LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088745.D
Acq On : 6 Jul 2016 20:31
Operator : UM/SJ
Sample : H3880-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C2.1-01

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-BF063016.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	1.701	8	10	19	rVB	179356	294648	10.00%	1.496%
2	1.827	19	21	58	rVB	1479888	2947261	100.00%	14.959%
3	4.902	287	290	293	rBV	136857	160936	5.46%	0.817%
4	5.336	325	328	330	rBV	1436633	1318544	44.74%	6.692%
5	6.376	416	419	422	rBV	1128410	1314057	44.59%	6.670%
6	6.513	428	431	433	rBV	1584038	1510634	51.26%	7.667%
7	6.742	449	451	454	rVB	521902	509669	17.29%	2.587%
8	6.902	462	465	467	rVB	1277842	1059813	35.96%	5.379%
9	7.313	498	501	503	rBV	784588	985177	33.43%	5.000%
10	8.033	561	564	566	rBV	806944	767362	26.04%	3.895%
11	9.108	655	658	660	rBV	2067268	1747667	59.30%	8.870%
12	9.496	690	692	695	rVV	212031	244010	8.28%	1.239%
13	9.782	714	717	719	rBV	885516	876625	29.74%	4.449%
14	10.559	783	785	788	rBV	816407	708535	24.04%	3.596%
15	10.696	795	797	803	rVB	37114	43838	1.49%	0.223%
16	11.142	833	836	837	rBV	47948	43589	1.48%	0.221%
17	11.256	843	846	848	rVB	996463	915713	31.07%	4.648%
18	12.834	982	984	987	rBV	1514895	1738006	58.97%	8.821%
19	13.268	1019	1022	1024	rBV	63015	57749	1.96%	0.293%
20	13.748	1061	1064	1073	rBV2	87060	150197	5.10%	0.762%
21	13.874	1073	1075	1078	rBV	887597	828516	28.11%	4.205%
22	14.731	1147	1150	1152	rBV	67659	74770	2.54%	0.380%
23	15.257	1193	1196	1199	rBV	563987	623592	21.16%	3.165%
24	17.509	1389	1393	1404	rVB2	23870	88797	3.01%	0.451%
25	17.817	1415	1420	1431	rVB4	28475	105702	3.59%	0.537%
26	18.491	1470	1479	1483	rBV6	9577	34668	1.18%	0.176%
27	18.937	1511	1518	1527	rVB	191328	551958	18.73%	2.802%

Sum of corrected areas: 19702033

LSC Report - Integrated Chromatogram

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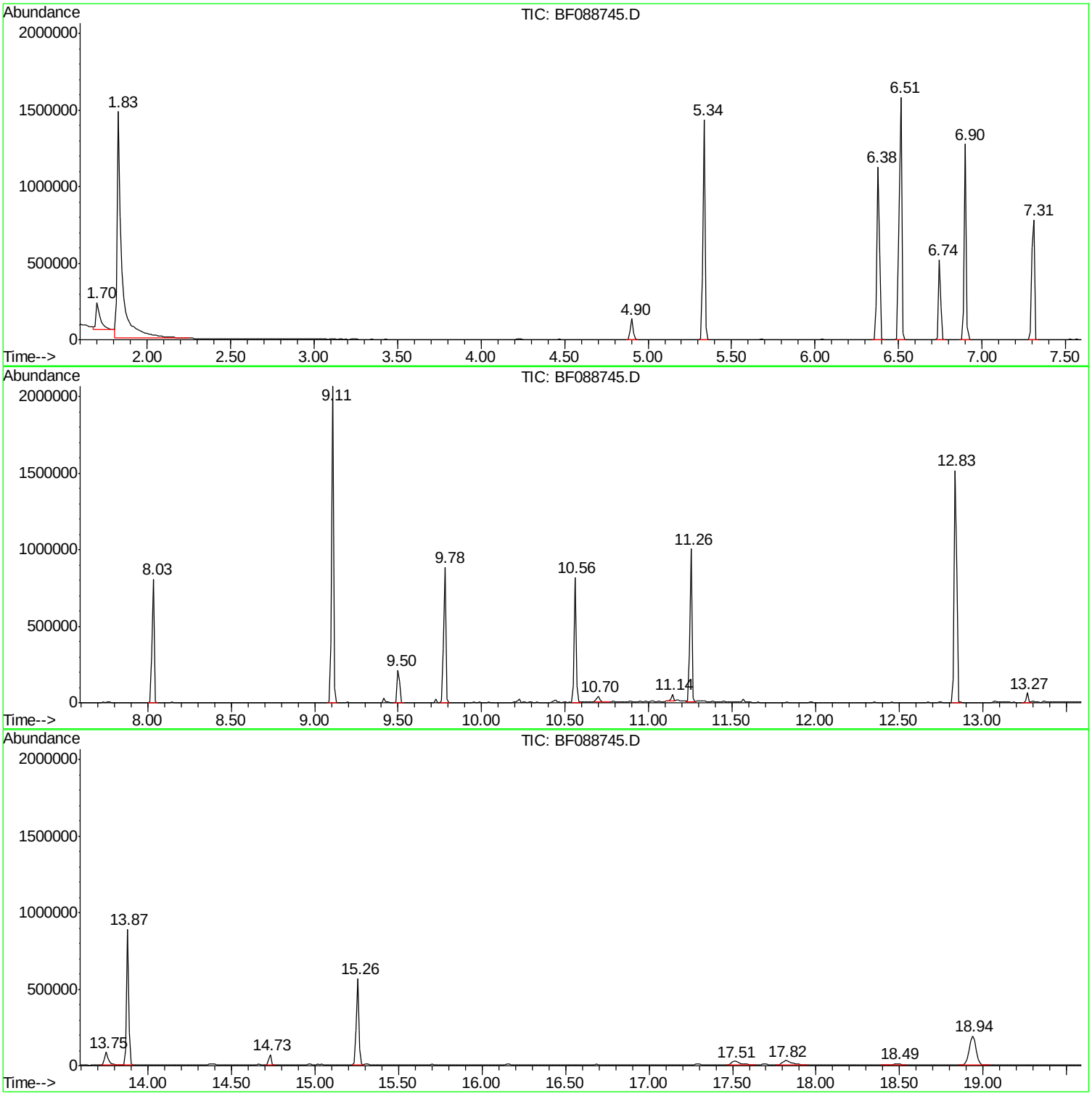
Sample : H3880-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C2.1-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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Data File : BF088745.D
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Operator : UM/SJ
Sample : H3880-01
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C2.1-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

