LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072016\
Data File : BF089156.D
Acq On : 21 Jul 2016 3:21
Operator : UM/SJ
Sample : H4019-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-SGS-33

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-BF072016.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	1.724	11	12	37	rVB	1044603	1533536	100.00%	10.479%
2	4.741	273	276	285	rBV	31979	57019	3.72%	0.390%
3	5.187	313	315	341	rBV	699075	1148548	74.90%	7.848%
4	6.261	406	409	416	rBV	902330	1271988	82.94%	8.692%
5	6.364	416	418	437	rVV	895329	1291988	84.25%	8.829%
6	6.604	437	439	449	rVV	194223	319923	20.86%	2.186%
7	6.753	449	452	469	rVV	997227	998553	65.11%	6.823%
8	7.164	486	488	498	rBV	529665	771788	50.33%	5.274%
9	7.885	548	551	561	rVB	407999	441082	28.76%	3.014%
10	8.959	642	645	648	rBV	1293925	1457242	95.02%	9.958%
11	9.359	678	680	683	rBV	445309	422231	27.53%	2.885%
12	9.622	701	703	706	rBV	348041	485469	31.66%	3.317%
13	10.410	770	772	775	rBV2	744761	870256	56.75%	5.947%
14	10.548	782	784	790	rBB	15995	19275	1.26%	0.132%
15	10.993	820	823	824	rBV	16507	16280	1.06%	0.111%
16	11.096	830	832	835	rBV	463074	514610	33.56%	3.517%
17	11.359	852	855	859	rBV	30764	73032	4.76%	0.499%
18	11.416	859	860	863	rVB	19999	17126	1.12%	0.117%
19	12.171	924	926	933	rBV	114603	259430	16.92%	1.773%
20	12.685	968	971	973	rBV	1560579	1496245	97.57%	10.224%
21	12.936	989	993	1000	rBV2	9171	23171	1.51%	0.158%
22	13.142	1008	1011	1013	rBV	32457	39036	2.55%	0.267%
23	13.234	1016	1019	1021	rBV	71384	63308	4.13%	0.433%
24	13.611	1049	1052	1058	rVB	34153	82488	5.38%	0.564%
25	13.714	1058	1061	1064	rBV	465752	626563	40.86%	4.282%
26	15.062	1176	1179	1182	rBV	306243	333848	21.77%	2.281%

