LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

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-BF080416.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	4.638	263	267	277	rBV	109022	269661	20.50%	2.493%
2	5.336	326	328	353	rBV	528425	1029292	78.23%	9.516%
3	6.982	470	472	478	rBV	655336	973914	74.02%	9.004%
4	7.073	478	480	503	rVV	779525	1222422	92.91%	11.301%
5	7.416	507	510	522	rVV	165321	246667	18.75%	2.280%
6	7.644	527	530	547	rVV	607923	867986	65.97%	8.024%
7	8.319	587	589	616	rBV	334213	654750	49.76%	6.053%
8	9.439	685	687	702	rBV	267704	362437	27.55%	3.351%
9	11.222	839	843	855	rBV	957482	1315704	100.00%	12.164%
10	12.102	916	920	925	rBV	6543	14080	1.07%	0.130%
11	12.262	931	934	942	rBB	313847	415882	31.61%	3.845%
12	13.554	1044	1047	1061	rBB	425000	577971	43.93%	5.343%
13	14.091	1084	1094	1105	rBV2	18016	113822	8.65%	1.052%
14	14.651	1141	1143	1150	rBV	285058	381526	29.00%	3.527%
15	15.691	1230	1234	1237	rBV3	6547	18216	1.38%	0.168%
16	16.034	1261	1264	1269	rBV2	11072	27805	2.11%	0.257%
17	16.708	1317	1323	1327	rBV2	42378	130614	9.93%	1.208%
18	16.777	1327	1329	1333	rVV3	14052	37431	2.84%	0.346%
19	16.891	1336	1339	1341	rVV	28384	34105	2.59%	0.315%
20	17.028	1348	1351	1354	rBV	954740	1097898	83.45%	10.150%
21	17.817	1418	1420	1424	rVB	21049	25516	1.94%	0.236%
22	18.366	1465	1468	1476	rVB	194767	318397	24.20%	2.944%
23	18.697	1495	1497	1506	rVB4	15381	47081	3.58%	0.435%
24	19.040	1523	1527	1530	rBV	72724	123900	9.42%	1.145%
25	20.023	1611	1613	1618	rBV	221680	269166	20.46%	2.488%
26	20.149	1622	1624	1626	rBV2	13690	26838	2.04%	0.248%
27	22.137	1793	1798	1802	rBV	51437	213672	16.24%	1.975%

Sum of corrected areas: 10816753

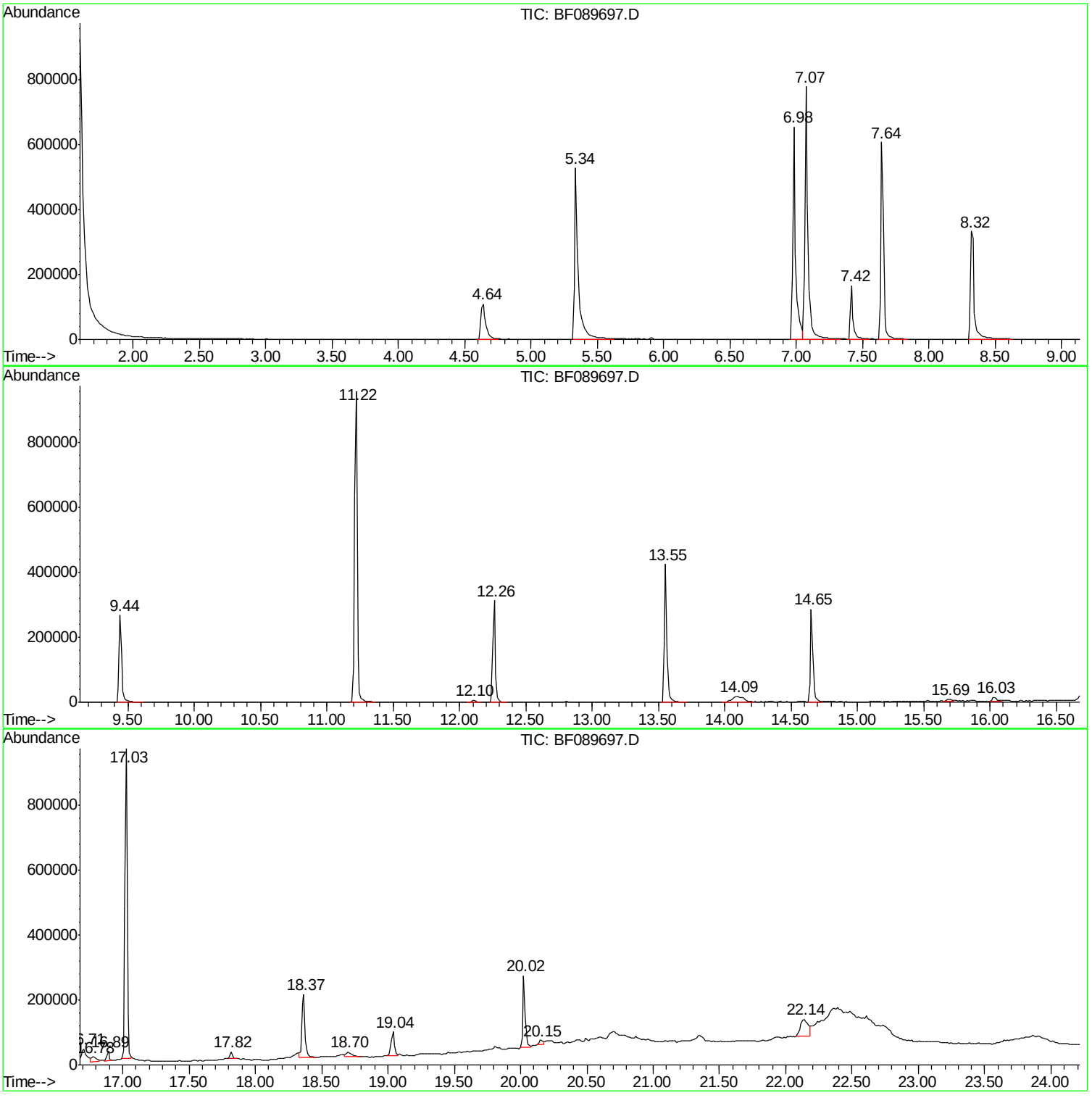
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.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\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

