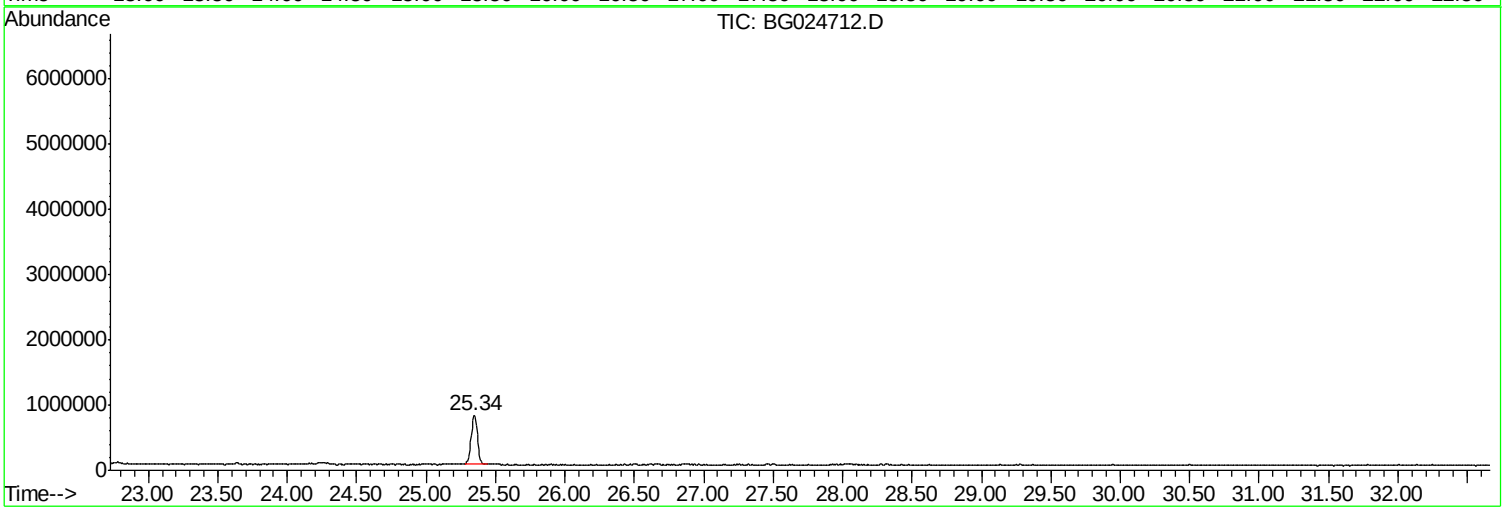
Instrument :
BNA_G
ClientSampleId :
GW-99-7.95-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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

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Sample : H5527-02
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Instrument :
BNA_G
ClientSampleId :
GW-99-7.95-15.0

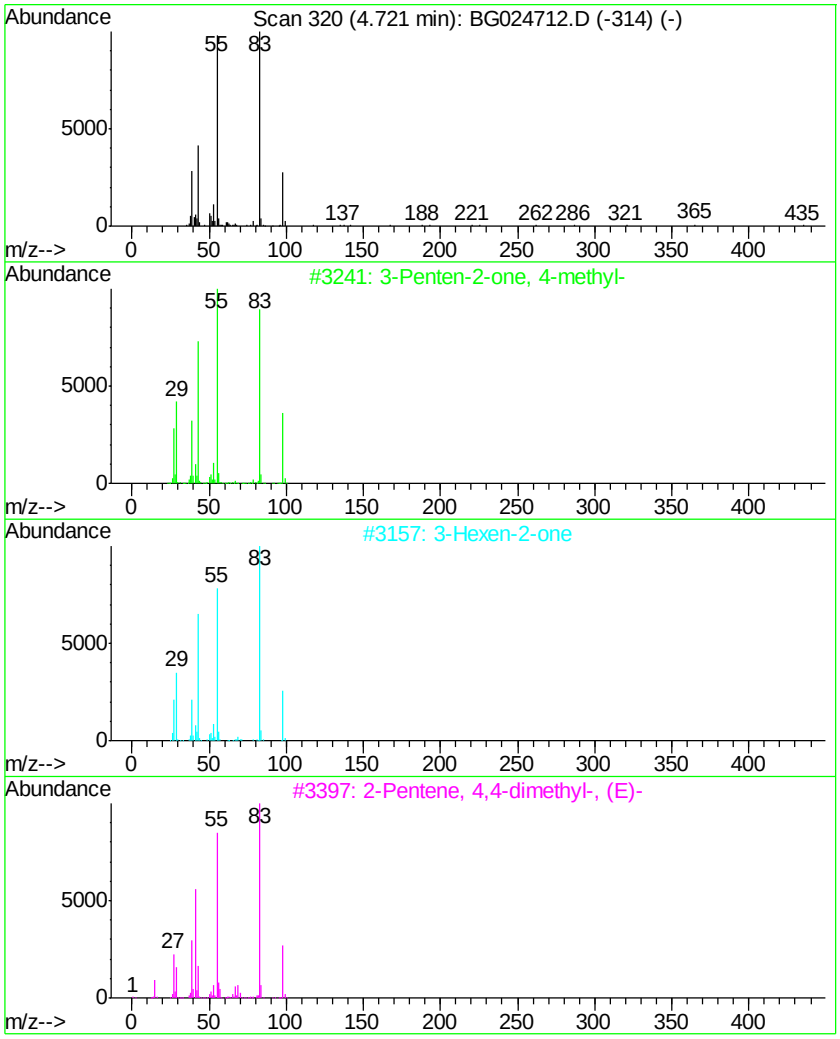
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