Sum of corrected areas: 14634035

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072016\
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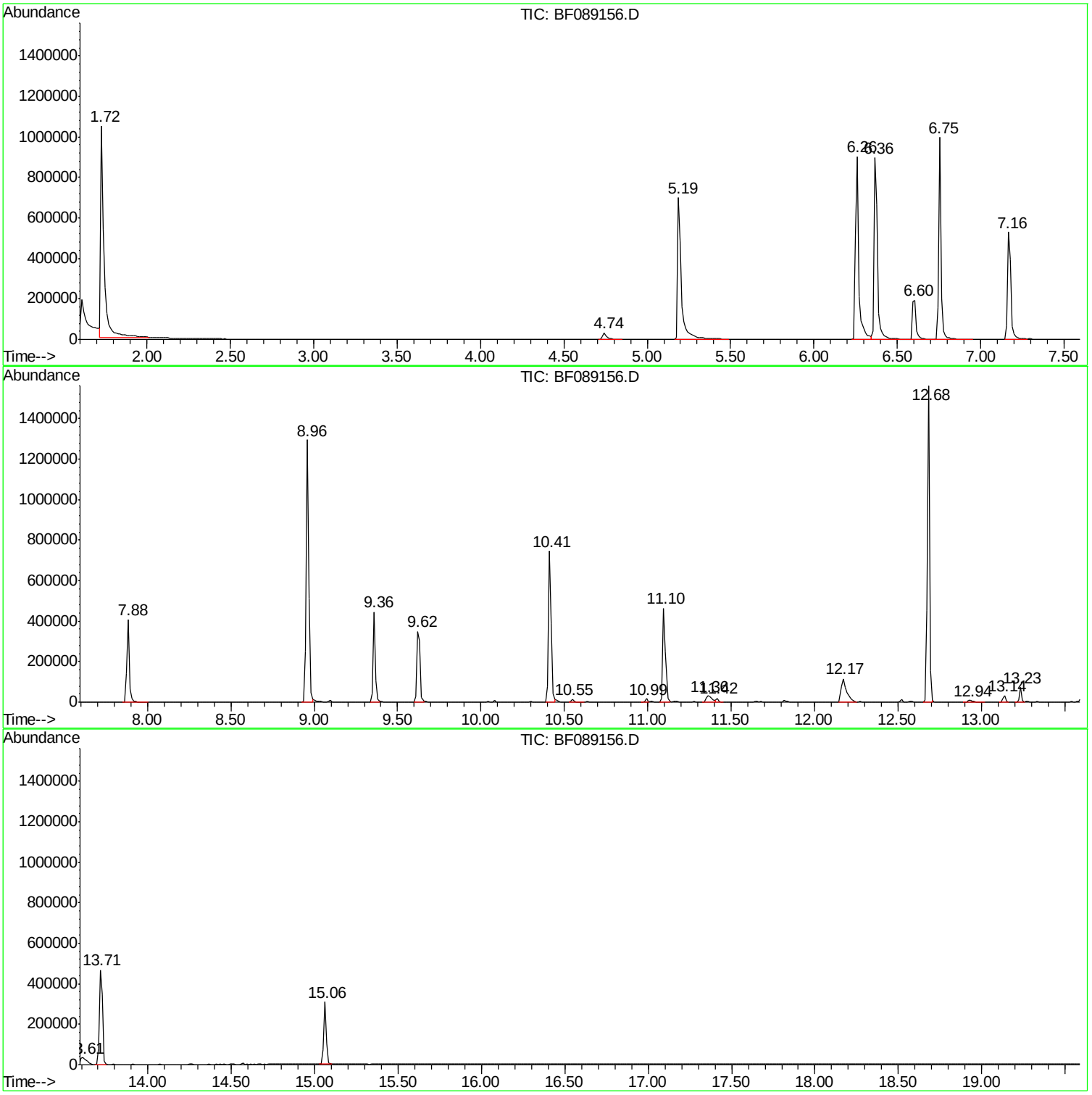
Operator : UM/SJ
Sample : H4019-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-SGS-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072016\
Data File : BF089156.D
Acq On : 21 Jul 2016 3:21
Operator : UM/SJ
Sample : H4019-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-SGS-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

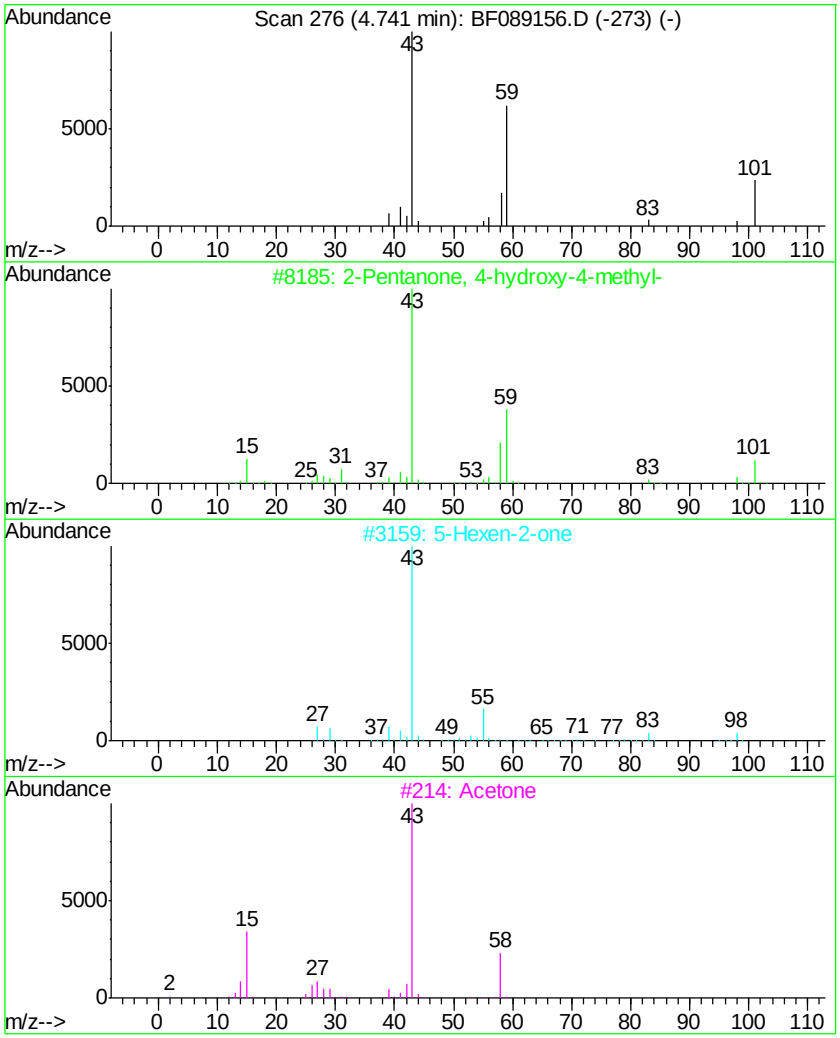
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

