LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100421.D
Acq On : 11 Nov 2017 5:16
Operator : SJ/JU
Sample : I6355-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110317-SIDI-E-D-B

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-BF110817.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	2.234	21	25	35	rVB	58605	94052	1.29%	0.220%
2	5.134	513	518	526	rVB	447030	548736	7.54%	1.284%
3	5.522	579	584	587	rBV	2894960	2904611	39.91%	6.799%
4	6.522	749	754	757	rBV	2212271	2066202	28.39%	4.836%
5	6.675	774	780	783	rBV	4247552	4470767	61.43%	10.464%
6	6.898	815	818	822	rVB	1093638	1000001	13.74%	2.341%
7	7.063	841	846	849	rBV	4854870	5467484	75.12%	12.797%
8	7.475	908	916	919	rBV	3891825	5025238	69.04%	11.762%
9	8.181	1032	1036	1040	rBV	1409929	1199609	16.48%	2.808%
10	9.263	1214	1220	1223	rBV	5667683	7278259	100.00%	17.036%
11	9.645	1282	1285	1289	rBV	163631	128261	1.76%	0.300%
12	9.939	1329	1335	1348	rVB	1289889	1227009	16.86%	2.872%
13	10.604	1445	1448	1451	rBV	187858	134961	1.85%	0.316%
14	10.651	1451	1456	1459	rBV	239031	191255	2.63%	0.448%
15	10.728	1464	1469	1472	rBV	2763257	2647351	36.37%	6.196%
16	11.422	1583	1587	1591	rBV	1140684	975449	13.40%	2.283%
17	13.016	1852	1858	1861	rBV2	4615786	5369176	73.77%	12.567%
18	14.063	2032	2036	2039	rBV	943299	853833	11.73%	1.999%
19	15.545	2282	2288	2298	rBV	508707	772387	10.61%	1.808%
20	16.010	2362	2367	2374	rVB2	89812	128884	1.77%	0.302%
21	16.527	2450	2455	2462	rVB2	85916	144115	1.98%	0.337%
22	17.139	2554	2559	2565	rVB2	50065	95938	1.32%	0.225%

Sum of corrected areas: 42723578

LSC Report - Integrated Chromatogram

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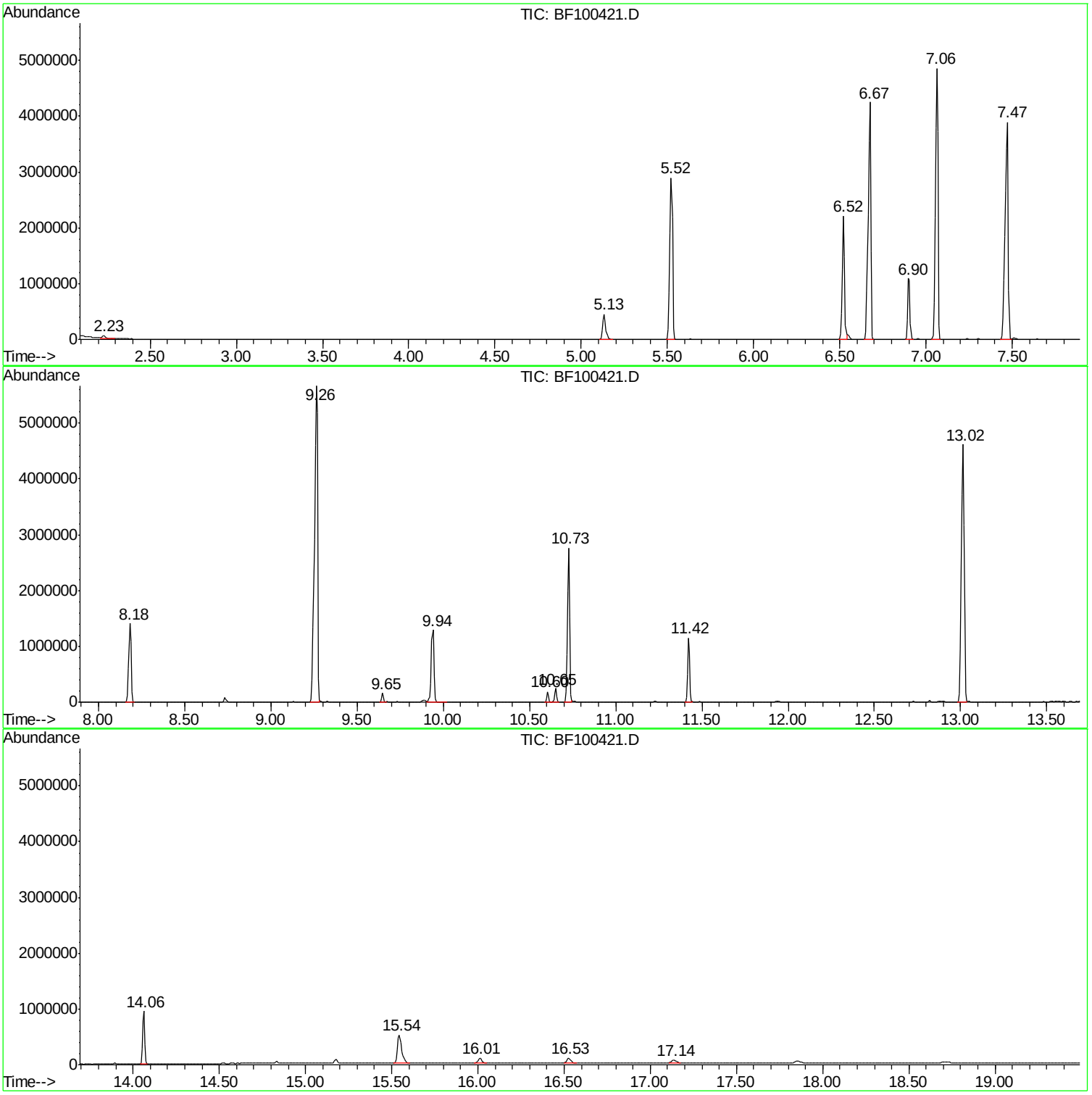
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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 : BF100421.D
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Operator : SJ/JU
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

