LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088762.D
Acq On : 7 Jul 2016 4:47
Operator : UM/SJ
Sample : H3879-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-06

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	17	rVB	148194	205431	8.56%	0.968%
2	1.827	19	21	77	rVB	1214247	2400683	100.00%	11.308%
3	4.913	289	291	296	rBB	84907	117536	4.90%	0.554%
4	5.347	326	329	331	rBV	1588064	2074801	86.43%	9.773%
5	6.387	417	420	423	rBV	1719639	1854639	77.25%	8.736%
6	6.513	429	431	434	rBV	1722151	1899763	79.13%	8.949%
7	6.753	449	452	454	rBV	522369	571720	23.81%	2.693%
8	6.902	463	465	468	rBB	1316696	1467997	61.15%	6.915%
9	7.313	498	501	503	rBV	1283234	1221500	50.88%	5.754%
10	8.033	562	564	566	rBV	985003	802671	33.44%	3.781%
11	9.108	656	658	661	rBV	1775723	2207729	91.96%	10.399%
12	9.508	691	693	695	rBV	295895	275602	11.48%	1.298%
13	9.725	711	712	715	rBV	27727	26541	1.11%	0.125%
14	9.782	715	717	719	rVB	945516	807231	33.63%	3.802%
15	10.228	754	756	757	rVB	52002	38365	1.60%	0.181%
16	10.445	773	775	778	rBV	17343	24447	1.02%	0.115%
17	10.571	783	786	788	rBV2	945401	1181160	49.20%	5.564%
18	10.696	795	797	802	rVB	59088	69108	2.88%	0.326%
19	11.142	834	836	838	rBV	64062	55805	2.32%	0.263%
20	11.256	844	846	849	rVV	797006	685135	28.54%	3.227%
21	11.325	849	852	856	rVB3	10129	26134	1.09%	0.123%
22	12.845	982	985	987	rBV	1553447	1718337	71.58%	8.094%
23	13.268	1021	1022	1024	rBV	31065	25158	1.05%	0.119%
24	13.748	1061	1064	1073	rBV2	83294	123608	5.15%	0.582%
25	13.874	1073	1075	1078	rBV	389724	532255	22.17%	2.507%
26	14.377	1116	1119	1124	rBV2	24569	48106	2.00%	0.227%
27	14.640	1140	1142	1146	rBV2	20119	28601	1.19%	0.135%
28	14.731	1148	1150	1154	rVV	28607	31084	1.29%	0.146%
29	15.268	1194	1197	1199	rVB	362244	494512	20.60%	2.329%
30	16.743	1323	1326	1330	rVB	58118	96068	4.00%	0.453%
31	17.108	1355	1358	1363	rBV5	8799	25157	1.05%	0.119%
32	17.554	1394	1397	1400	rVB3	30060	57375	2.39%	0.270%
33	17.863	1418	1424	1427	rBV4	12213	35197	1.47%	0.166%

LSC Area Percent Report

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Acq On : 7 Jul 2016 4:47
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Sample : H3879-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-06