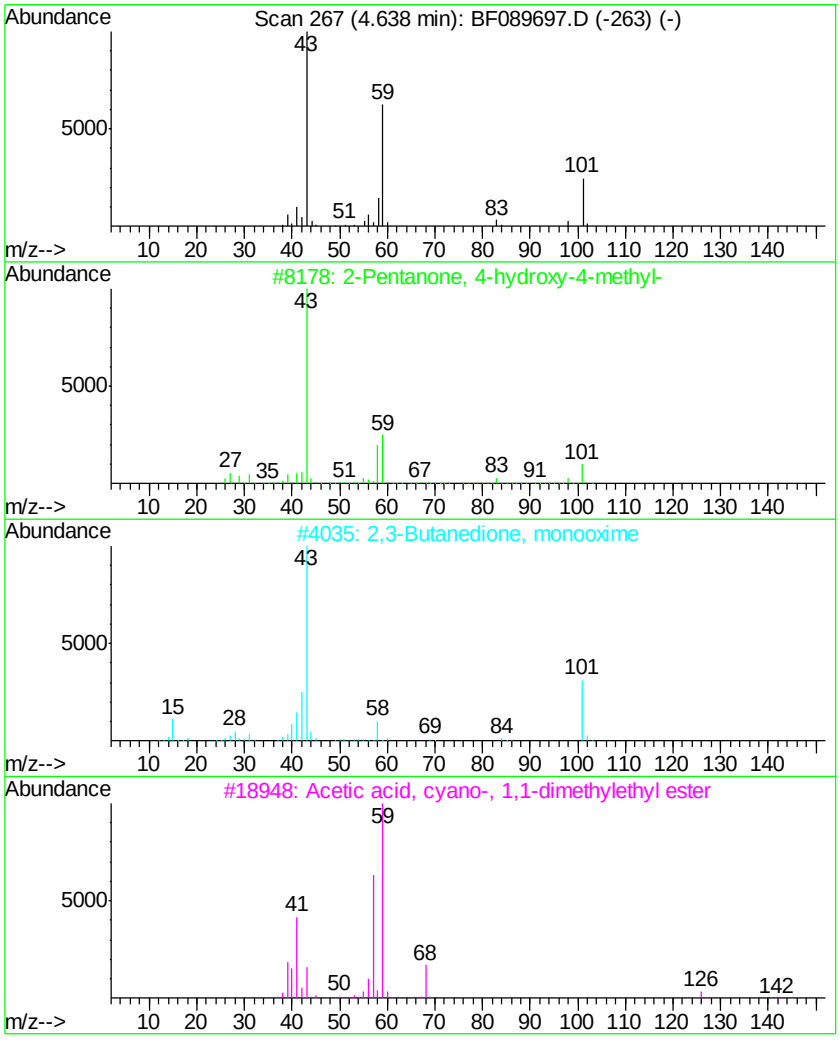
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

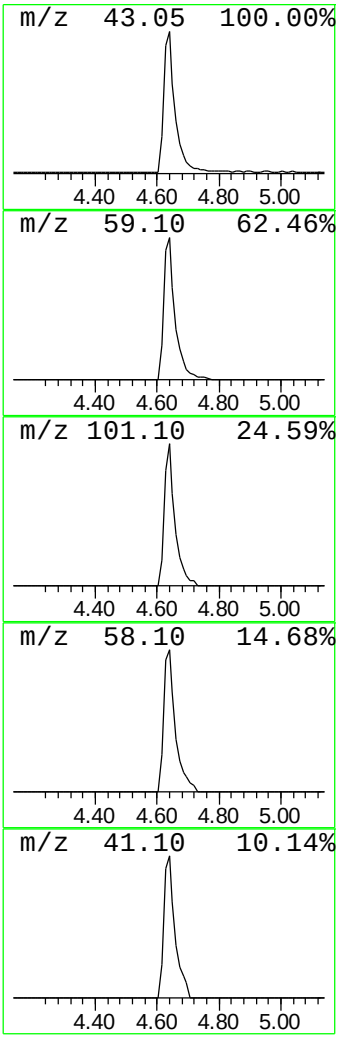
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	21.86 ng	269661	1,4-Dichlorobenzene-d4	7.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

