LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088757.D
Acq On : 7 Jul 2016 2:22
Operator : UM/SJ
Sample : H3879-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-03

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	9	10	16	rVV	140139	193941	5.31%	0.983%
2	1.827	19	21	62	rVB	1811538	3655732	100.00%	18.535%
3	4.901	287	290	294	rBB	66315	86914	2.38%	0.441%
4	5.336	325	328	330	rBV	1294309	1321017	36.14%	6.698%
5	6.376	416	419	422	rBV	1035507	1237894	33.86%	6.276%
6	6.513	428	431	433	rBV	1545175	1411040	38.60%	7.154%
7	6.742	449	451	453	rBV	453801	526187	14.39%	2.668%
8	6.902	463	465	467	rVB	1220752	1024712	28.03%	5.195%
9	7.313	498	501	503	rBV	846241	930522	25.45%	4.718%
10	8.033	561	564	566	rBV	910641	815678	22.31%	4.136%
11	9.108	656	658	661	rVB	1837380	1611234	44.07%	8.169%
12	9.508	691	693	695	rVB	176402	221706	6.06%	1.124%
13	9.782	714	717	719	rBV	1041802	890060	24.35%	4.513%
14	10.559	783	785	788	rBV2	795182	862542	23.59%	4.373%
15	10.696	795	797	802	rVB2	54885	83517	2.28%	0.423%
16	11.142	834	836	837	rBV	62412	48816	1.34%	0.248%
17	11.256	843	846	848	rBV	1046625	876948	23.99%	4.446%
18	11.496	864	867	872	rVV3	28815	57310	1.57%	0.291%
19	12.319	935	939	941	rBV2	72179	136202	3.73%	0.691%
20	12.685	968	971	972	rVB2	37275	48971	1.34%	0.248%
21	12.731	972	975	978	rVB2	25974	43641	1.19%	0.221%
22	12.845	982	985	987	rBV	1117447	1568008	42.89%	7.950%
23	13.085	1001	1006	1007	rBV	45783	59986	1.64%	0.304%
24	13.394	1030	1033	1034	rBV	30359	48469	1.33%	0.246%
25	13.748	1061	1064	1068	rBV2	132337	186331	5.10%	0.945%
26	13.874	1073	1075	1078	rBV	599844	702959	19.23%	3.564%
27	14.377	1116	1119	1127	rBV3	48619	140637	3.85%	0.713%
28	14.731	1148	1150	1152	rVV	58211	55935	1.53%	0.284%
29	14.868	1160	1162	1166	rVB	18525	38763	1.06%	0.197%
30	15.257	1193	1196	1199	rVV	413034	506920	13.87%	2.570%
31	16.743	1322	1326	1330	rVV	127801	242305	6.63%	1.229%
32	16.880	1333	1338	1342	rVB6	14796	49412	1.35%	0.251%
33	17.863	1418	1424	1427	rBV3	12147	39307	1.08%	0.199%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : C2.1-03