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: 21229456

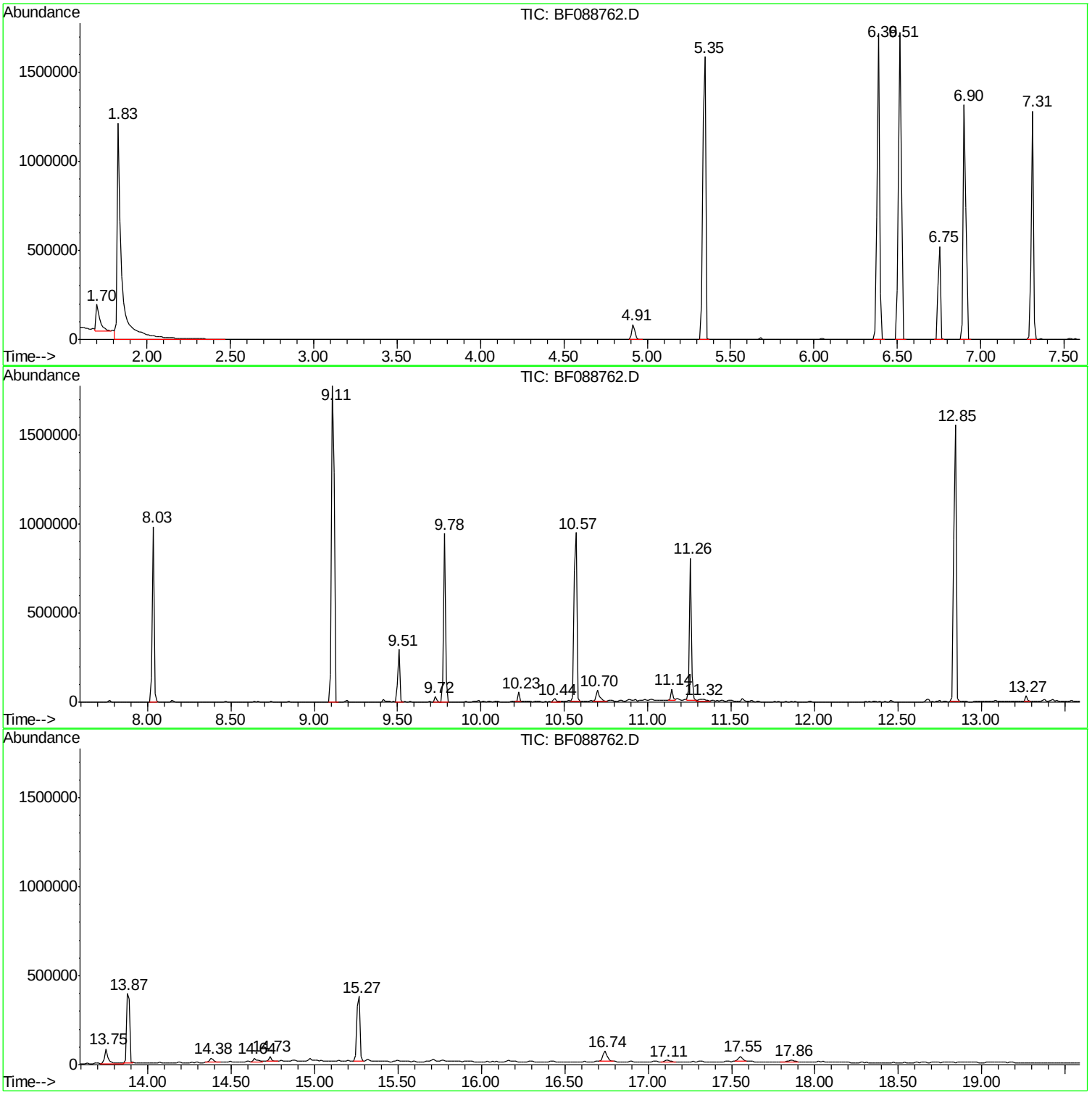
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088762.D
Acq On : 7 Jul 2016 4:47
Operator : UM/SJ
Sample : H3879-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-06

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 : BF088762.D
Acq On : 7 Jul 2016 4:47
Operator : UM/SJ
Sample : H3879-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-06