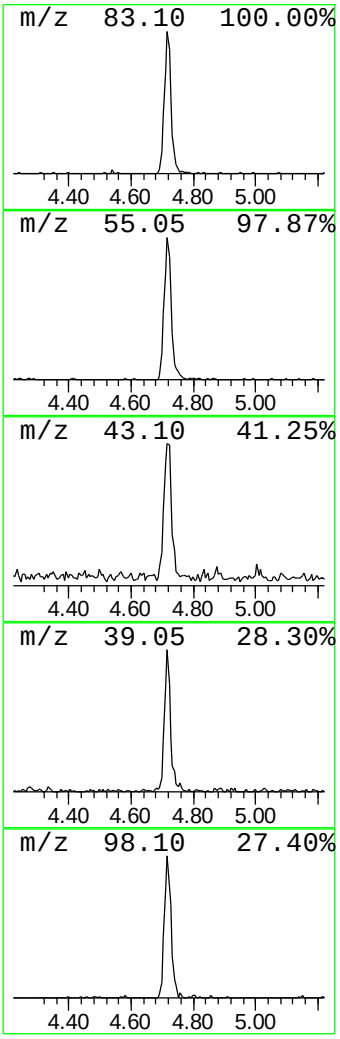
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	11.81 ng	383362	1,4-Dichlorobenzene-d4	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72





Library Search Compound Report

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Operator : UM/SJ
Sample : H5527-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-99-7.95-15.0

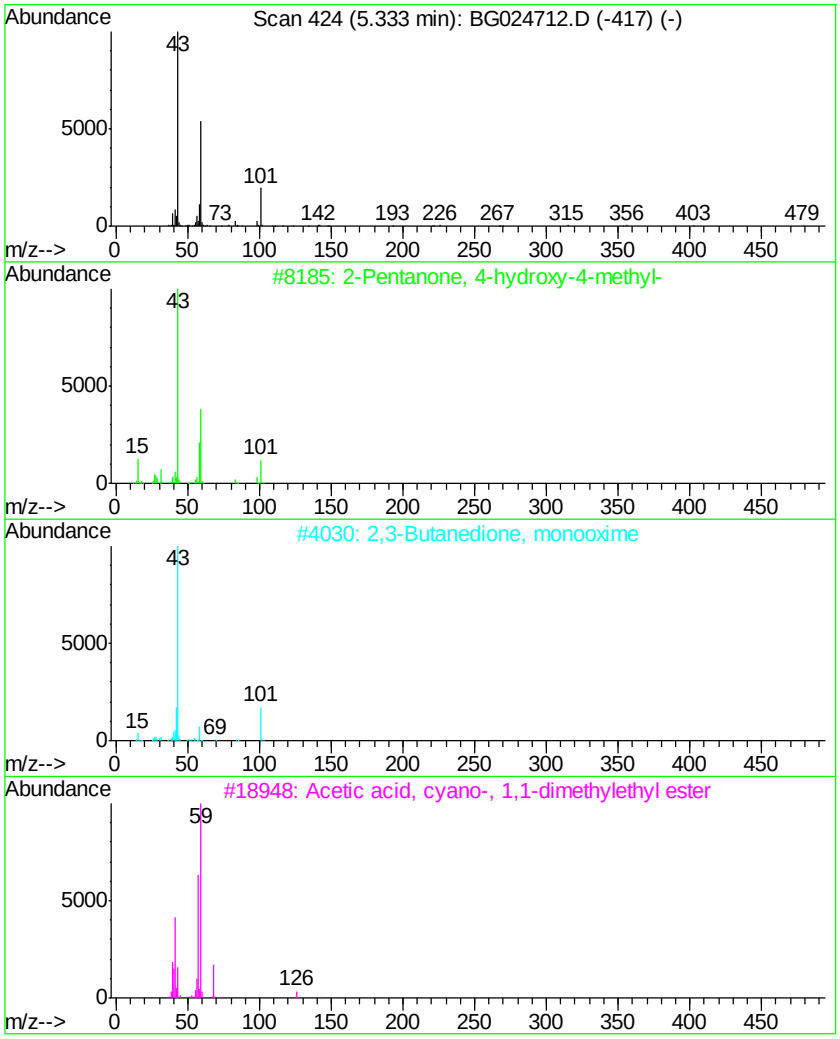
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