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

Sum of corrected areas: 19723616

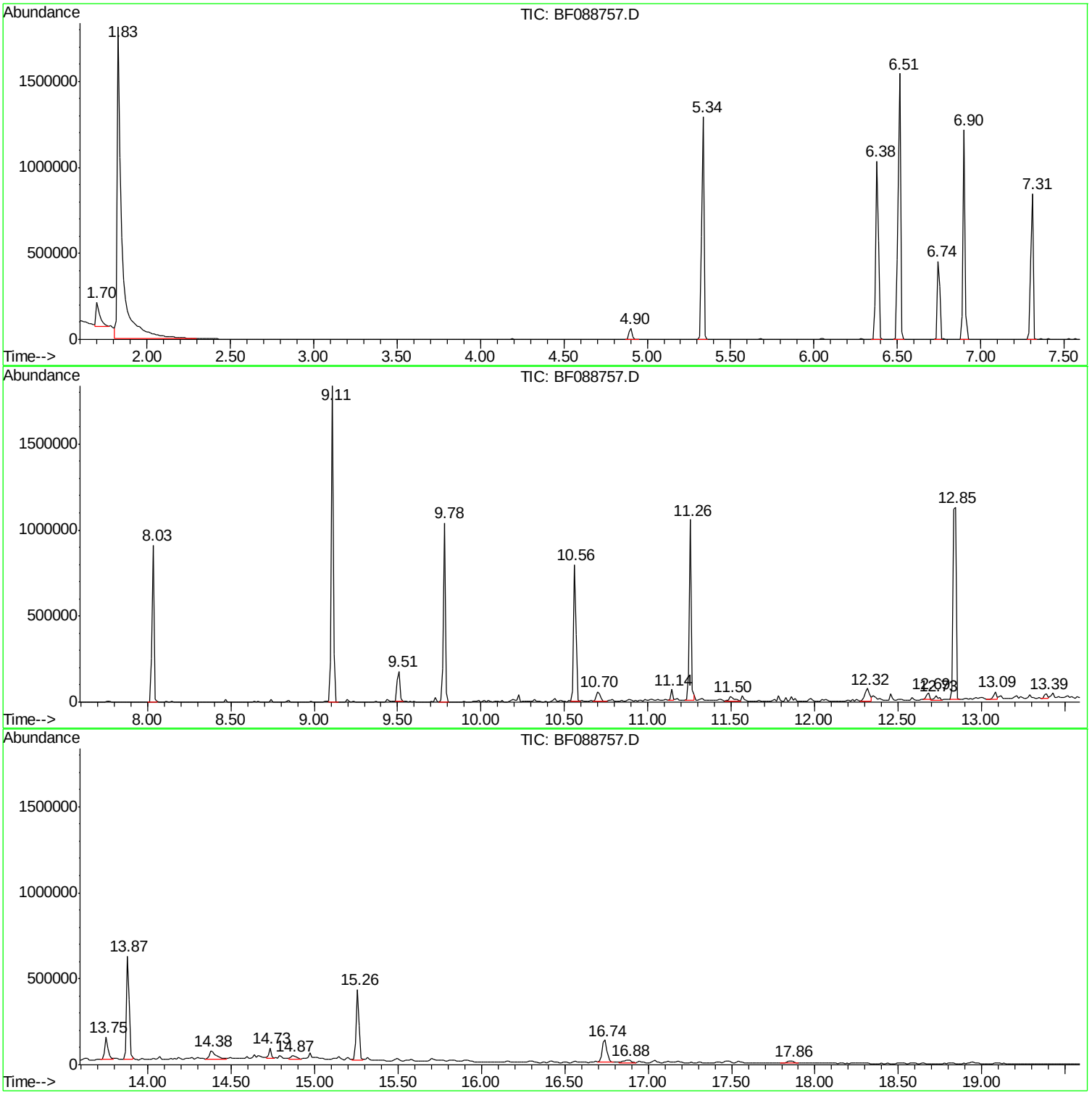
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088757.D
Acq On : 7 Jul 2016 2:22
Operator : UM/SJ
Sample : H3879-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-03

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088757.D
Acq On : 7 Jul 2016 2:22
Operator : UM/SJ
Sample : H3879-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-03

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

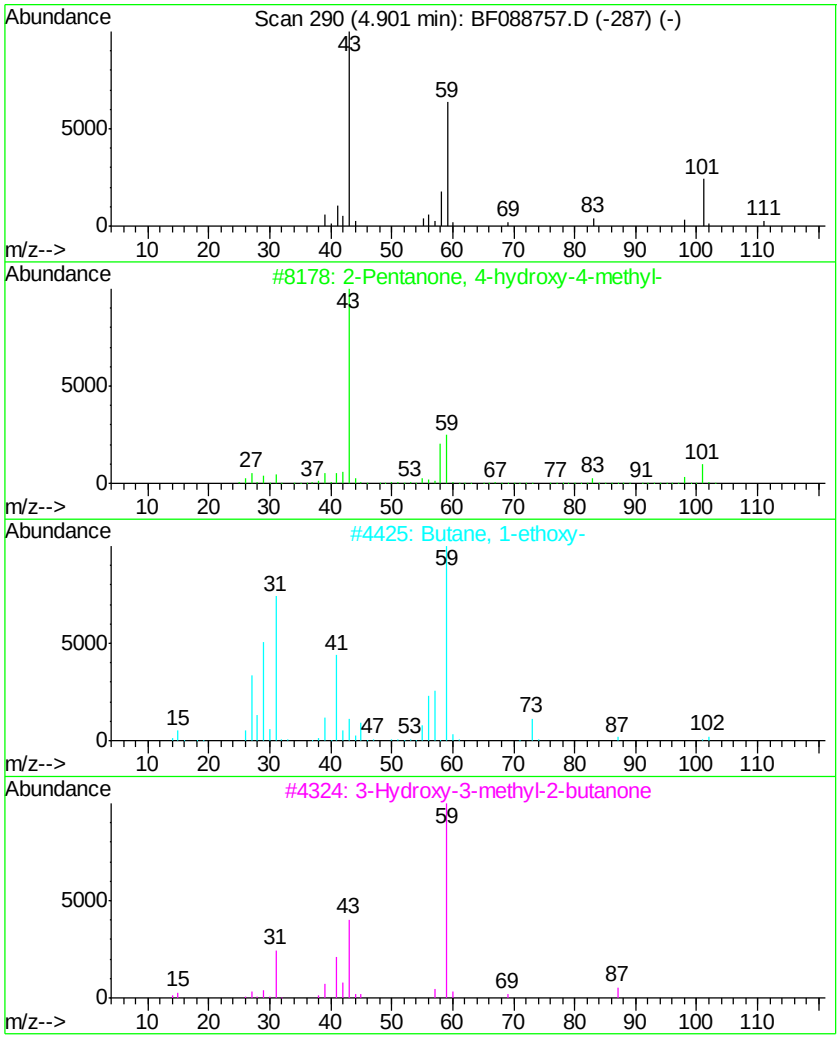
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