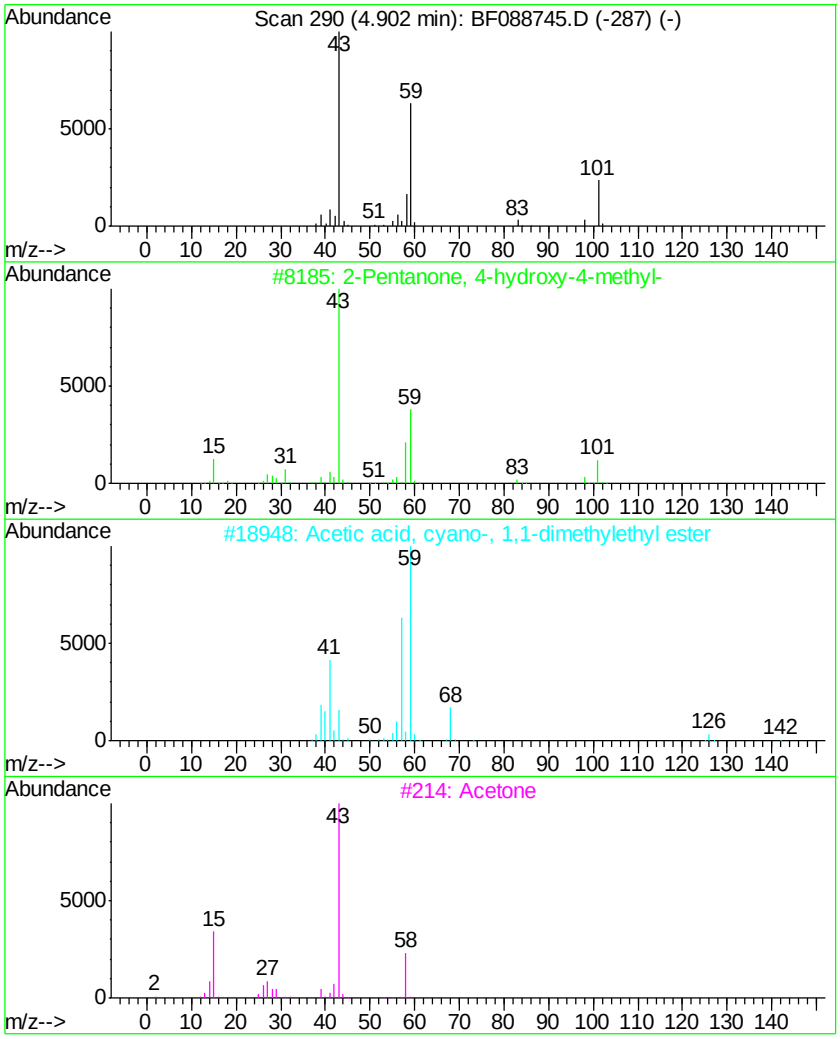
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