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

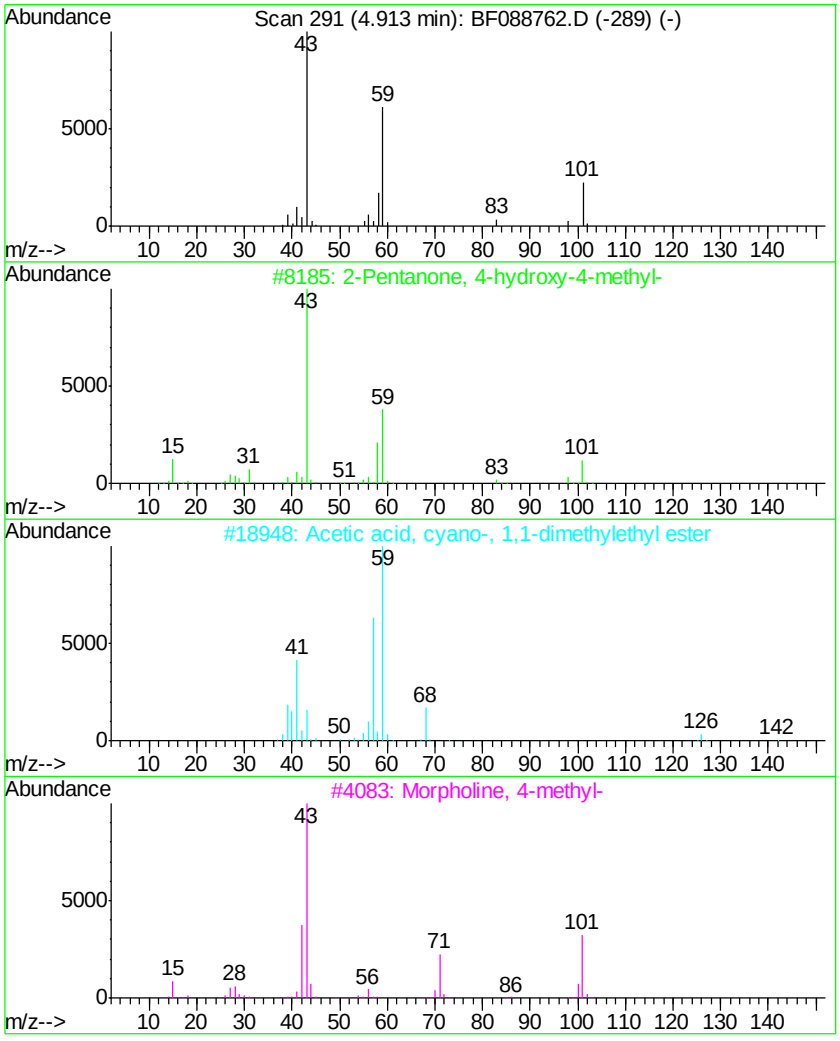
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

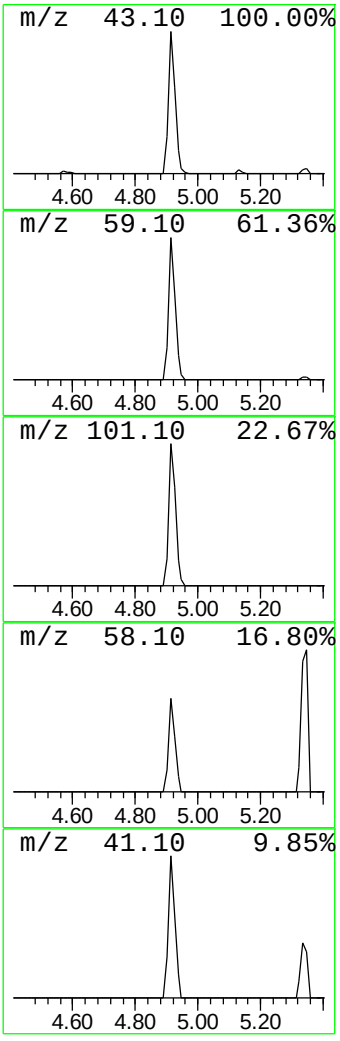
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	4.11 ng	117536	1,4-Dichlorobenzene-d4	6.75

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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088762.D
Acq On : 7 Jul 2016 4:47
Operator : UM/SJ
Sample : H3879-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-06