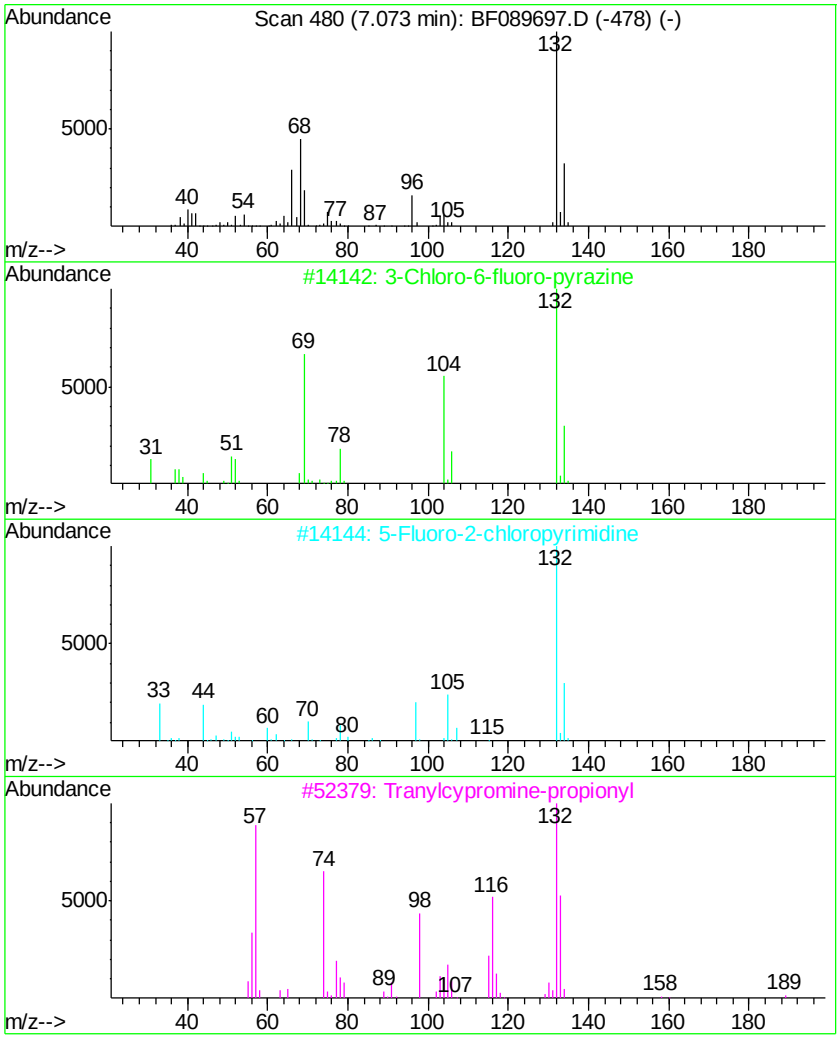
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

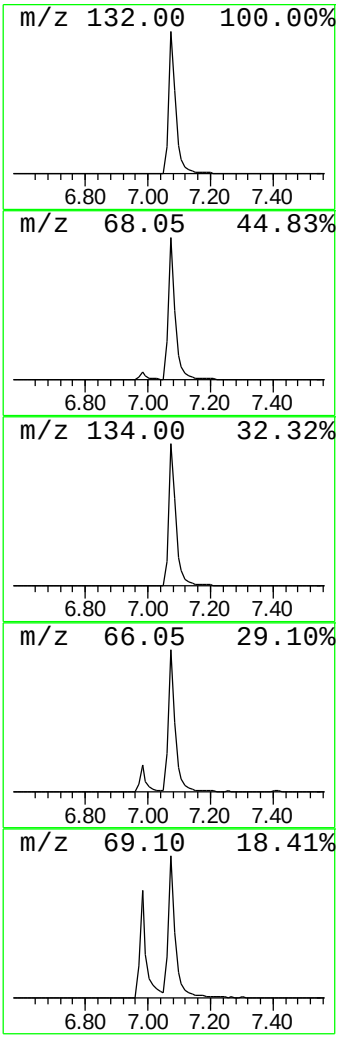
****

Peak Number 2 unknown7.07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	99.12 ng	1222420	1,4-Dichlorobenzene-d4	7.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Xenon	132	Xe	007440-63-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

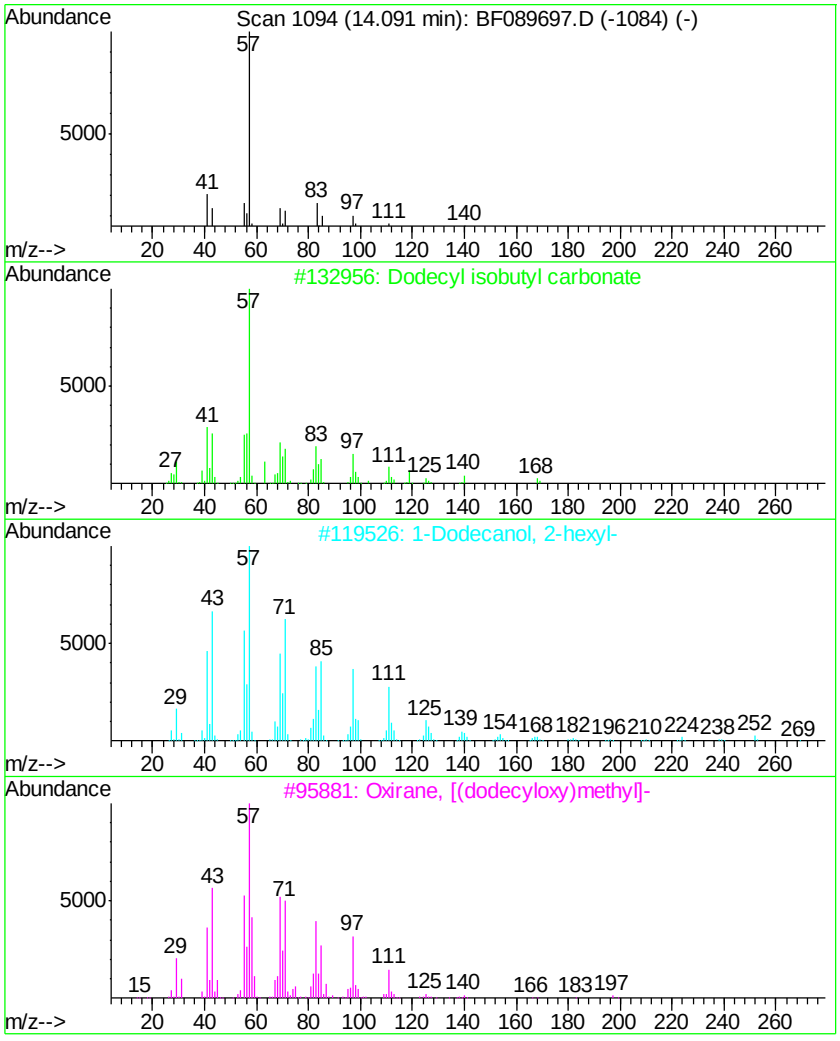
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