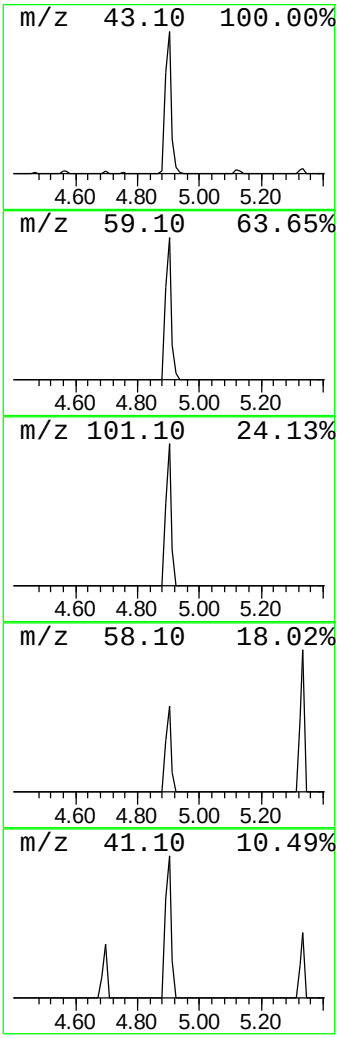
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.30 ng	86914	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	59
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	16
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088757.D
Acq On : 7 Jul 2016 2:22
Operator : UM/SJ
Sample : H3879-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-03

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

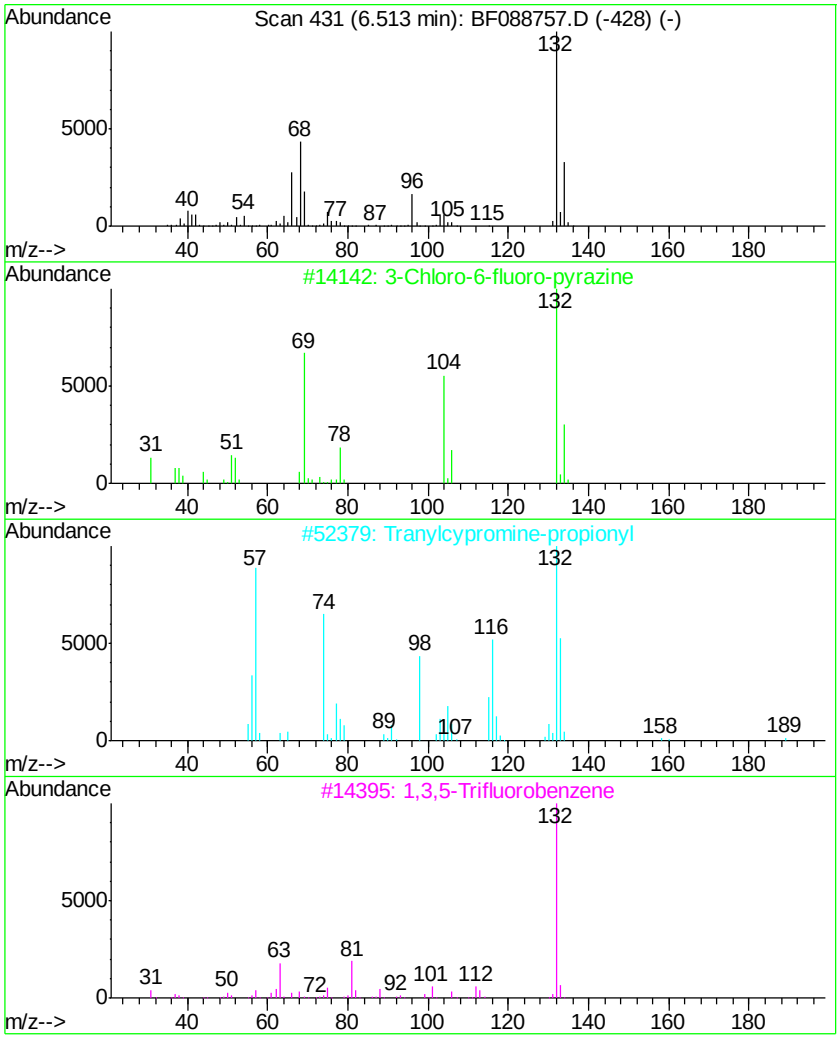
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