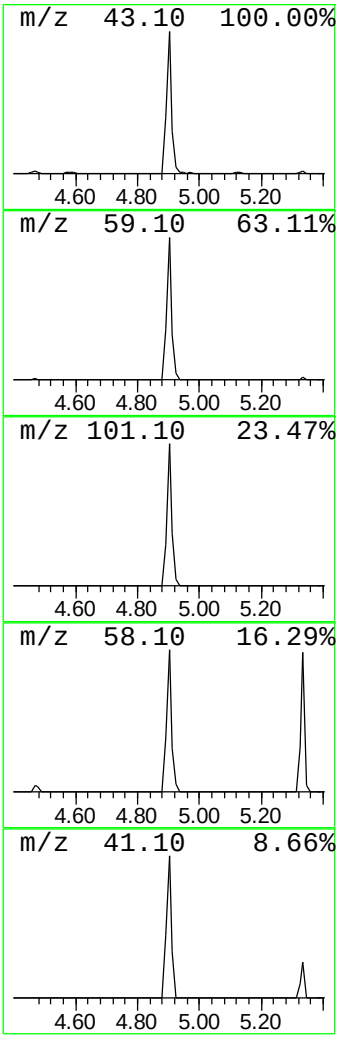
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	6.32 ng	160936	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Acetone	58	C3H6O	000067-64-1	10
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H3880-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C2.1-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

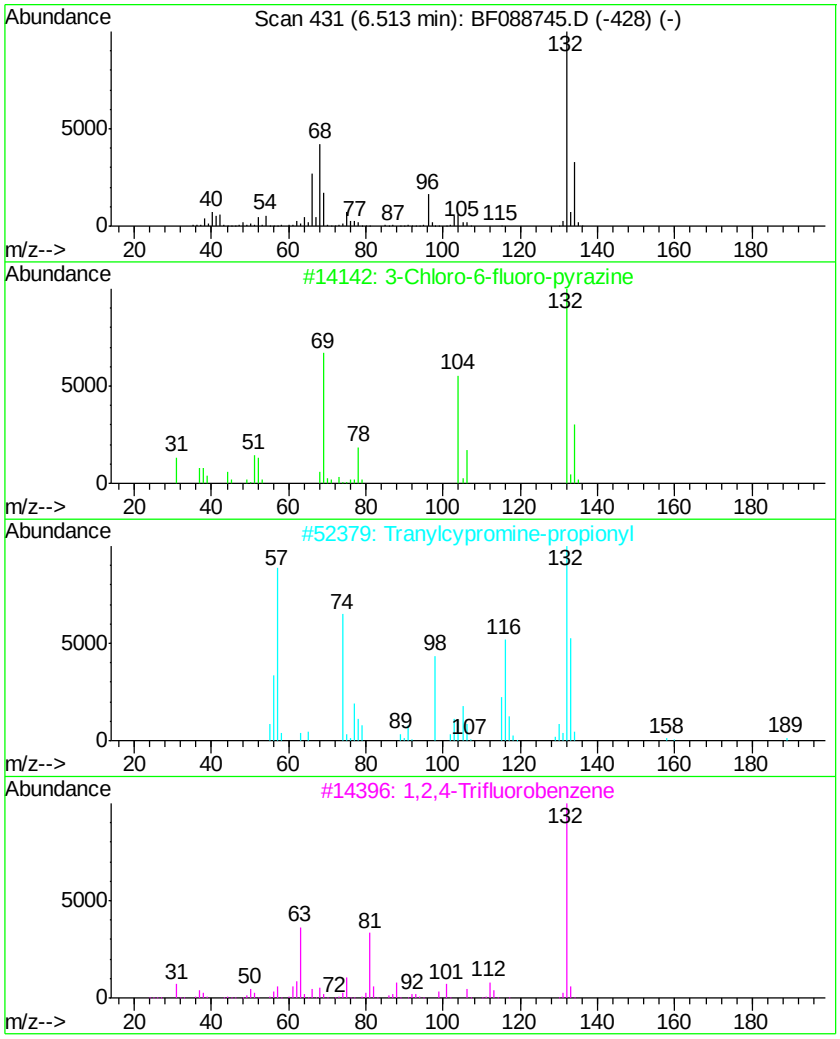
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