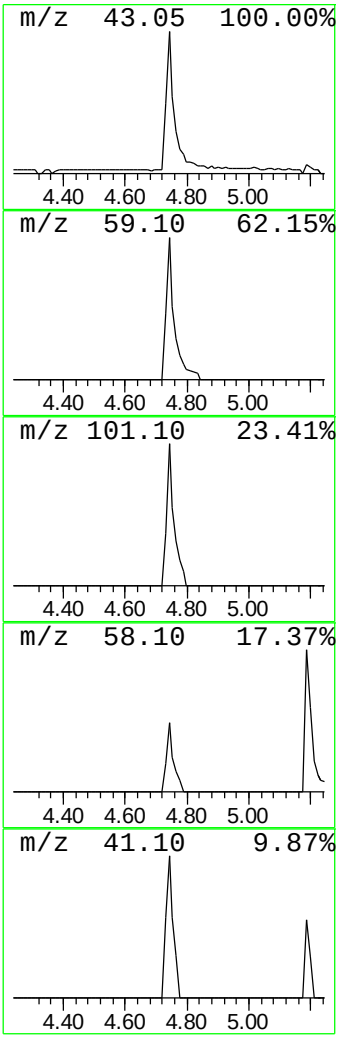
****

Peak Number 2 unknown4.74 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	3.56 ng	57019	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Acetone	58	C3H6O	000067-64-1	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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Operator : UM/SJ
Sample : H4019-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-SGS-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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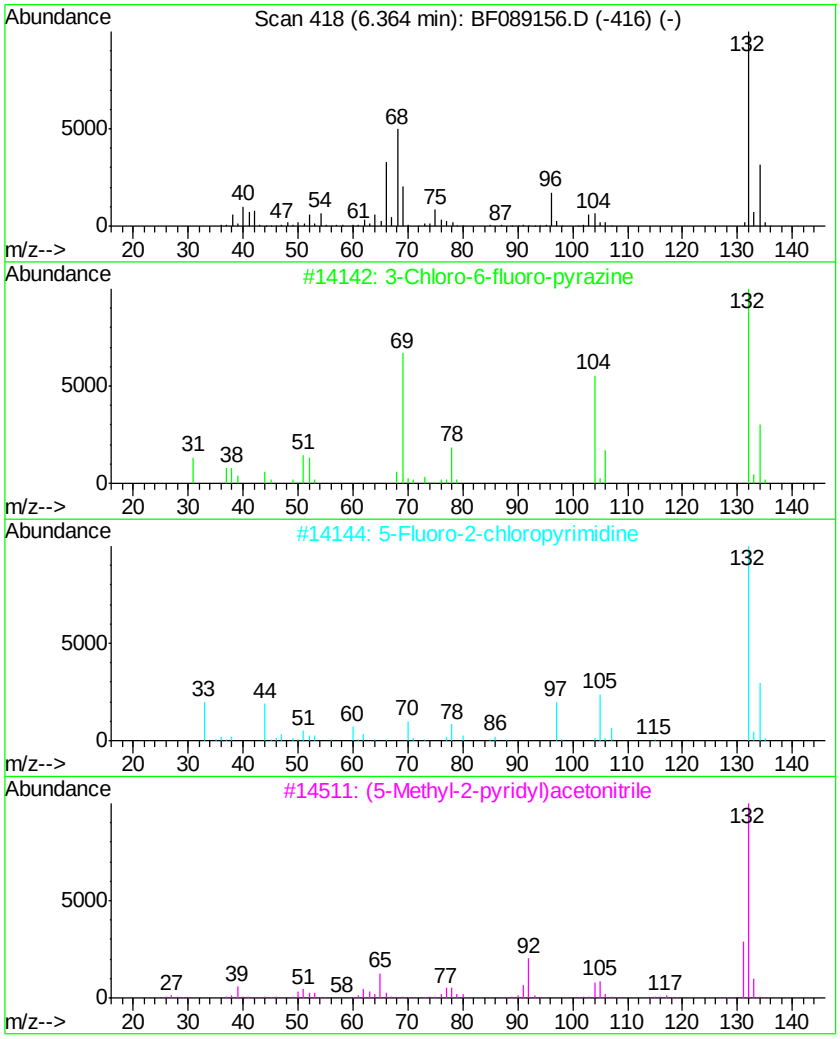