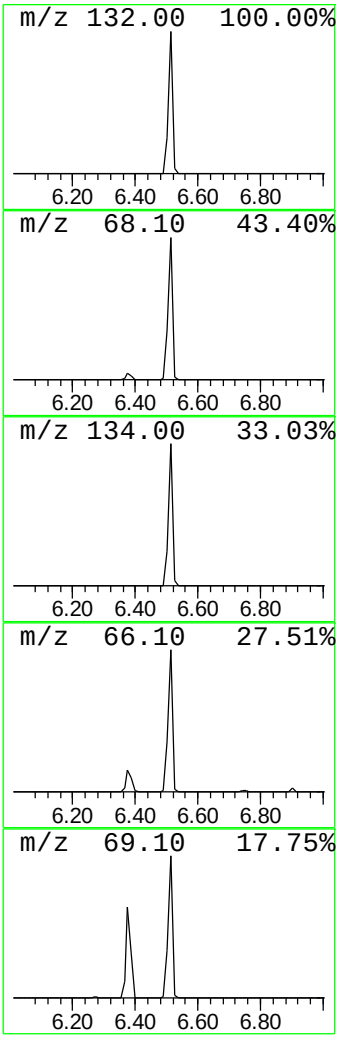
****

Peak Number 4 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	53.63 ng	1411040	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	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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 : BF088757.D
Acq On : 7 Jul 2016 2:22
Operator : UM/SJ
Sample : H3879-14
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-03

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

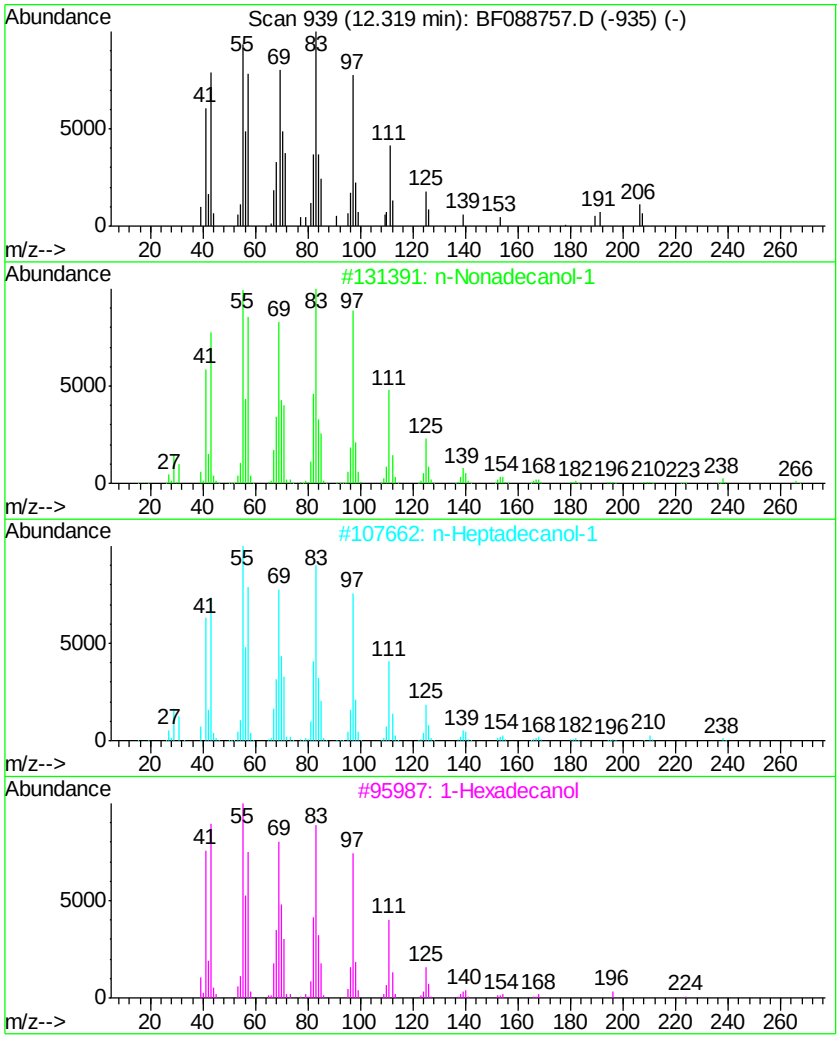
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