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

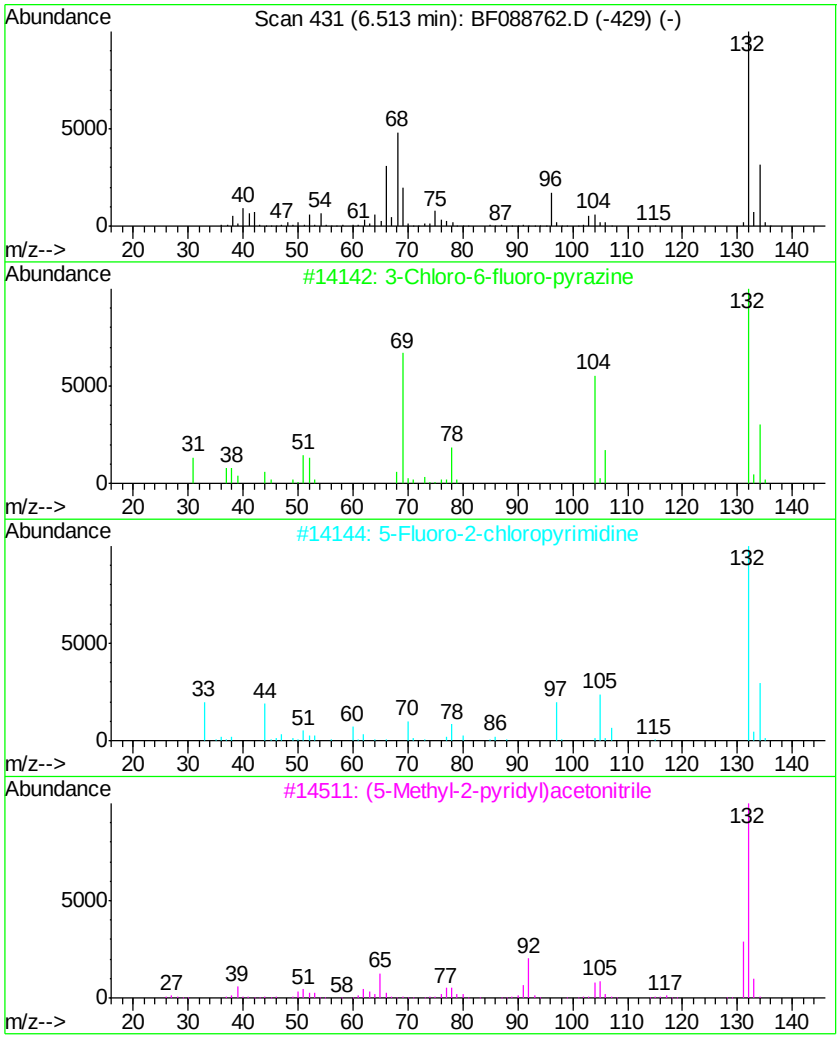
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

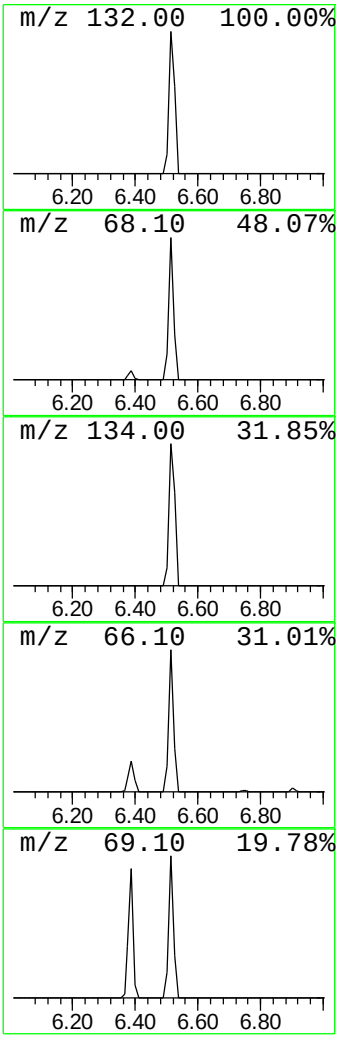
****

Peak Number 4 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	66.46 ng	1899760	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088762.D
Acq On : 7 Jul 2016 4:47
Operator : UM/SJ
Sample : H3879-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-06