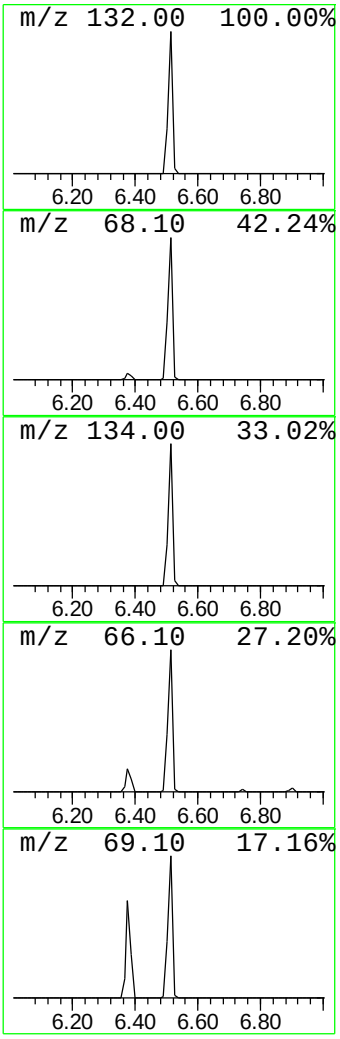
****

Peak Number 4 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	59.28 ng	1510630	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088745.D
Acq On : 6 Jul 2016 20:31
Operator : UM/SJ
Sample : H3880-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C2.1-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

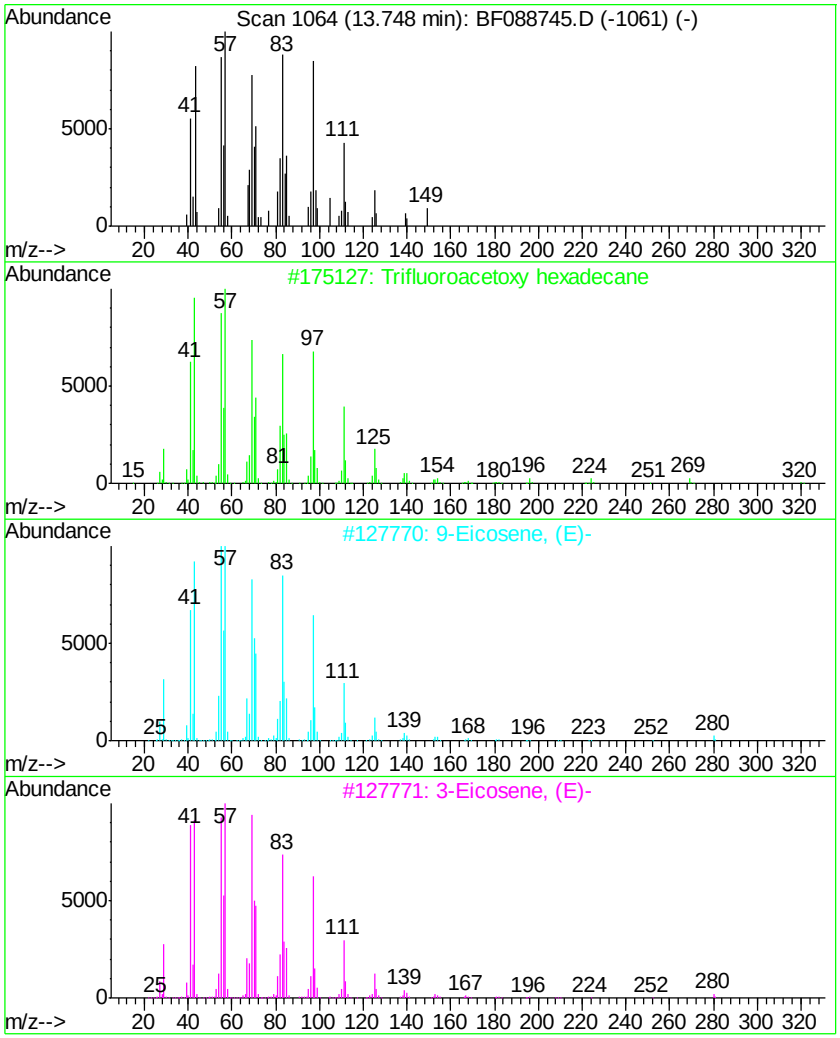
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

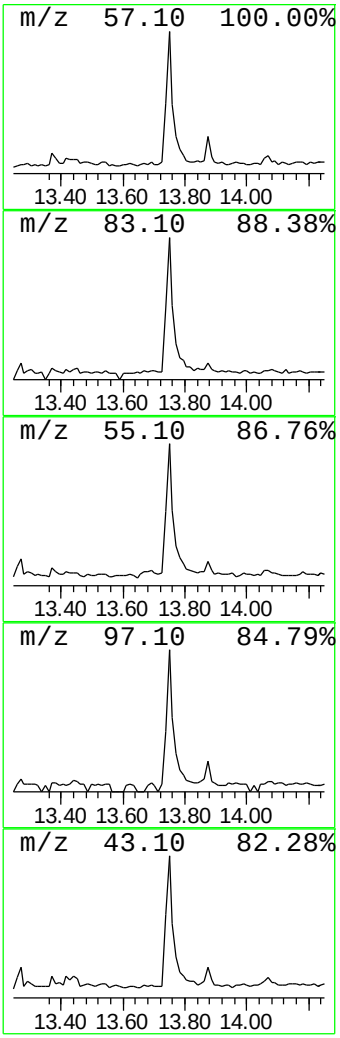
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.63 ng	150197	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	90
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088745.D
Acq On : 6 Jul 2016 20:31
Operator : UM/SJ
Sample : H3880-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C2.1-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