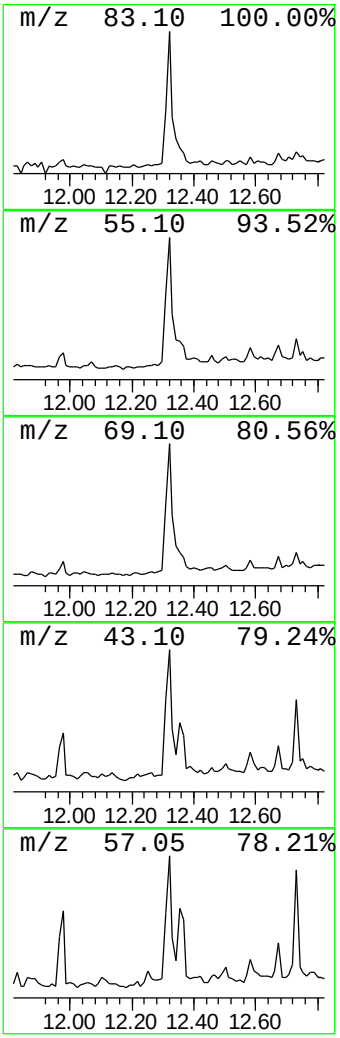
****

Peak Number 6 n-Nonadecanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	3.11 ng	136202	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
3	1-Hexadecanol	242	C16H34O	036653-82-4	95
4	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	94
5	n-Pentadecanol	228	C15H32O	000629-76-5	94





Library Search Compound Report

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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-03

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

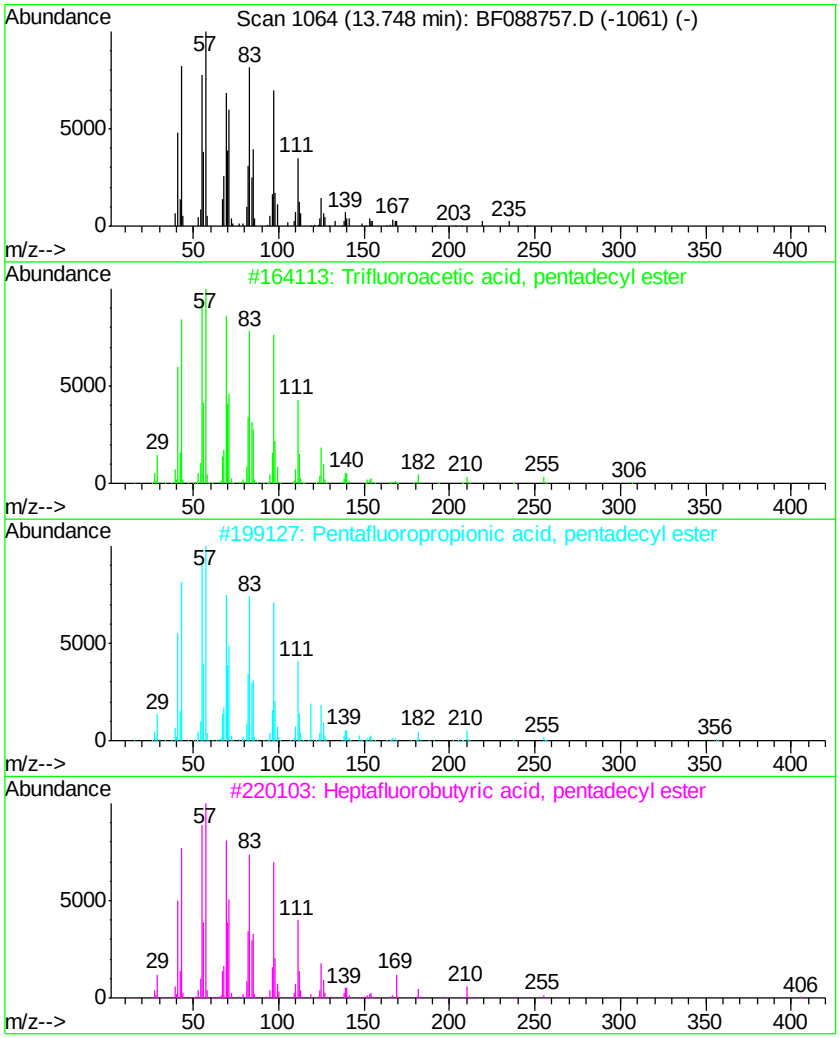
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

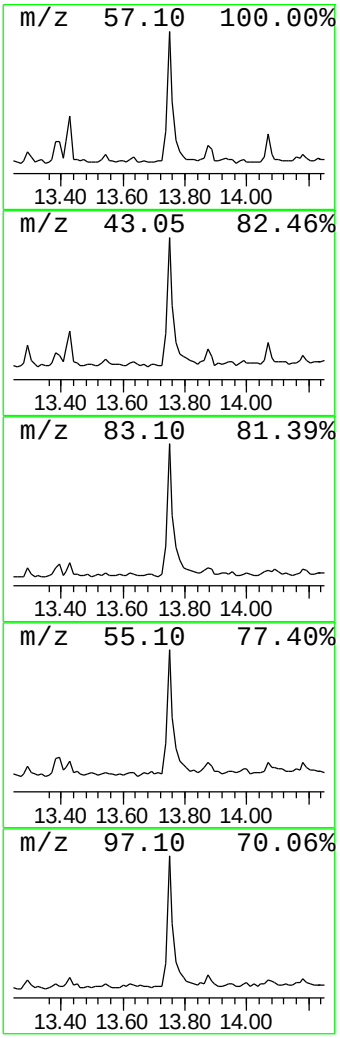
****

Peak Number 7 Trifluoroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	5.30 ng	186331	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