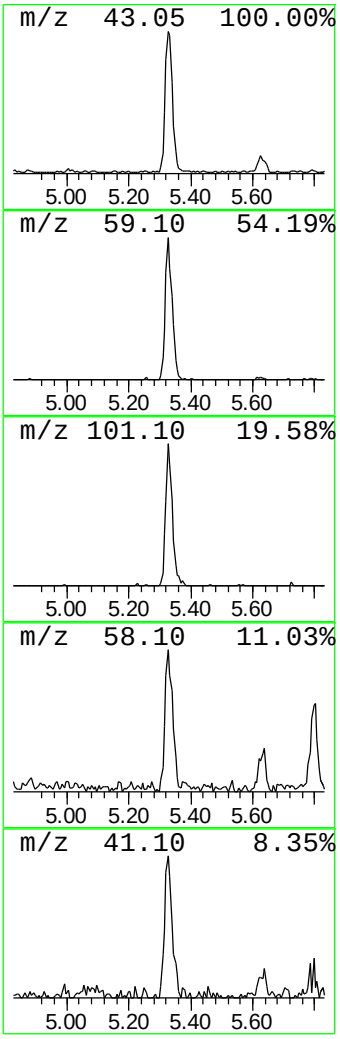
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	12.82 ng	416141	1,4-Dichlorobenzene-d4	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	12
5	3-Pentanol	88	C5H12O	000584-02-1	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H5527-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-99-7.95-15.0

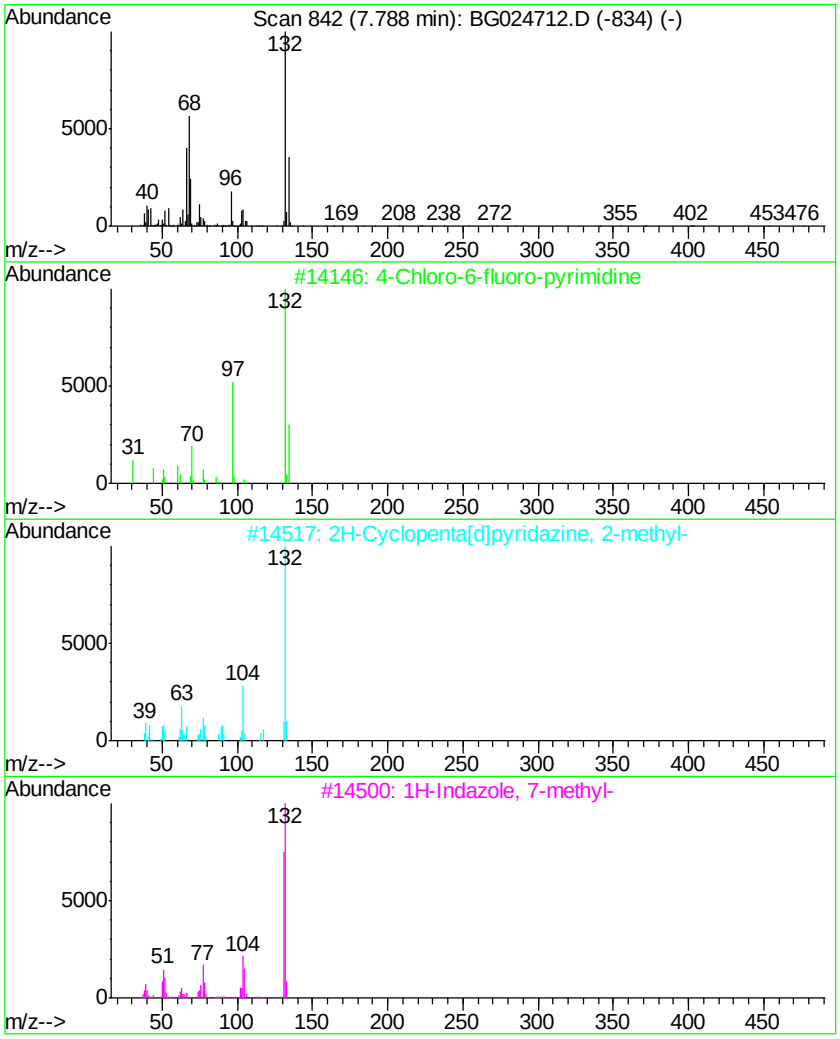
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