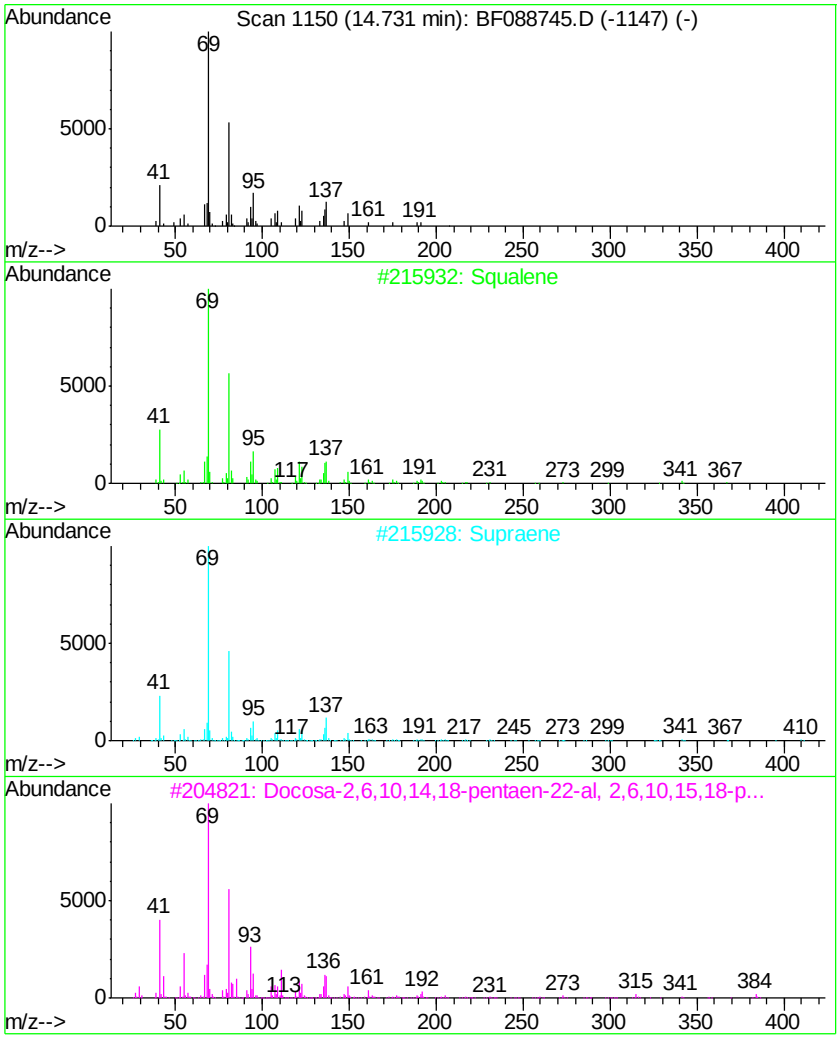
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

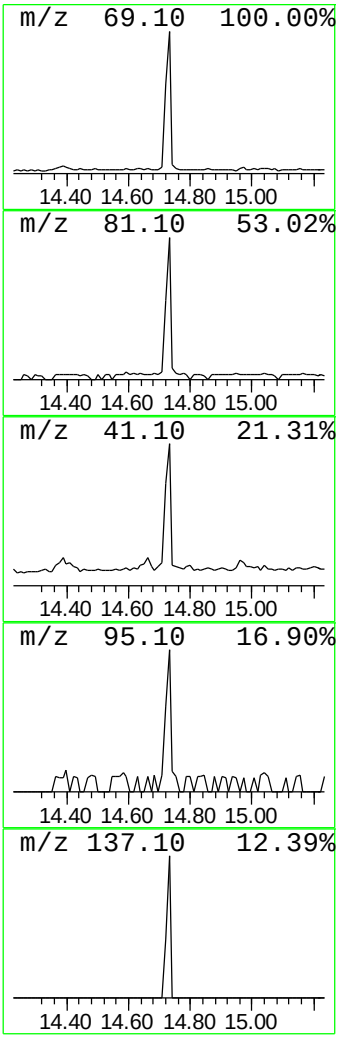
****

Peak Number 7 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.40 ng	74770	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	64
5	trans-Farnesol	222	C15H26O	000106-28-5	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
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Acq On : 6 Jul 2016 20:31
Operator : UM/SJ
Sample : H3880-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C2.1-01