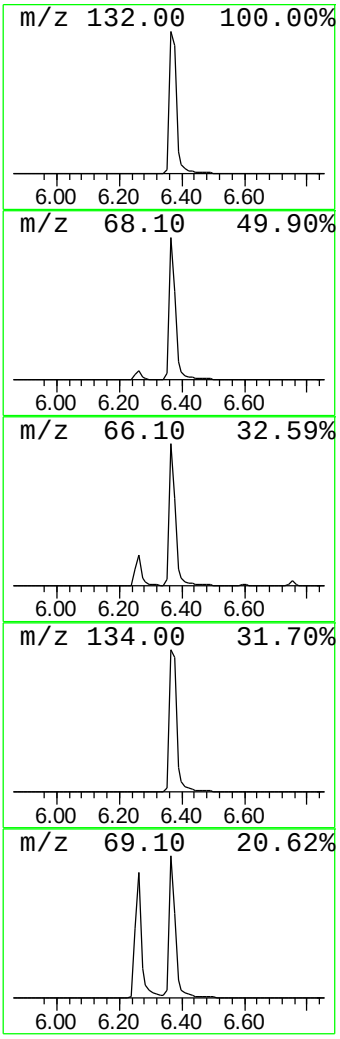
Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	80.77 ng	1291990	1,4-Dichlorobenzene-d4	6.60

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	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072016\
Data File : BF089156.D
Acq On : 21 Jul 2016 3:21
Operator : UM/SJ
Sample : H4019-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-SGS-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

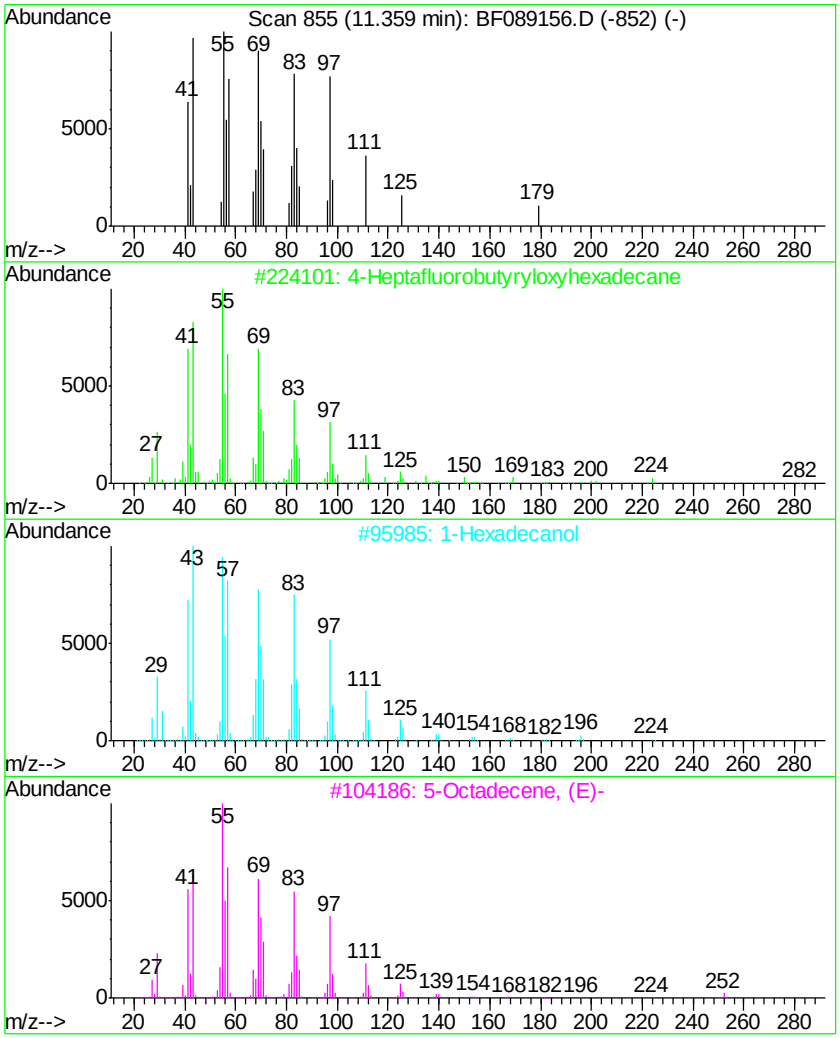
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