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

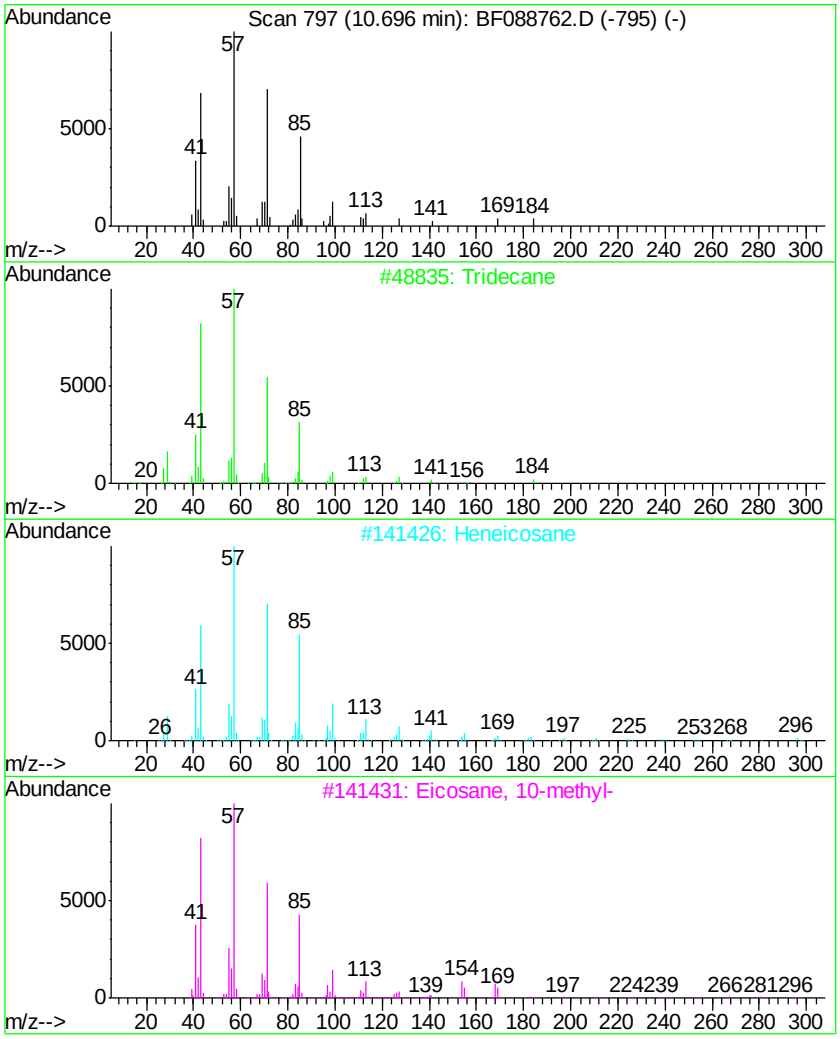
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

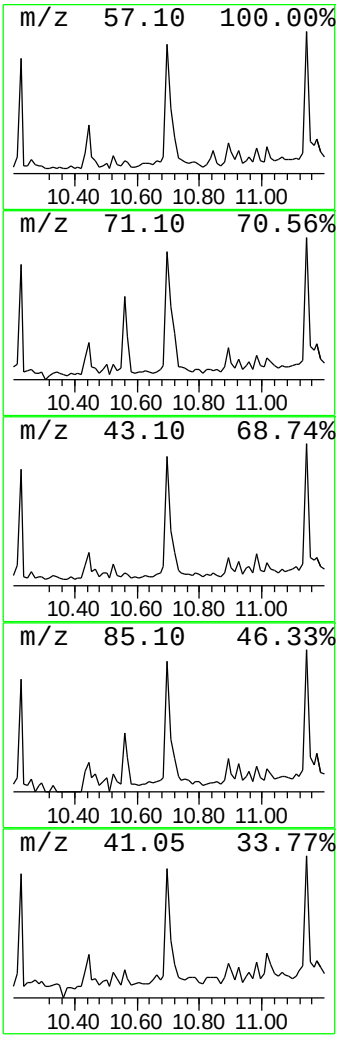
****

Peak Number 6 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.02 ng	69108	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Heneicosane	296	C21H44	000629-94-7	86
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088762.D
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Sample : H3879-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-06