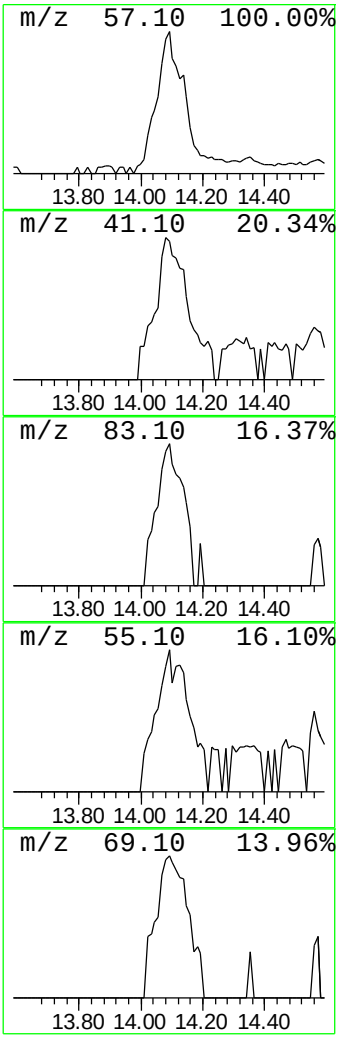
****

Peak Number 4 Dodecyl isobutyl carbonate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	5.97 ng	113822	Phenanthrene-d10	14.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	53
2	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	47
3	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	45
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	45
5	Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

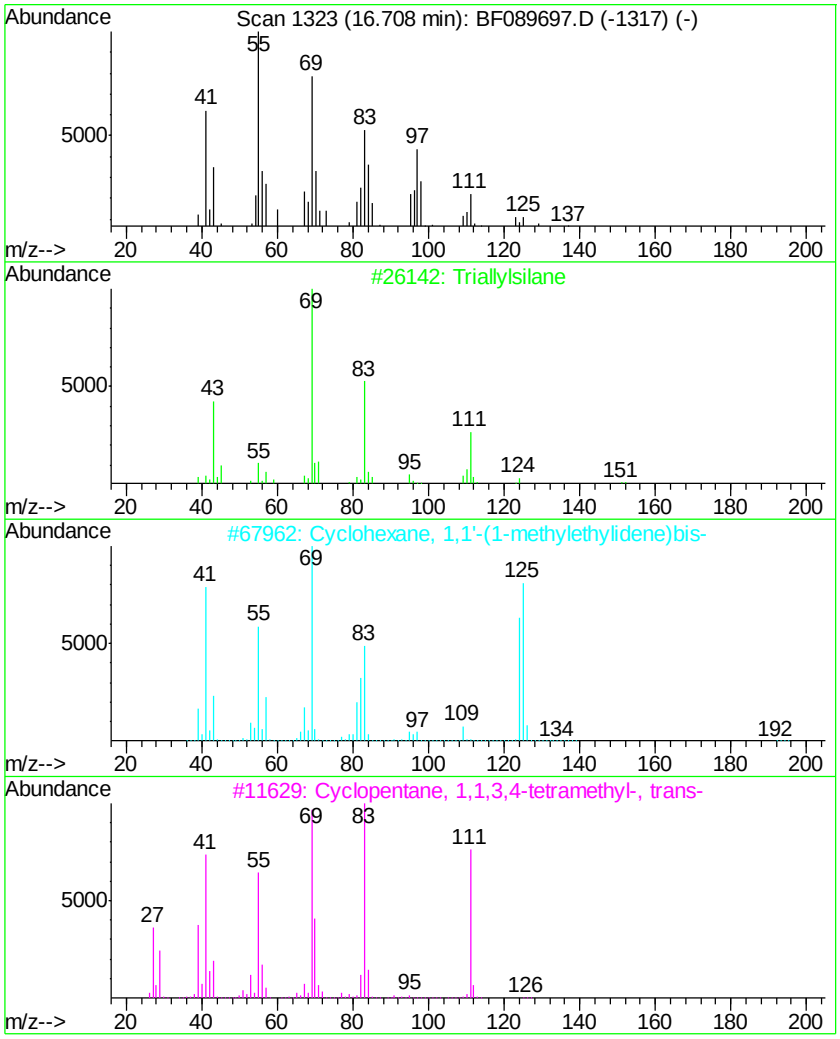
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

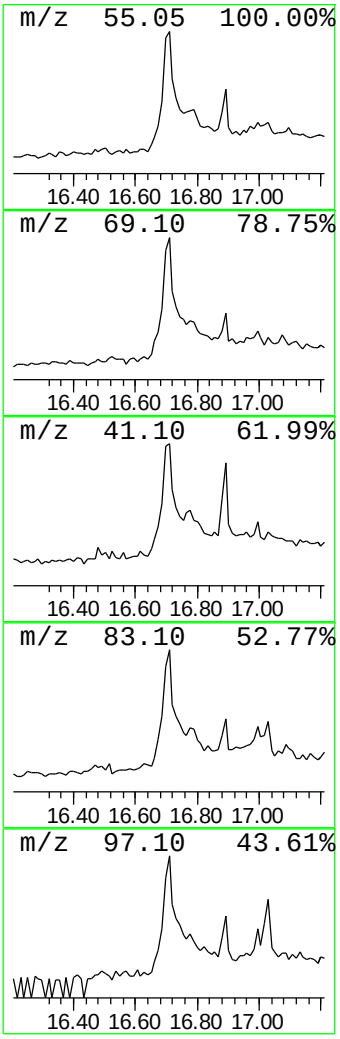
****

Peak Number 5 unknown16.71 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.71	8.20 ng	130614	Chrysene-d12	18.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triallylsilane	152	C9H16Si	001116-62-7	38
2	Cyclohexane, 1,1'-(1-methylethyl...	208	C15H28	054934-90-6	38
3	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	35
4	1,4-Heptadiene, 3,3,6-trimethyl-	138	C10H18	074498-89-8	27
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