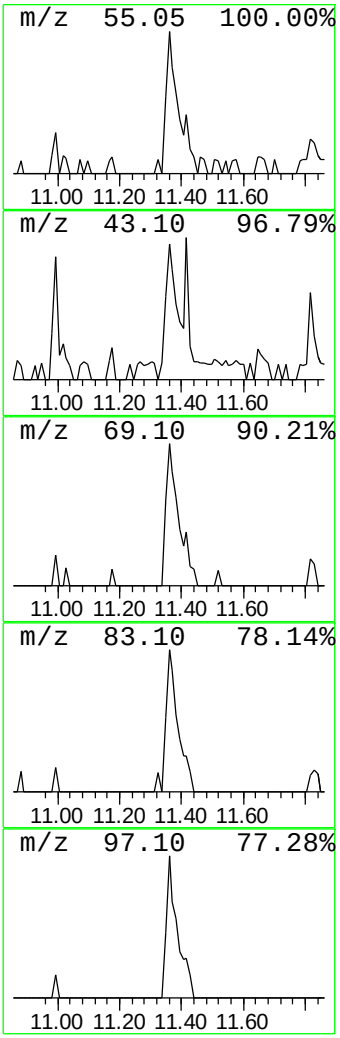
****

Peak Number 5 4-Heptafluorobutyryloxyhexa... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.36	2.84 ng	73032	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
4	1-Tetradecanol	214	C14H30O	000112-72-1	90
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072016\
Data File : BF089156.D
Acq On : 21 Jul 2016 3:21
Operator : UM/SJ
Sample : H4019-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-SGS-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