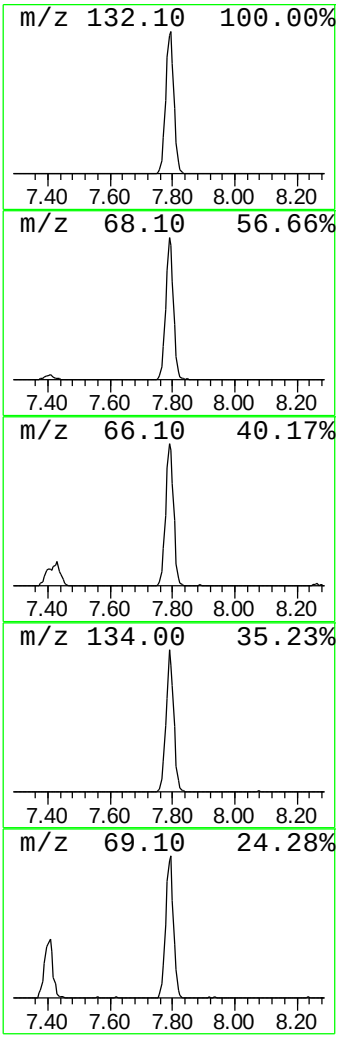
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown7.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	94.02 ng	3052740	1,4-Dichlorobenzene-d4	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