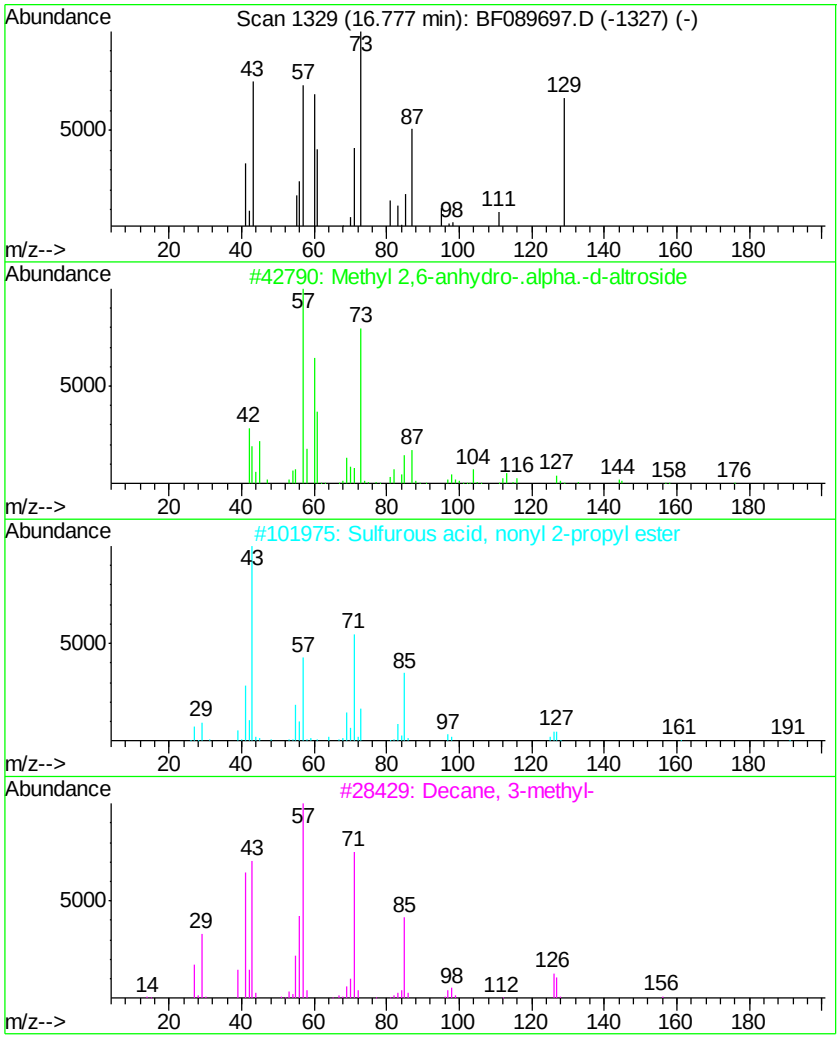
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

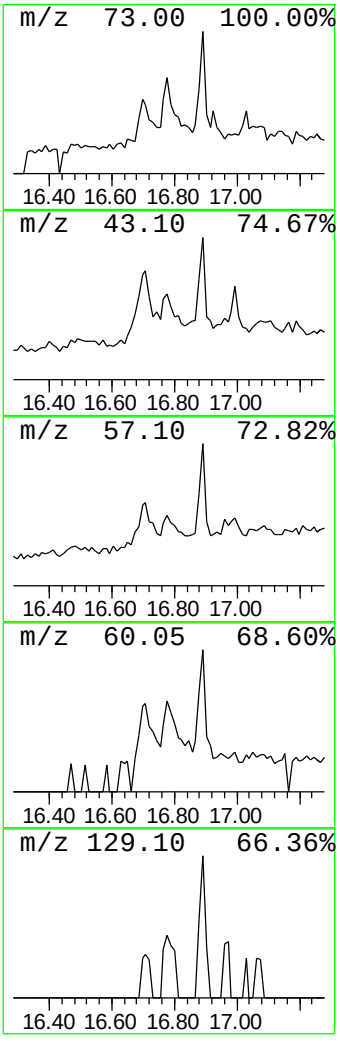
****

Peak Number 6 unknown16.78 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.78	2.35 ng	37431	Chrysene-d12	18.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	32
2	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	10
3	Decane, 3-methyl-	156	C11H24	013151-34-3	10
4	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	9
5	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