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Instrument : BNA_F
ClientSampleId : C2.1-03

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

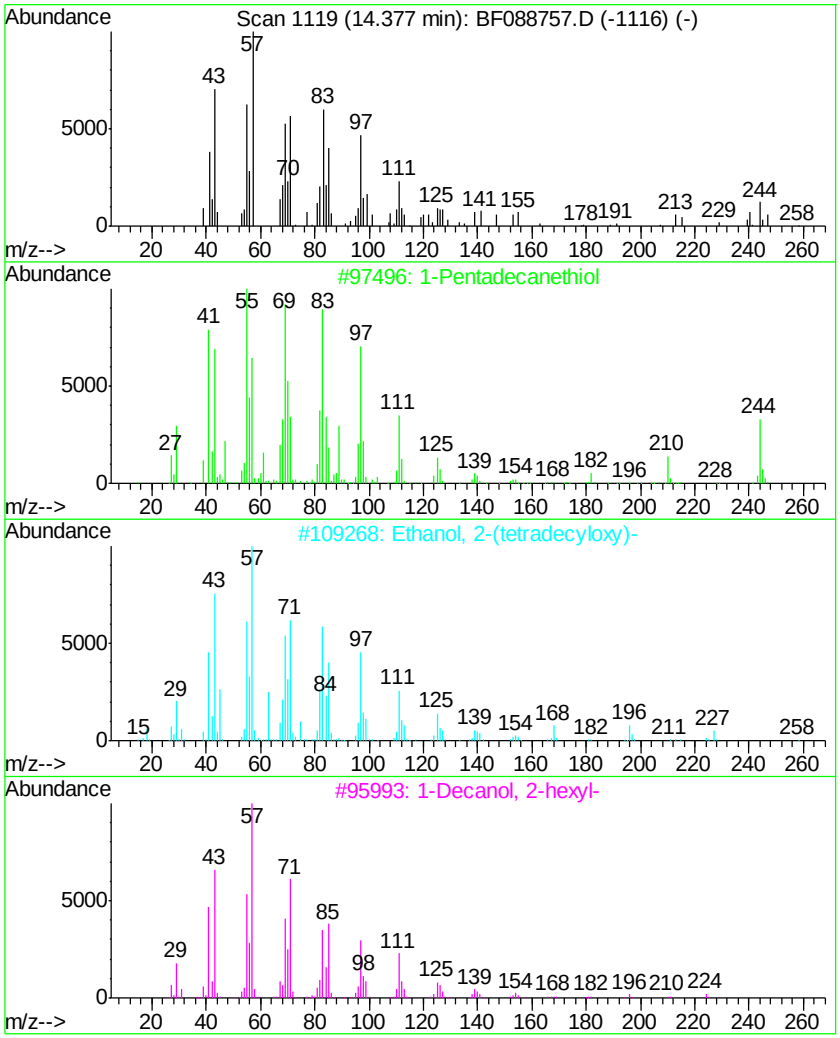
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

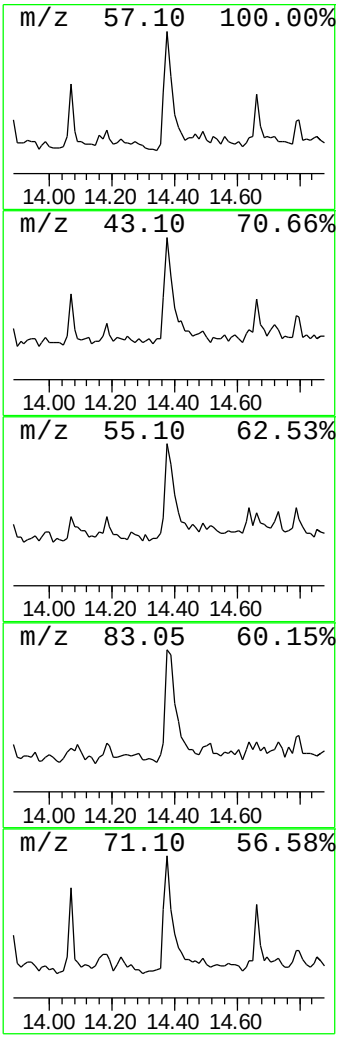
****

Peak Number 8 1-Pentadecanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	4.00 ng	140637	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	93
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	74
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	70
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	68
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64