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Operator : UM/SJ
Sample : H5527-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-99-7.95-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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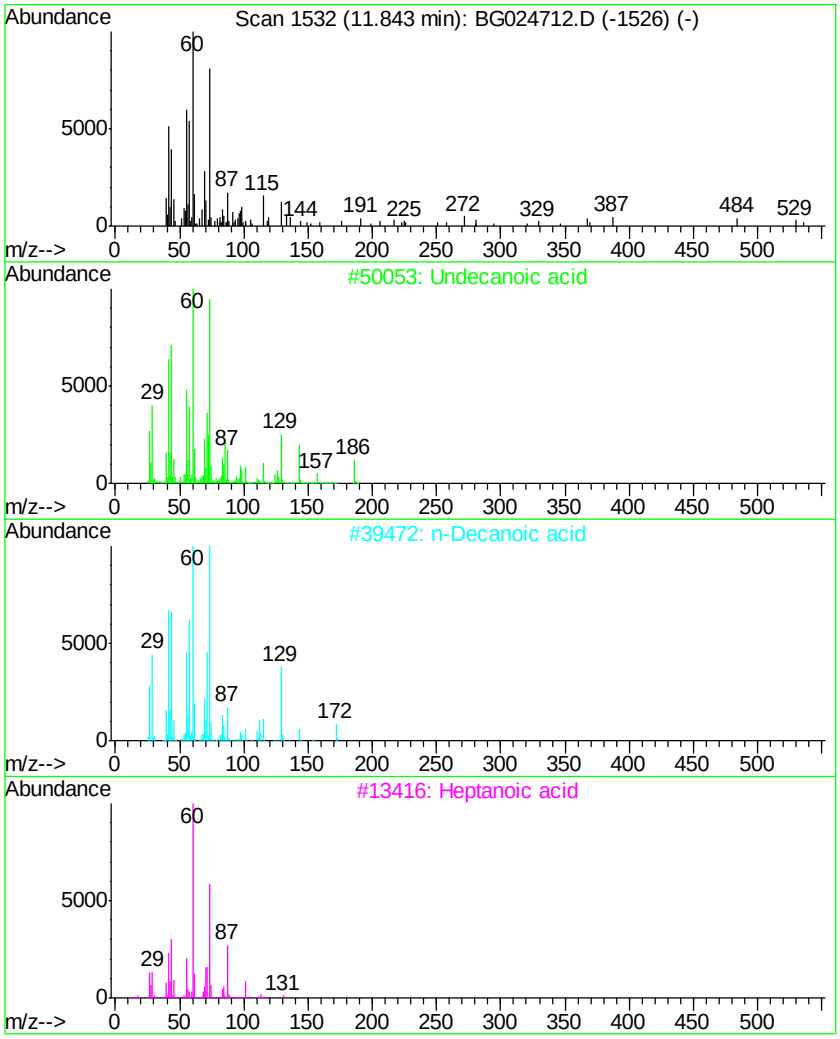
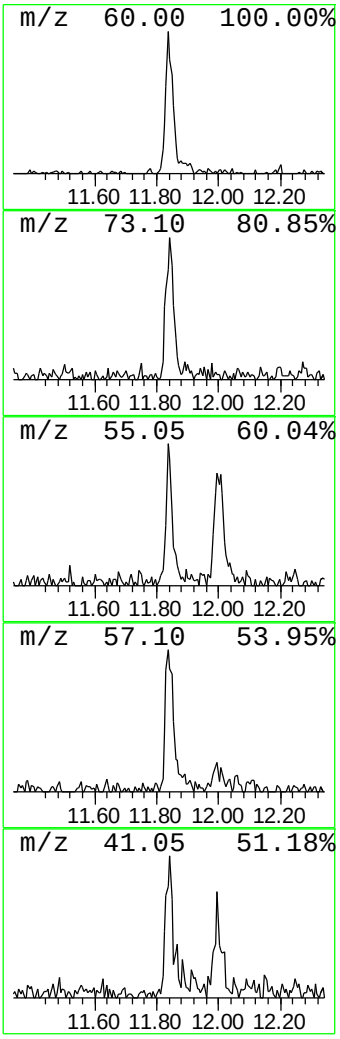
****

Peak Number 6 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	3.29 ng	144605	Naphthalene-d8	11.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	n-Decanoic acid	172	C10H20O2	000334-48-5	59
3	Heptanoic acid	130	C7H14O2	000111-14-8	50
4	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	47
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	45





Library Search Compound Report

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ClientSampleId :
GW-99-7.95-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