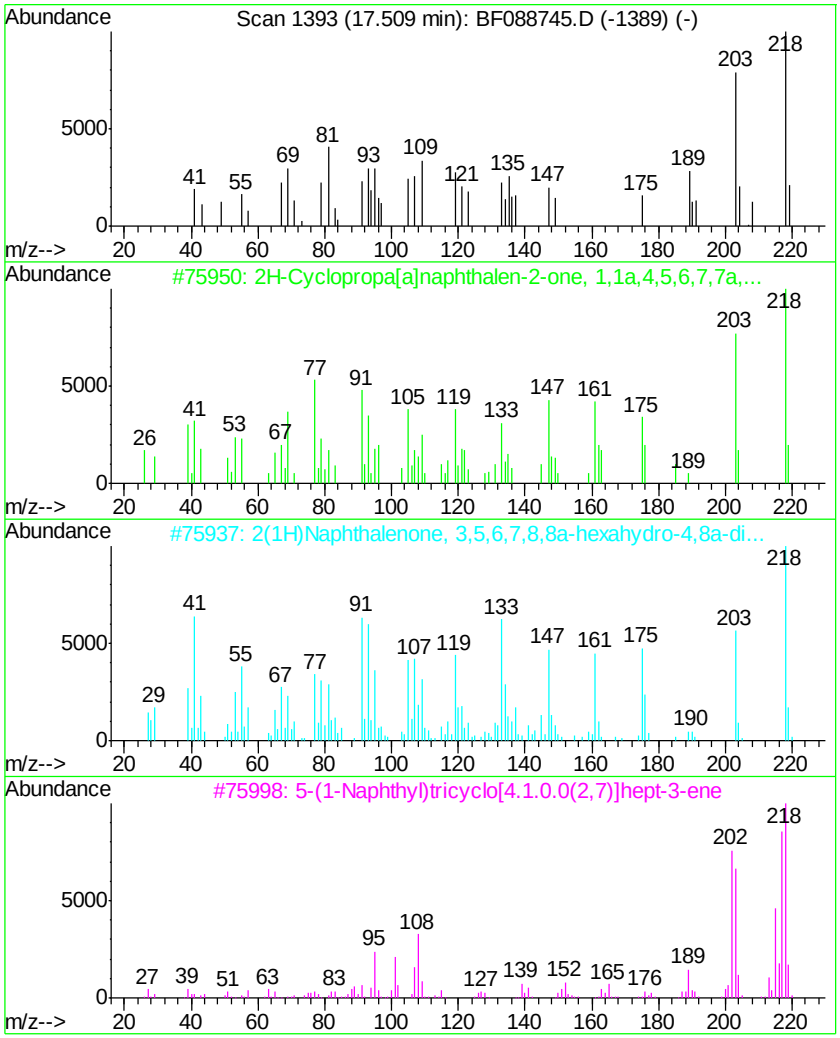
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

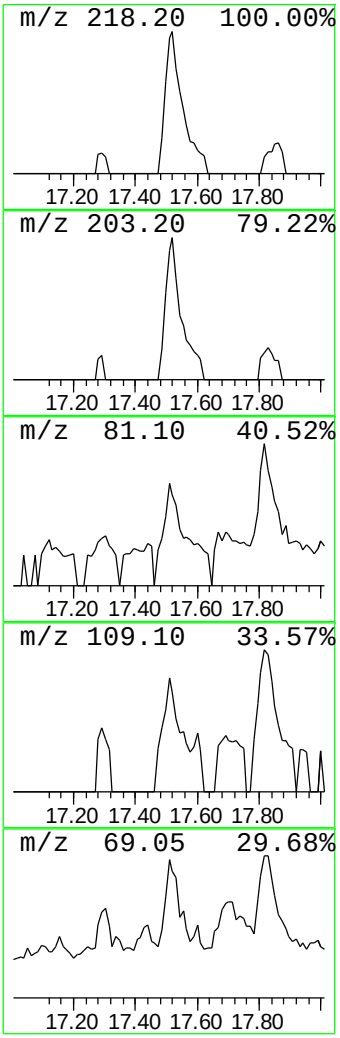
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2H-Cyclopropa[a]naphthalen-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.51	2.85 ng	88797	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	59
2	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	58
3	5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	52
4	7b-Phenyl-2a,7b-dihydro-3H-cyclo...	218	C17H14	138089-70-0	50
5	1,2,3,4-Tetrahydro-1-phenyl-1,2,...	218	C17H14	138089-69-7	50