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

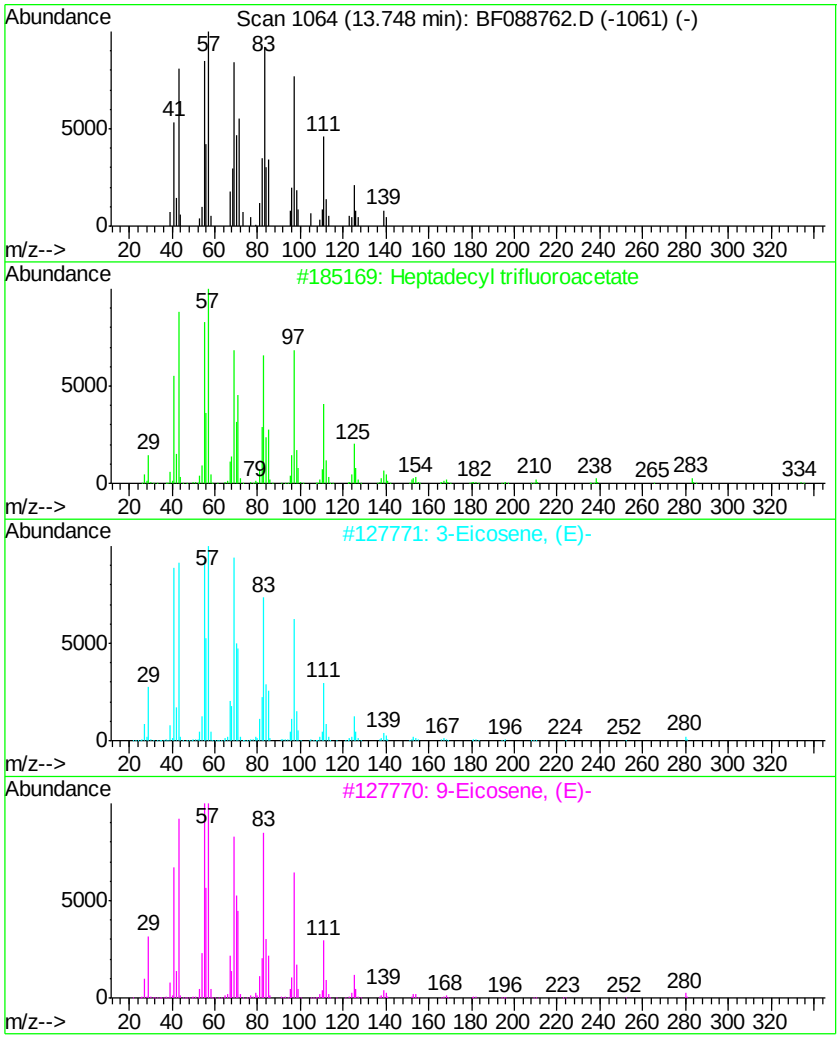
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

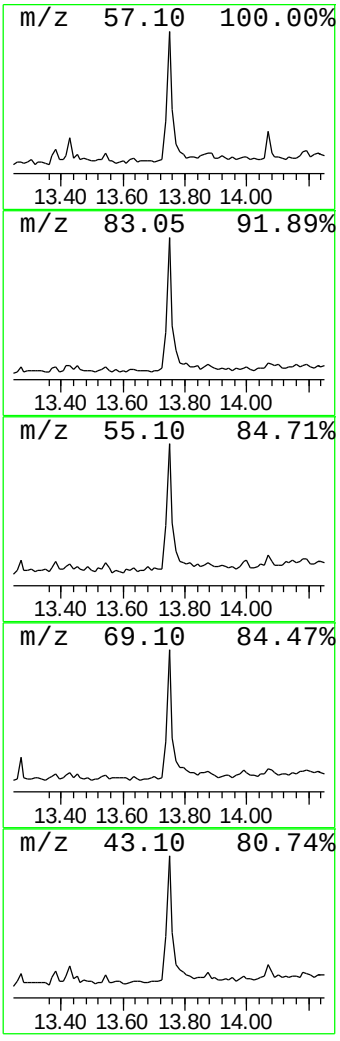
****

Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	4.64 ng	123608	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





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Sample : H3879-04
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-06