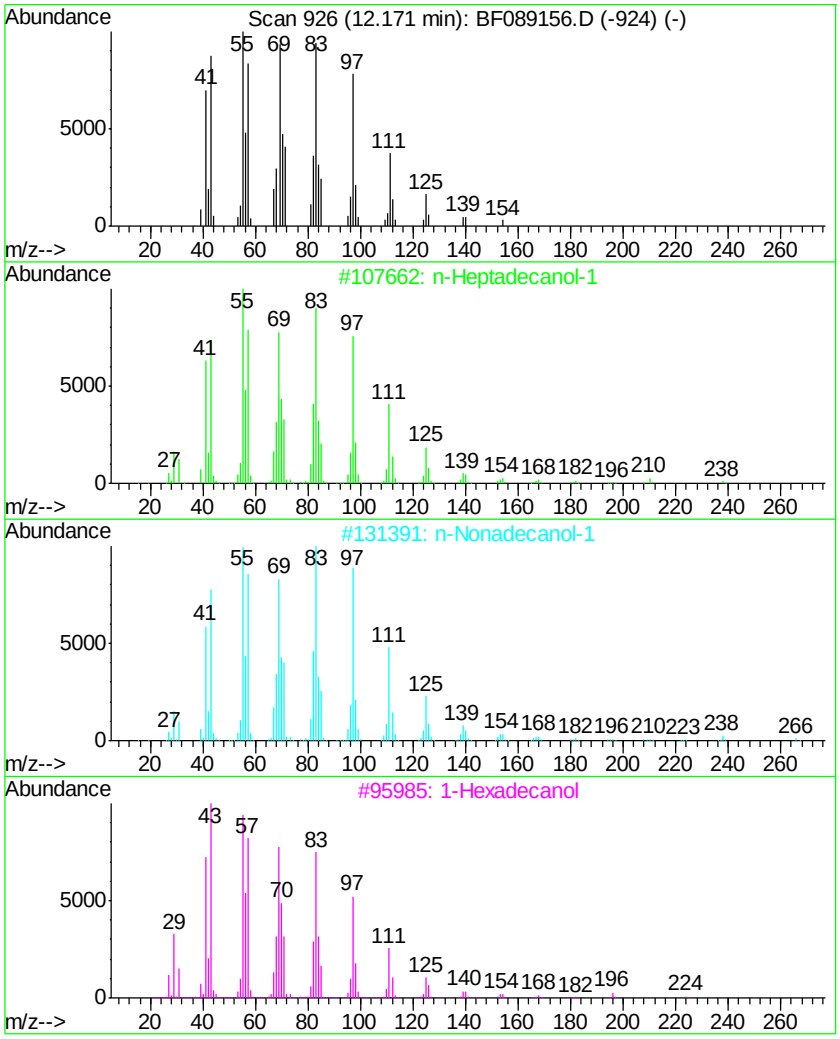
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

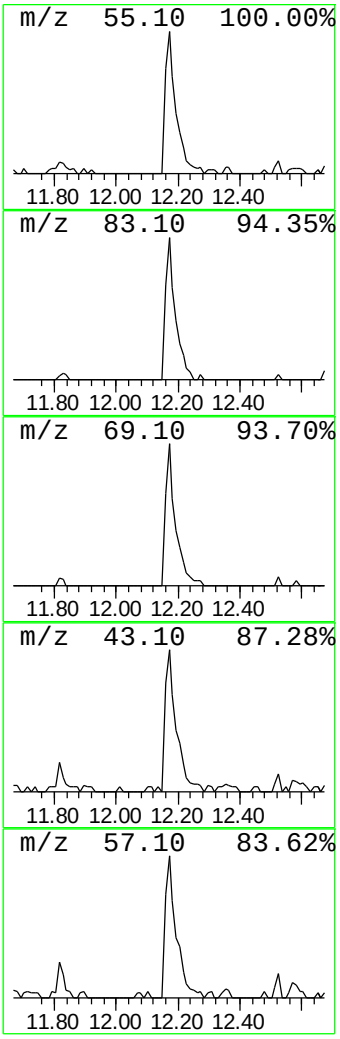
****

Peak Number 6 n-Heptadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.17	10.08 ng	259430	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	1-Hexadecanol	242	C16H34O	036653-82-4	91
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072016\
Data File : BF089156.D
Acq On : 21 Jul 2016 3:21
Operator : UM/SJ
Sample : H4019-02
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-SGS-33

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

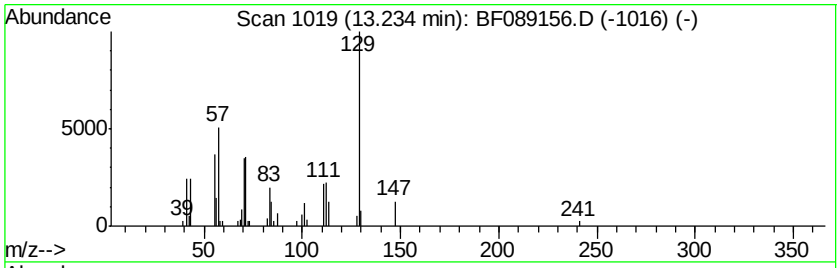
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