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ClientSampleId : C2.1-03

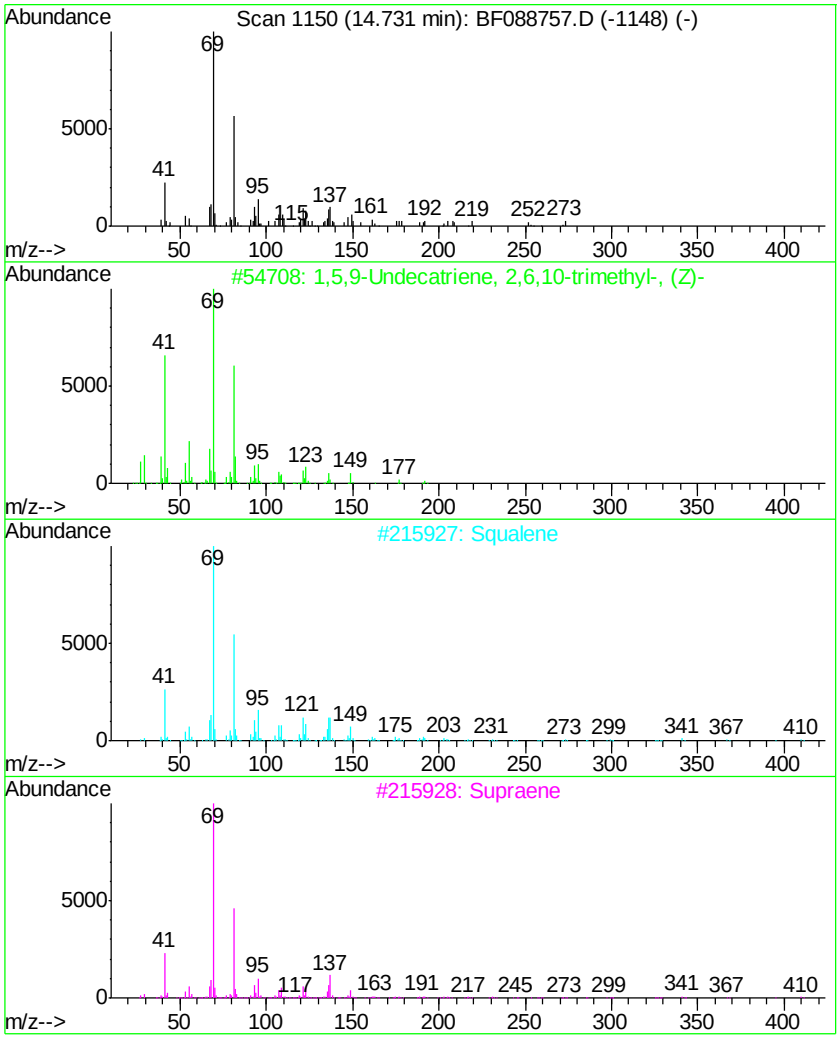
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

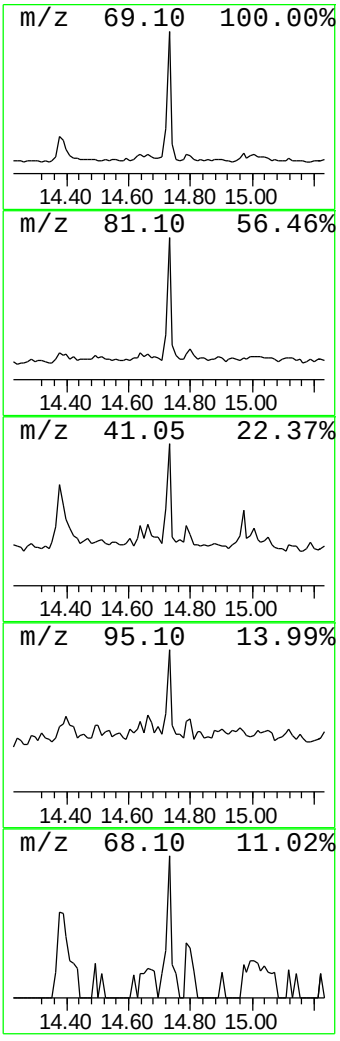
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.21 ng	55935	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	90
2	Squalene	410	C30H50	000111-02-4	87
3	Supraene	410	C30H50	007683-64-9	83
4	trans-Farnesol	222	C15H26O	000106-28-5	59
5	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