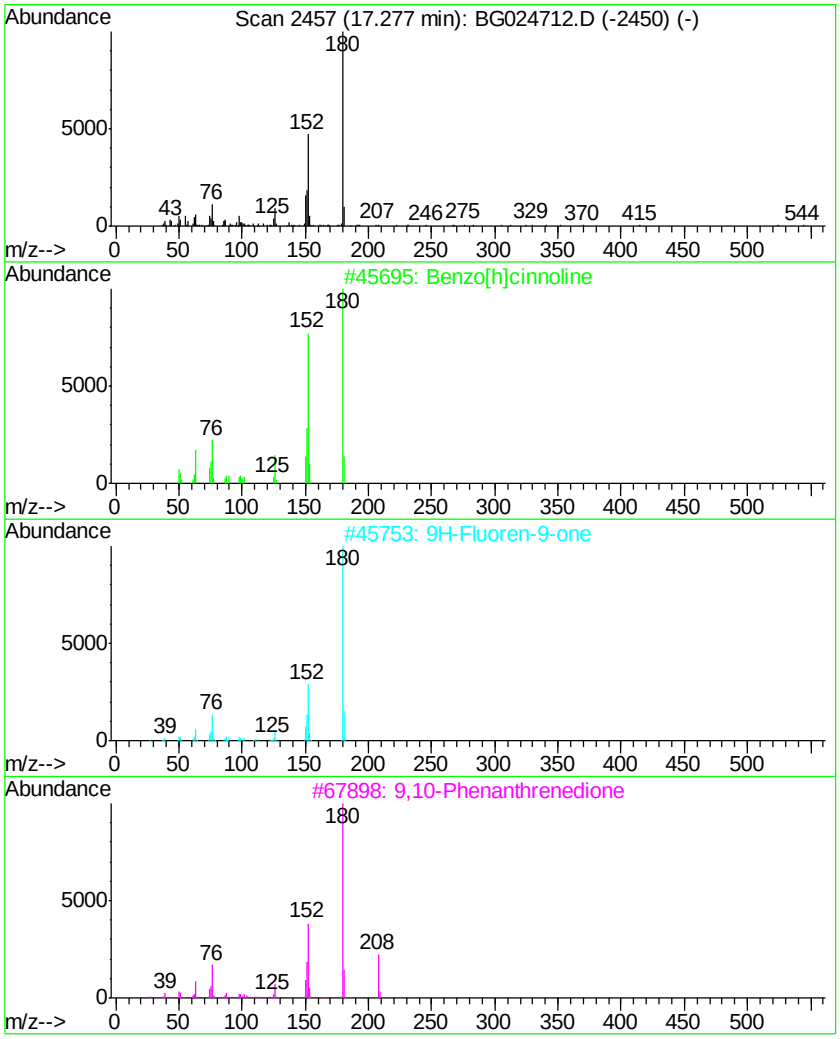
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

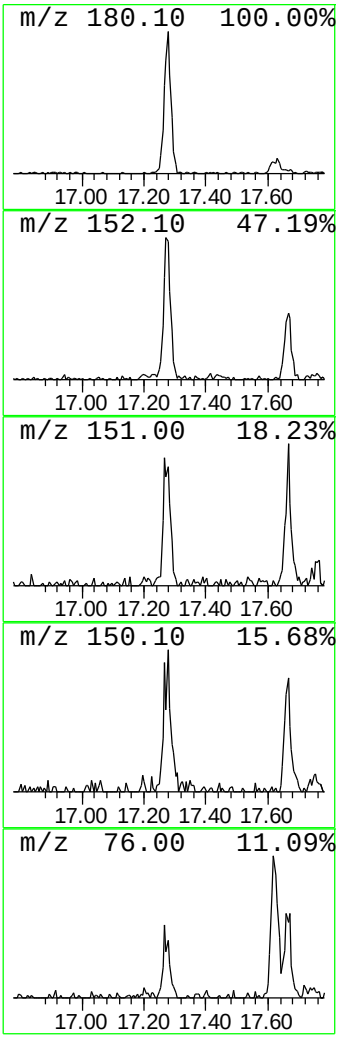
****

Peak Number 7 Benzo[h]cinnoline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.28	2.38 ng	211806	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	90
2	9H-Fluoren-9-one	180	C13H8O	000486-25-9	86
3	9,10-Phenanthrenedione	208	C14H8O2	000084-11-7	83
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	78
5	2,3-Diazaphenanthrene	180	C12H8N2	000229-72-1	59





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BNA_G
ClientSampleId :
GW-99-7.95-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