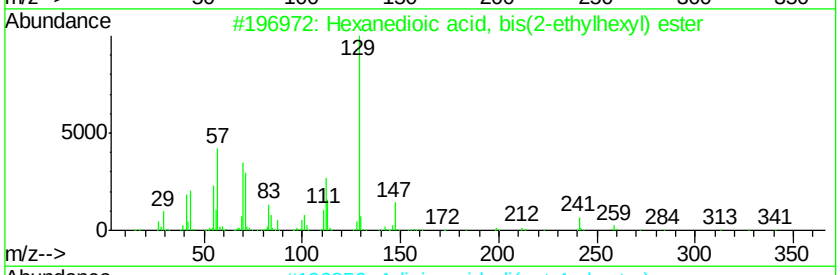
****

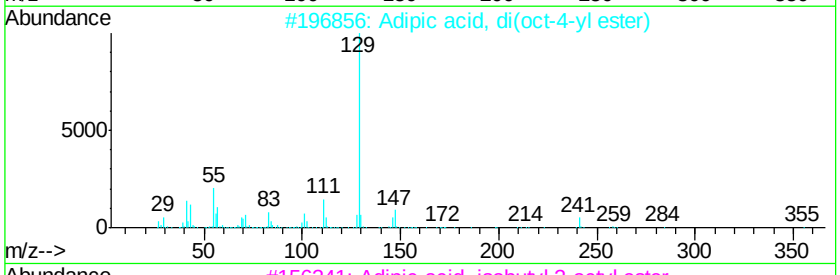
Peak Number 7 Hexanedioic acid, bis(2-eth... Concentration Rank 8

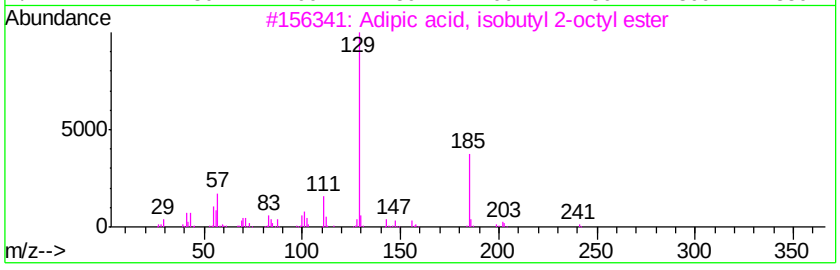
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	2.02 ng	63308	Chrysene-d12	13.71

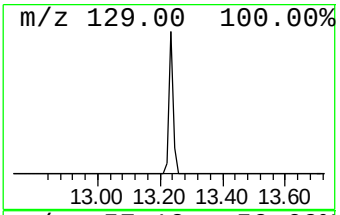
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	80
2	Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	50
3	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	38
4	Adipic acid, isobutyl isohexyl e...	286	C16H30O4	1000324-09-5	38
5	Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	37