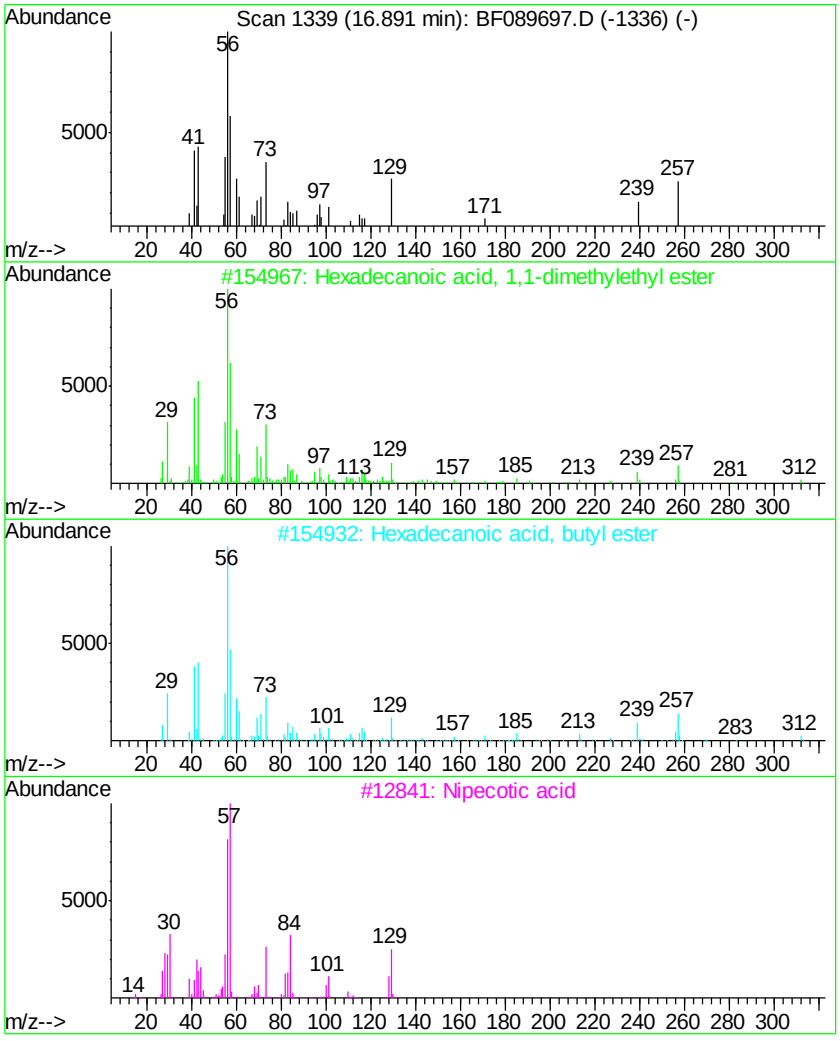
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

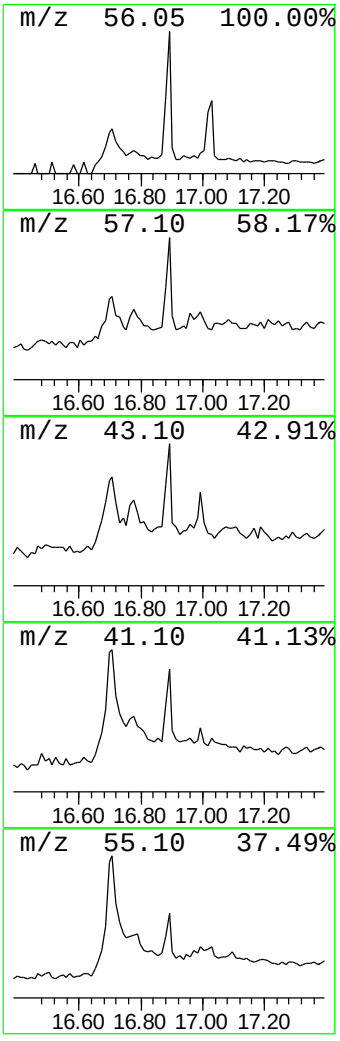
****

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	2.14 ng	34105	Chrysene-d12	18.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	64
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	38
5	Chloromethyl 2-chloroundecanoate	268	C12H22Cl2O2	080418-88-8	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

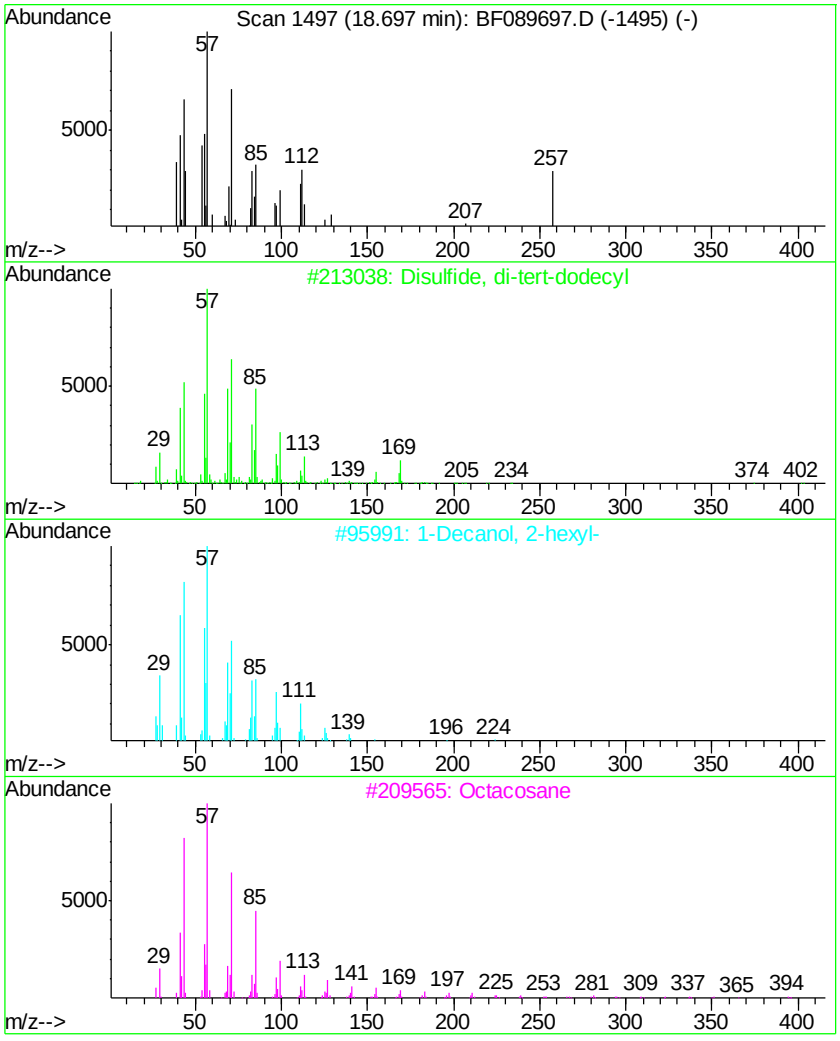
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