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

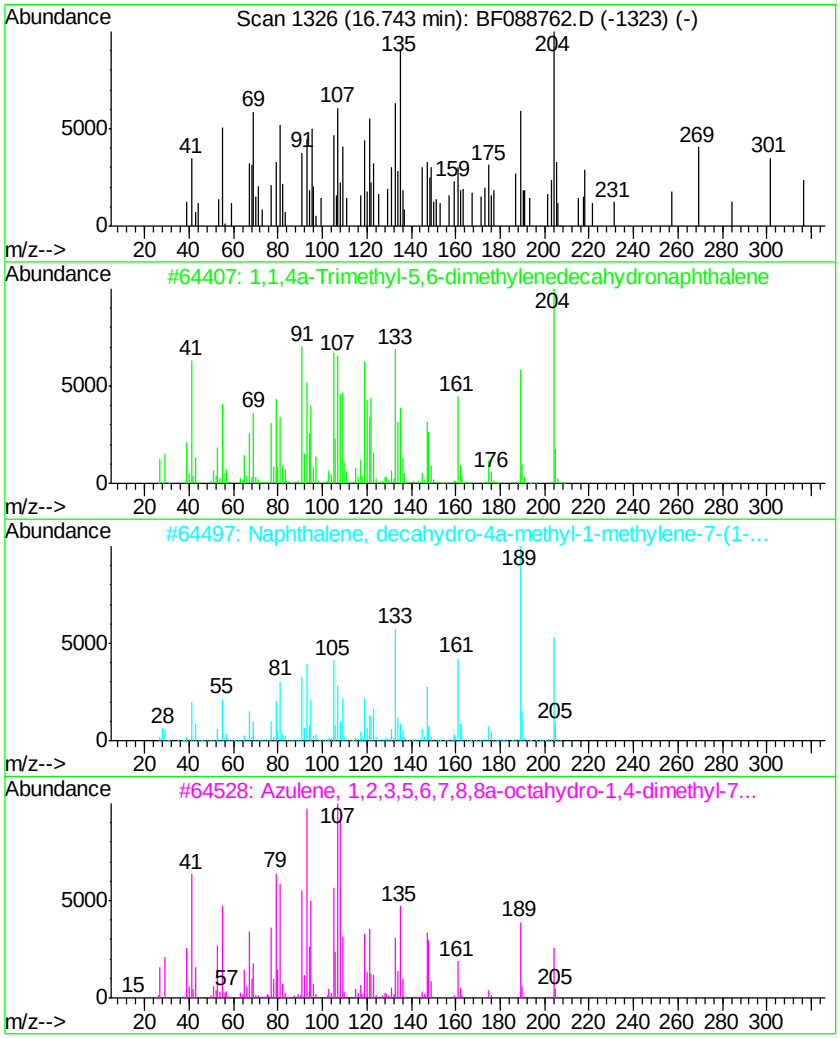
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

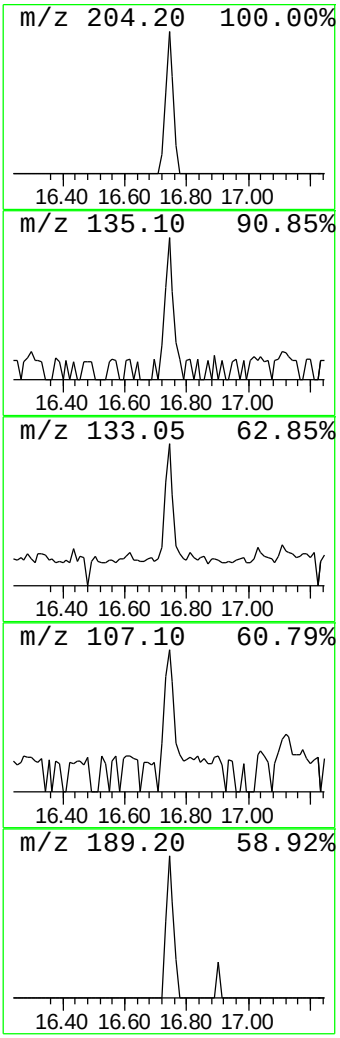
****

Peak Number 8 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	3.89 ng	96068	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	64
2	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	60
3	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	60
4	.beta.-Humulene	204	C15H24	000116-04-1	55
5	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	53