Library Search Compound Report

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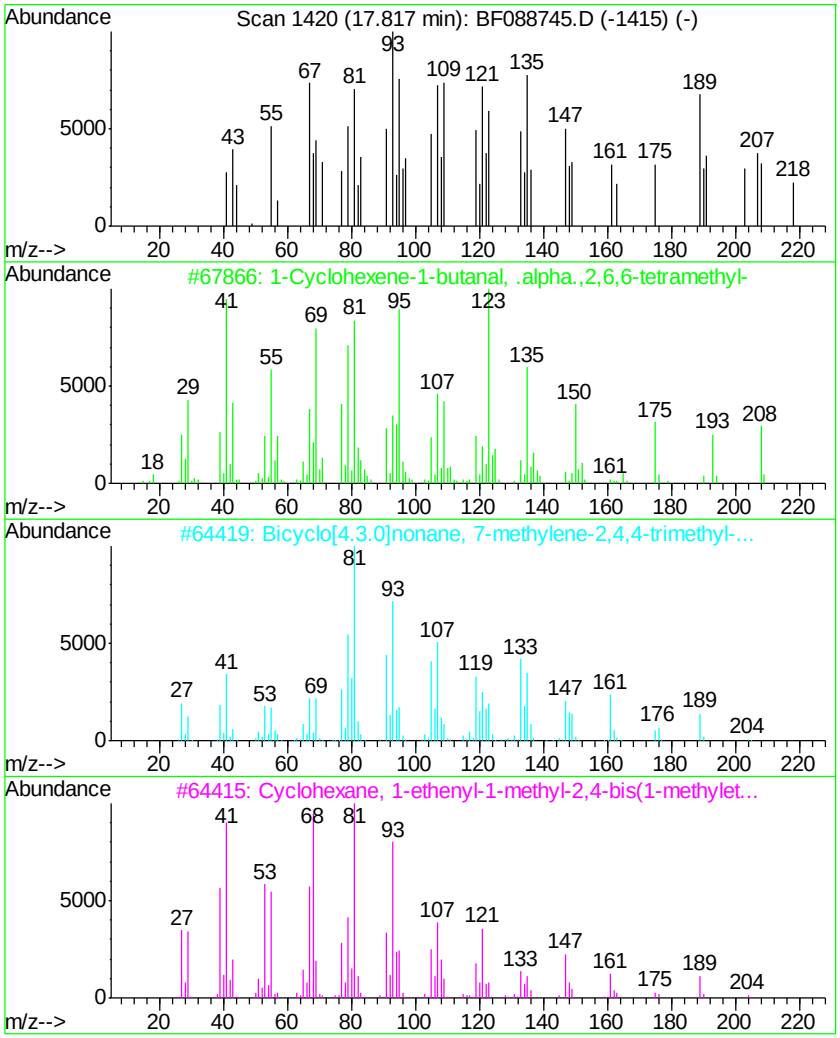
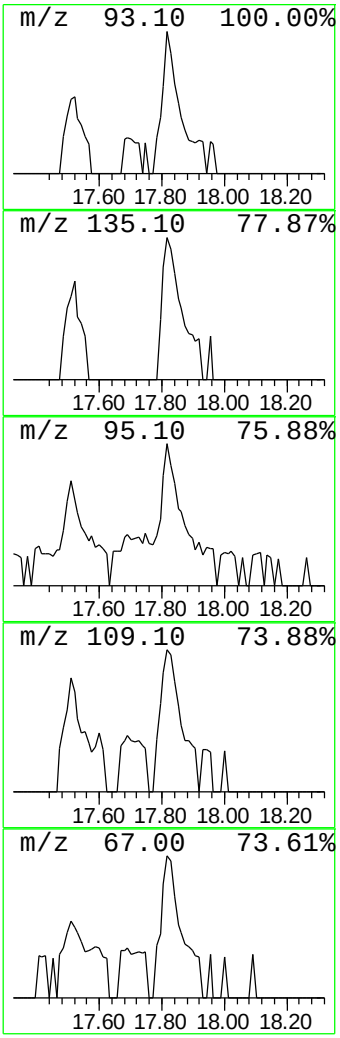
****

Peak Number 9 unknown17.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	3.39 ng	105702	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cyclohexene-1-butanal, .alpha....	208	C14H24O	021632-06-4	27
2	Bicyclo[4.3.0]nonane, 7-methylen...	204	C15H24	1000156-11-9	27
3	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	110823-68-2	22
4	5,10-Undecadienoic acid, 2-methy...	208	C13H20O2	051788-60-4	18
5	1,5-Cycloundecadiene, 9-(1-methy...	190	C14H22	062338-55-0	15