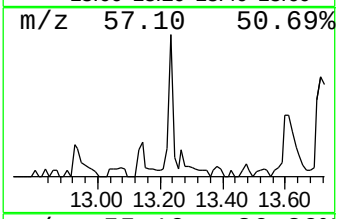


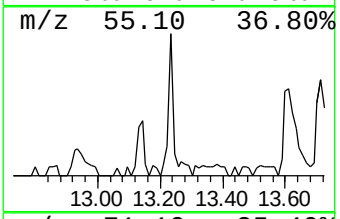


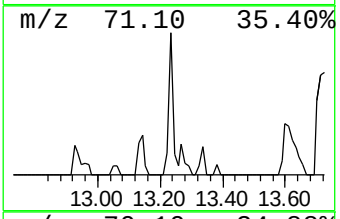


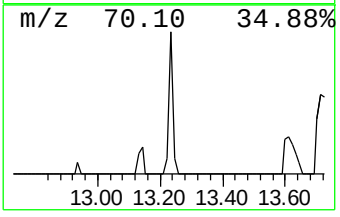












Library Search Compound Report

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

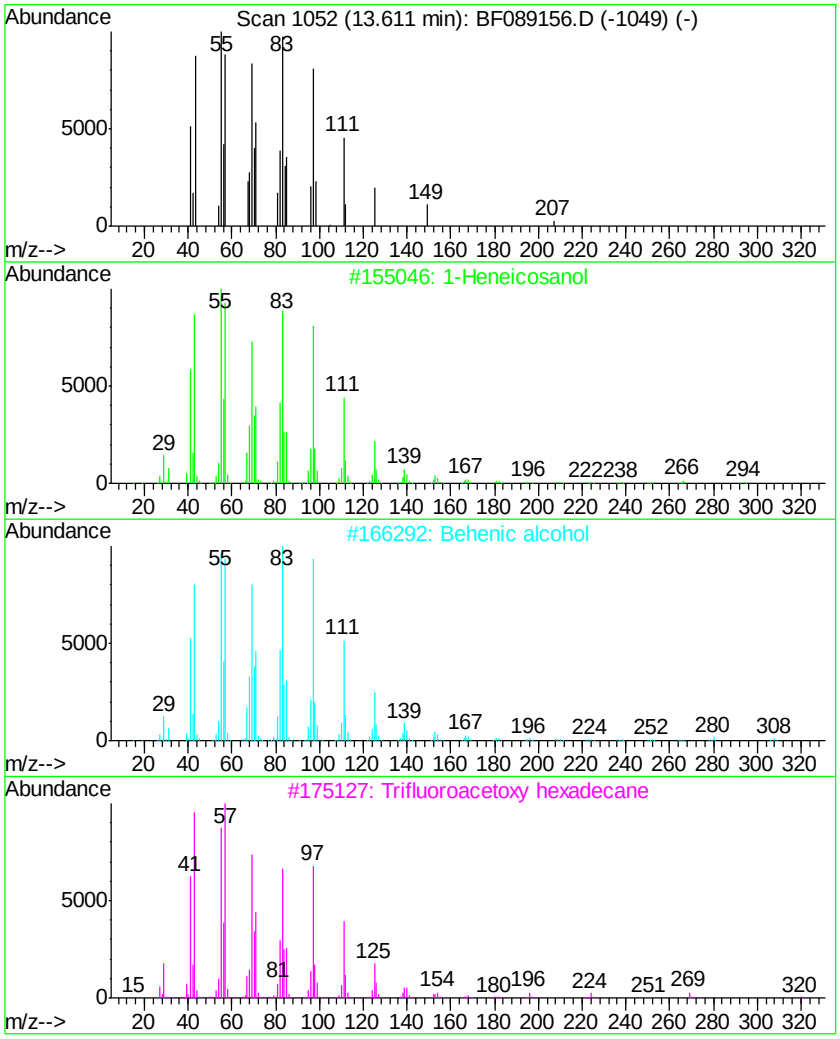
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

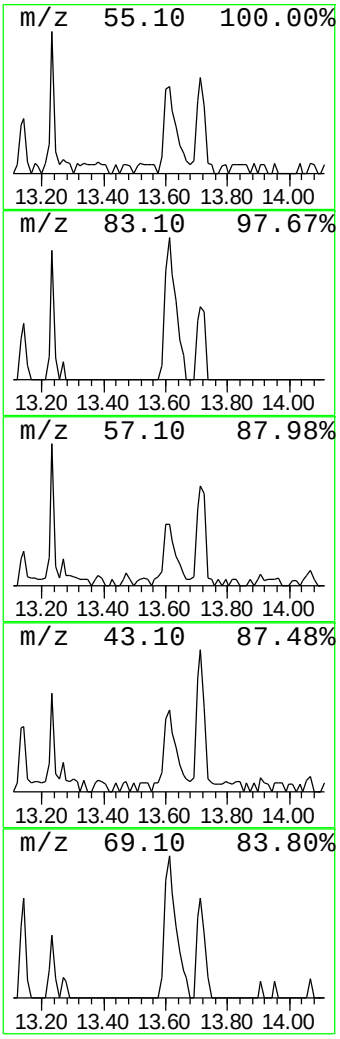
****

Peak Number 8 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	2.63 ng	82488	Chrysene-d12	13.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown4.74	4.74	3.6	ng	57019	1	6.60	319923	20.0
unknown6.36	6.36	80.8	ng	1291990	1	6.60	319923	20.0
4-Heptafluorobuty...	11.36	2.8	ng	73032	4	11.10	514610	20.0
n-Heptadecanol-1	12.17	10.1	ng	259430	4	11.10	514610	20.0
Hexanedioic acid,...	13.23	2.0	ng	63308	5	13.71	626563	20.0
1-Heneicosanol	13.61	2.6	ng	82488	5	13.71	626563	20.0