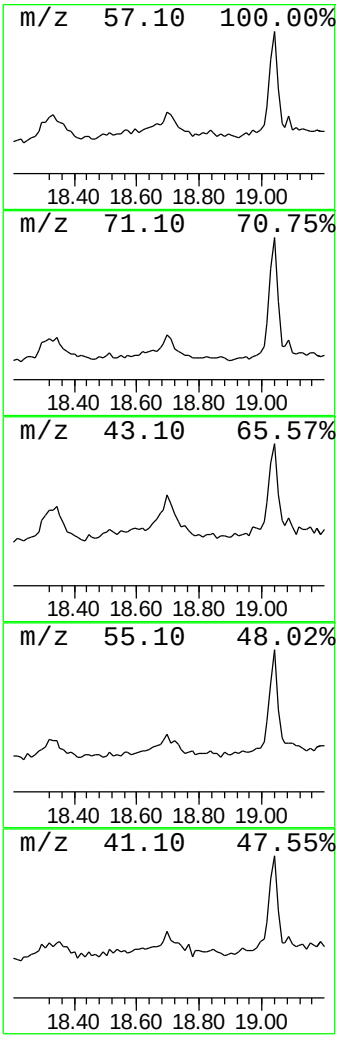
****

Peak Number 8 unknown18.70 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.70	2.96 ng	47081	Chrysene-d12	18.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	38
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	38
3	Octacosane	394	C28H58	000630-02-4	38
4	Oxalic acid, 2-ethylhexyl tetrad...	398	C24H46O4	1000309-39-7	35
5	Hexacosane	366	C26H54	000630-01-3	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

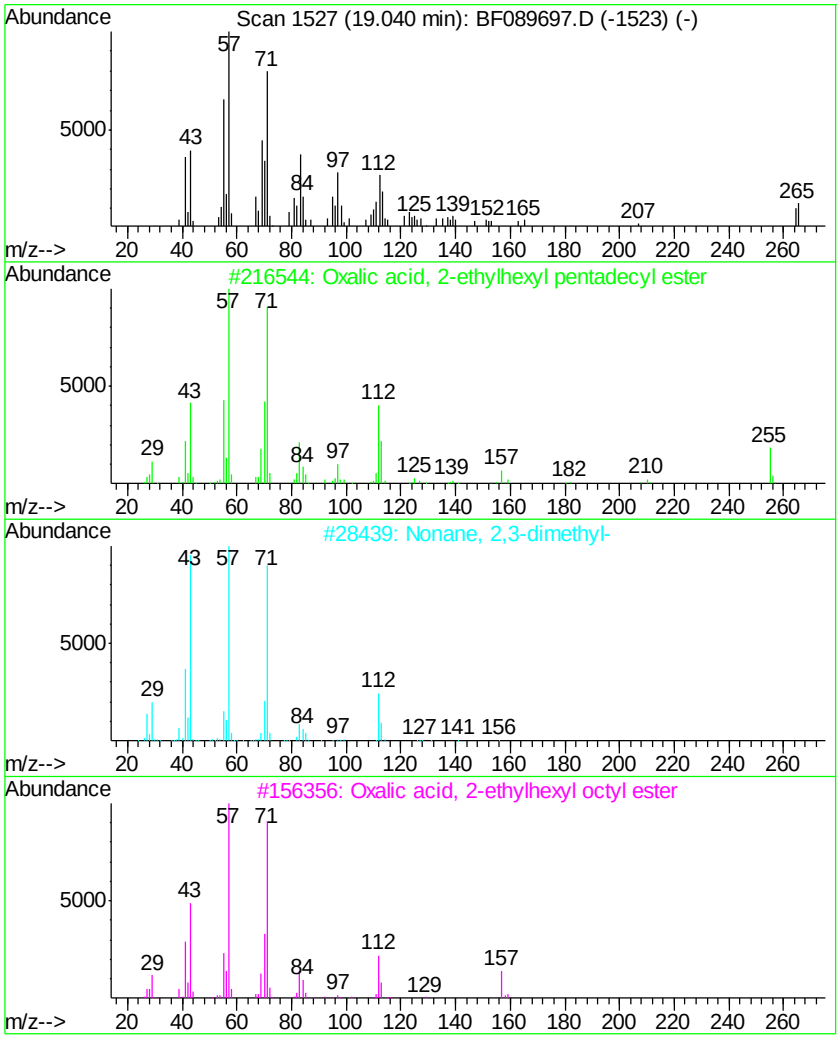
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

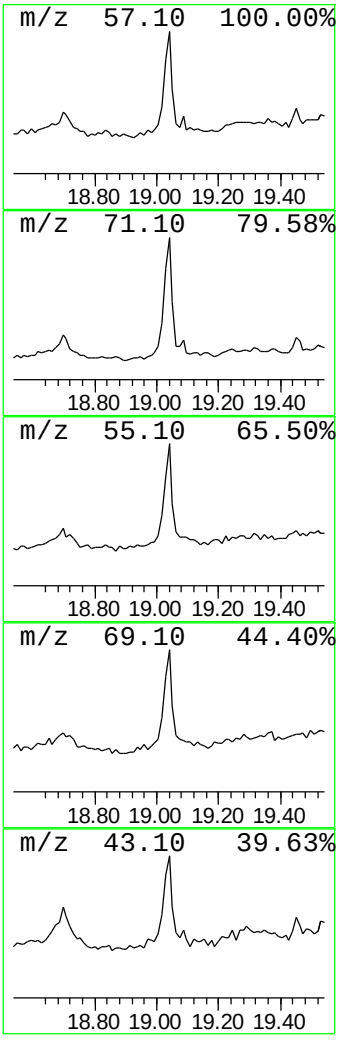
****

Peak Number 9 Oxalic acid, 2-ethylhexyl p... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	7.78 ng	123900	Chrysene-d12	18.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, 2-ethylhexyl pentad...	412	C25H48O4	1000309-39-8	50
2	Nonane, 2,3-dimethyl-	156	C11H24	002884-06-2	43
3	Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	43
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	35
5	Cyclopropanecarboxamide, N-metha...	139	C8H13NO	1000340-05-6	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