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TIC Library : C:\Database\NIST11.L
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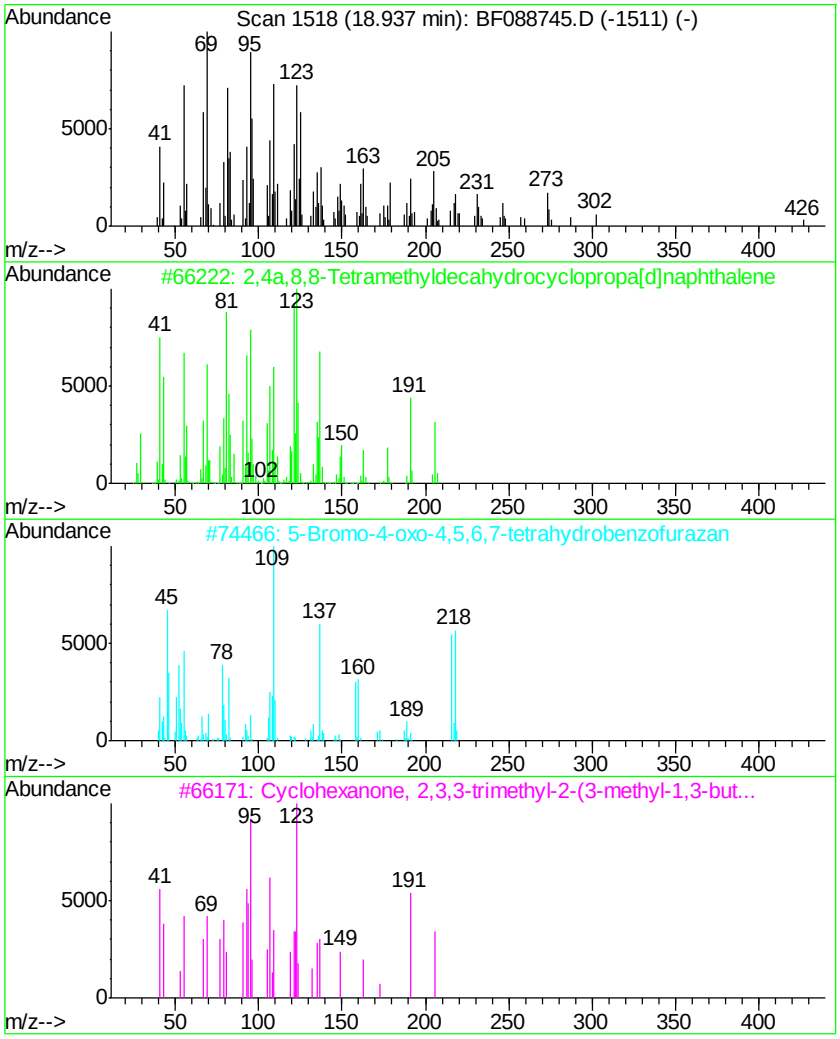
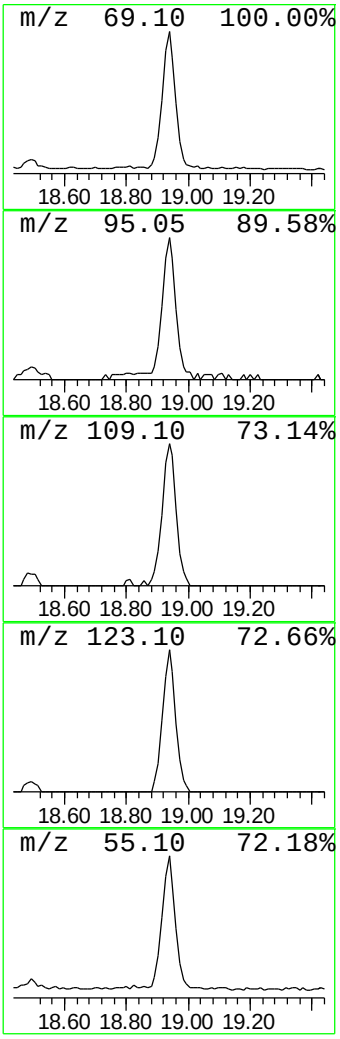
Peak Number 10 2,4a,8,8-Tetramethyldecahyd... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.94	17.70 ng	551958	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	62
2	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	60
3	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	60
4	Sesquirosefuran	218	C15H22O	039007-93-7	60
5	Methyl Camphorsulfonates	246	C11H18O4S	046471-67-4	56





Tentatively Identified Compound (LSC) summary

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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	6.3	ng	160936	1	6.74	509669	20.0
unknown6.51	6.51	59.3	ng	1510630	1	6.74	509669	20.0
Trifluoroacetoxy ...	13.75	3.6	ng	150197	5	13.87	828516	20.0
Squalene	14.73	2.4	ng	74770	6	15.26	623592	20.0
2H-Cyclopropa[a]n...	17.51	2.9	ng	88797	6	15.26	623592	20.0
unknown17.82	17.82	3.4	ng	105702	6	15.26	623592	20.0
2,4a,8,8-Tetramet...	18.94	17.7	ng	551958	6	15.26	623592	20.0