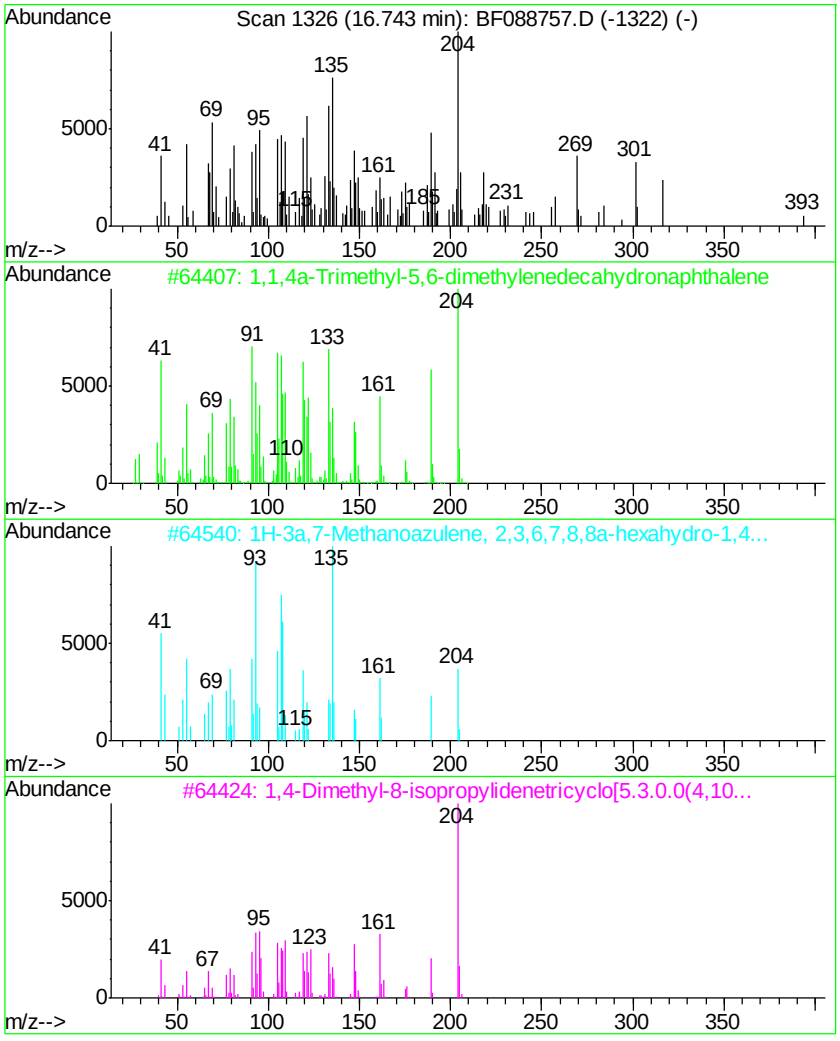
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

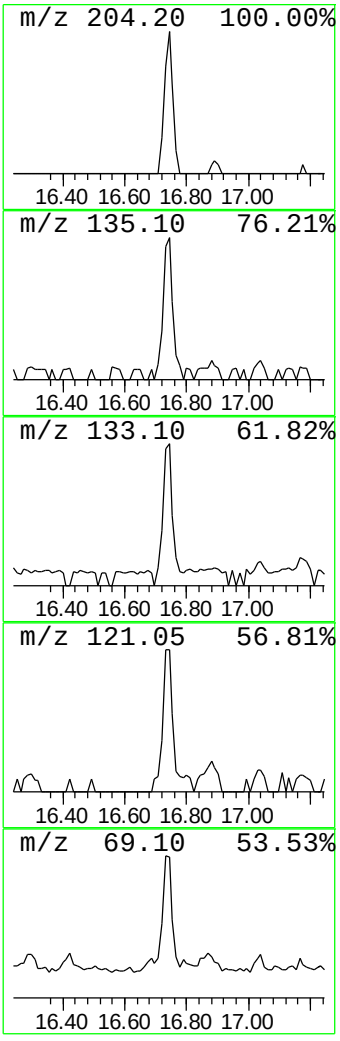
****

Peak Number 10 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	9.56 ng	242305	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	70
2	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	58
3	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	53
4	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	49
5	Farnesyl bromide	284	C15H25Br	006874-67-5	43





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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	3.3	ng	86914	1	6.74	526187	20.0
unknown6.51	6.51	53.6	ng	1411040	1	6.74	526187	20.0
n-Nonadecanol-1	12.32	3.1	ng	136202	4	11.26	876948	20.0
Trifluoroacetic a...	13.75	5.3	ng	186331	5	13.87	702959	20.0
1-Pentadecanethiol	14.38	4.0	ng	140637	5	13.87	702959	20.0
1,5,9-Undecatrien...	14.73	2.2	ng	55935	6	15.26	506920	20.0
1,1,4a-Trimethyl-...	16.74	9.6	ng	242305	6	15.26	506920	20.0