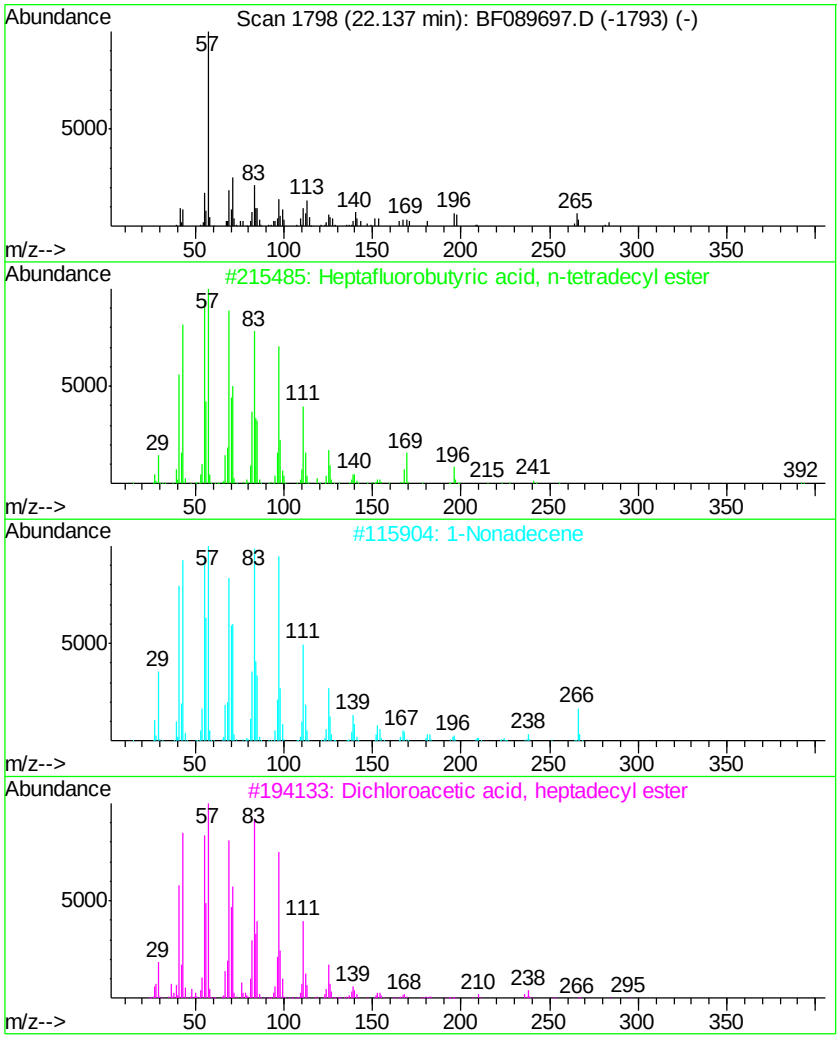
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

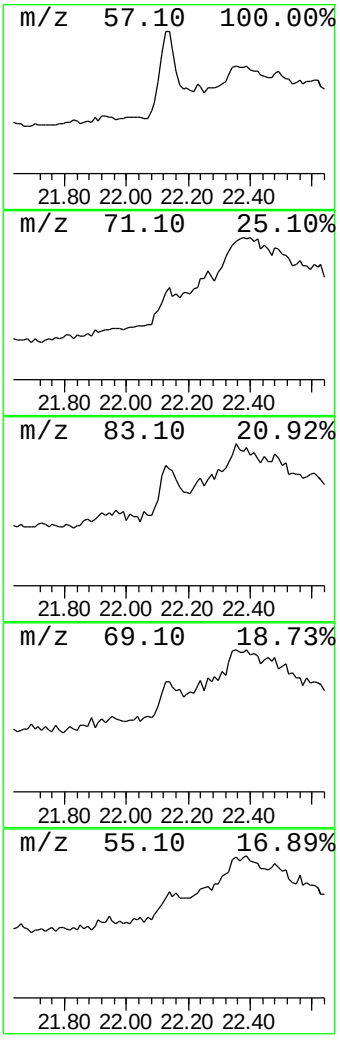
****

Peak Number 10 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.14	15.88 ng	213672	Perylene-d12	20.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	58
2	1-Nonadecene	266	C19H38	018435-45-5	53
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	52
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	52
5	Tetradecanal	212	C14H28O	000124-25-4	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080916\
Data File : BF089697.D
Acq On : 9 Aug 2016 19:58
Operator : UM/SJ
Sample : PB92711BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB92711BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
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...	4.64	21.9	ng	269661	1	7.42	246667	20.0
unknown7.07	7.07	99.1	ng	1222420	1	7.42	246667	20.0
Dodecyl isobutyl ...	14.09	6.0	ng	113822	4	14.65	381526	20.0
unknown16.71	16.71	8.2	ng	130614	5	18.37	318397	20.0
unknown16.78	16.78	2.4	ng	37431	5	18.37	318397	20.0
Hexadecanoic acid...	16.89	2.1	ng	34105	5	18.37	318397	20.0
unknown18.70	18.70	3.0	ng	47081	5	18.37	318397	20.0
Oxalic acid, 2-et...	19.04	7.8	ng	123900	5	18.37	318397	20.0
Heptafluorobutyri...	22.14	15.9	ng	213672	6	20.02	269166	20.0