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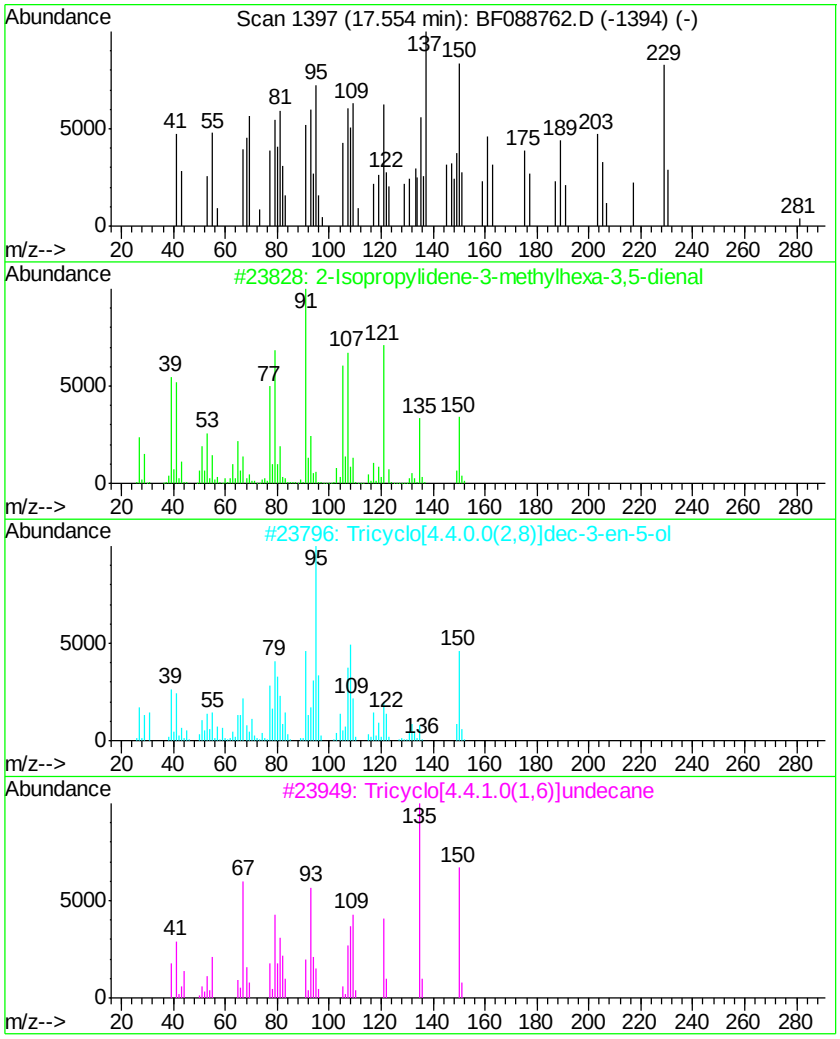
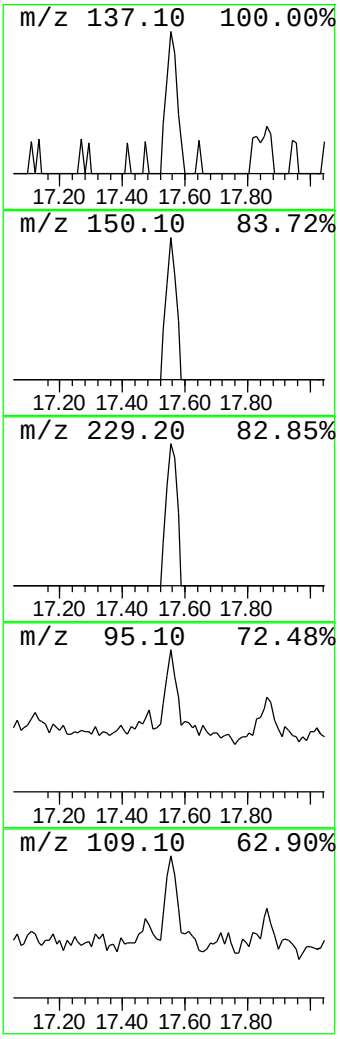
****

Peak Number 9 unknown17.55 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.55	2.32 ng	57375	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropylidene-3-methylhexa-3,...	150	C10H14O	1000191-76-5	25
2	Tricyclo[4.4.0.0(2,8)]dec-3-en-5-ol	150	C10H14O	1000193-38-7	15
3	Tricyclo[4.4.1.0(1,6)]undecane	150	C11H18	006571-73-9	15
4	2(1H)-Pyridone, 1-ethyl-4-methyl-	137	C8H11NO	019006-62-3	15
5	2-Cyclohexen-1-one, 2-(2-methyl-...	150	C10H14O	018926-98-2	11





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...	4.91	4.1	ng	117536	1	6.75	571720	20.0
unknown6.51	6.51	66.5	ng	1899760	1	6.75	571720	20.0
Tridecane	10.70	2.0	ng	69108	4	11.26	685135	20.0
Heptadecyl triflu...	13.75	4.6	ng	123608	5	13.89	532255	20.0
1,1,4a-Trimethyl-...	16.74	3.9	ng	96068	6	15.27	494512	20.0
unknown17.55	17.55	2.3	ng	57375	6	15.27	494512	20.0