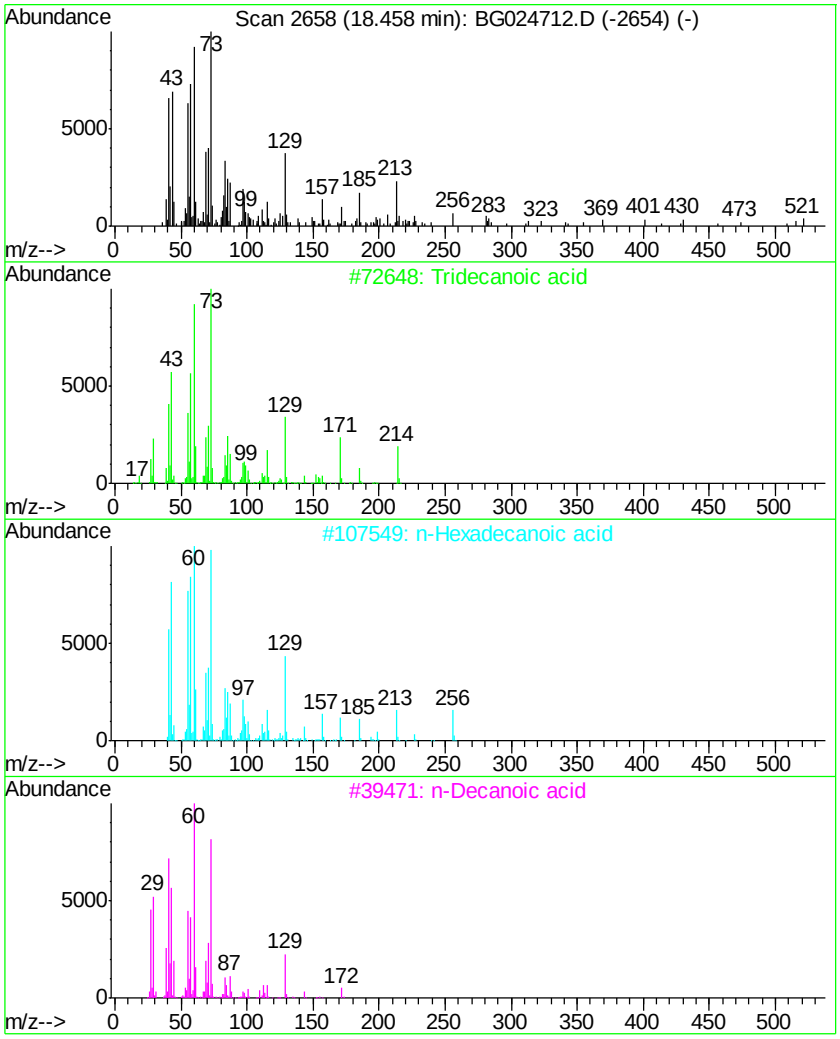
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

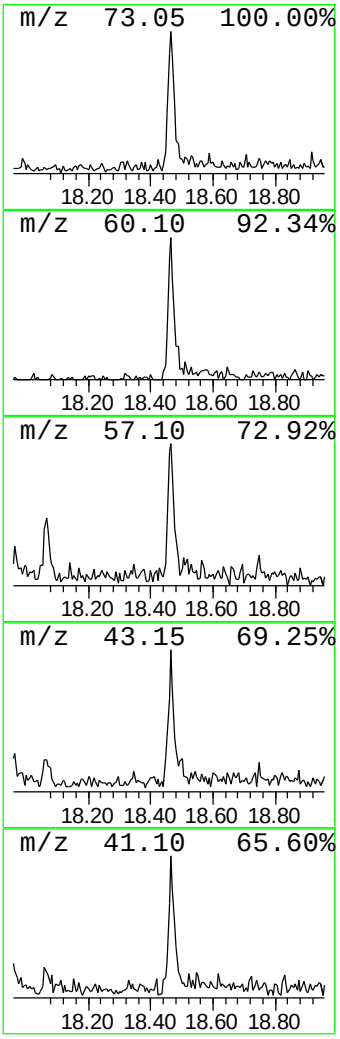
****

Peak Number 8 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.46	3.04 ng	270051	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	n-Decanoic acid	172	C10H20O2	000334-48-5	60
4	Undecanoic acid	186	C11H22O2	000112-37-8	52
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	50





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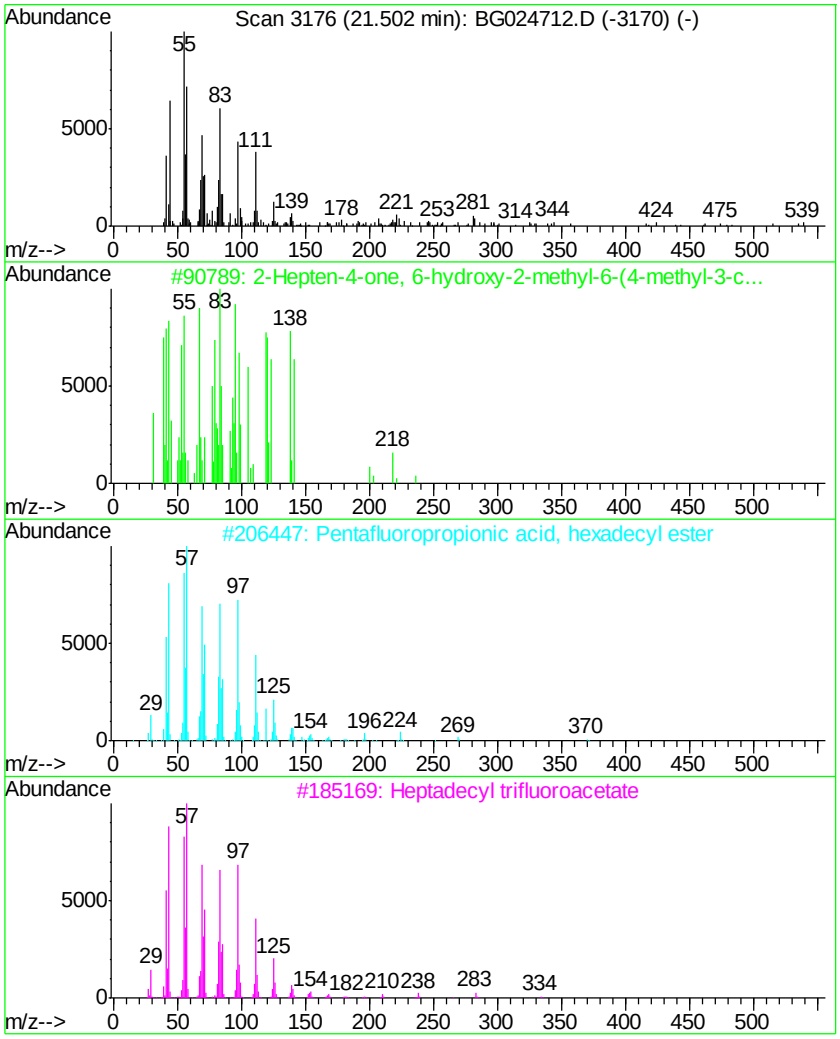
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

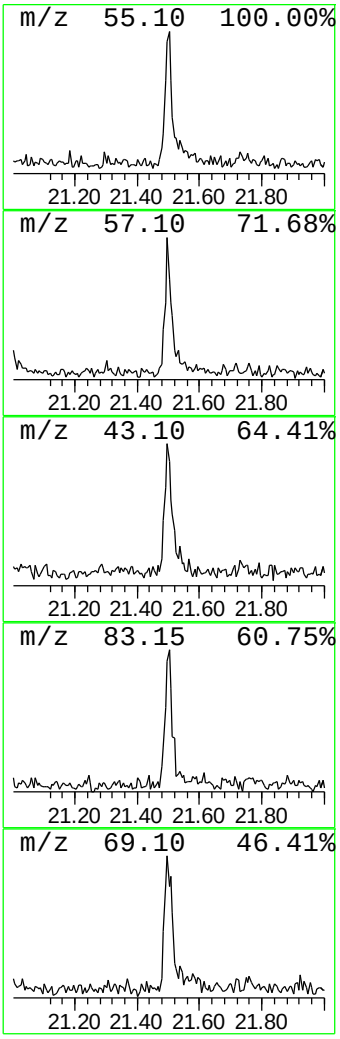
****

Peak Number 9 2-Hepten-4-one, 6-hydroxy-2... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	2.94 ng	351563	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-4-one, 6-hydroxy-2-meth...	236	C15H24O2	038043-98-0	94
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
4	Fumaric acid, 2-decyl tridecyl e...	438	C27H50O4	1000348-59-4	87
5	Octacosanol	410	C28H58O	000557-61-9	87





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
3-Penten-2-one, 4...	4.72	11.8	ng	383362	1	8.26	649409	20.0
2-Pentanone, 4-hy...	5.33	12.8	ng	416141	1	8.26	649409	20.0
unknown7.79	7.79	94.0	ng	3052740	1	8.26	649409	20.0
Undecanoic acid	11.84	3.3	ng	144605	2	11.09	878003	20.0
Benzo[h]cinnoline	17.28	2.4	ng	211806	4	17.62	1778940	20.0
Tridecanoic acid	18.46	3.0	ng	270051	4	17.62	1778940	20.0
2-Hepten-4-one, 6...	21.50	2.9	ng	351563	5	21.92	2390610	20.0