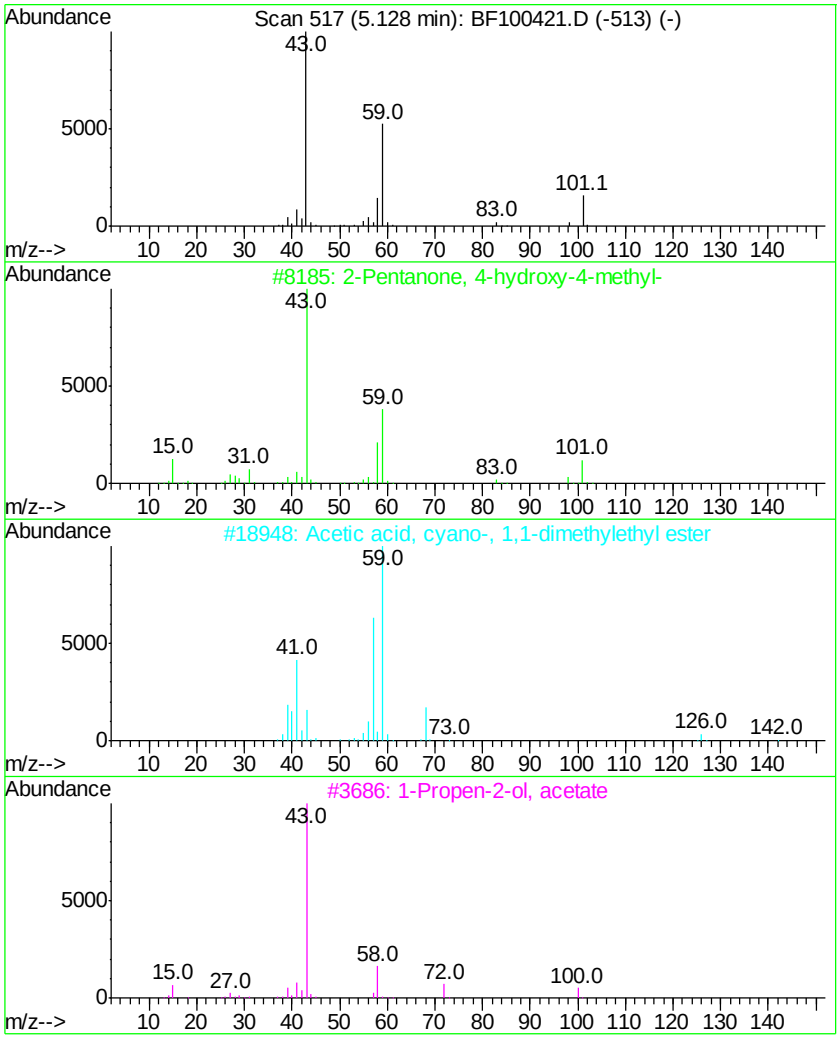
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

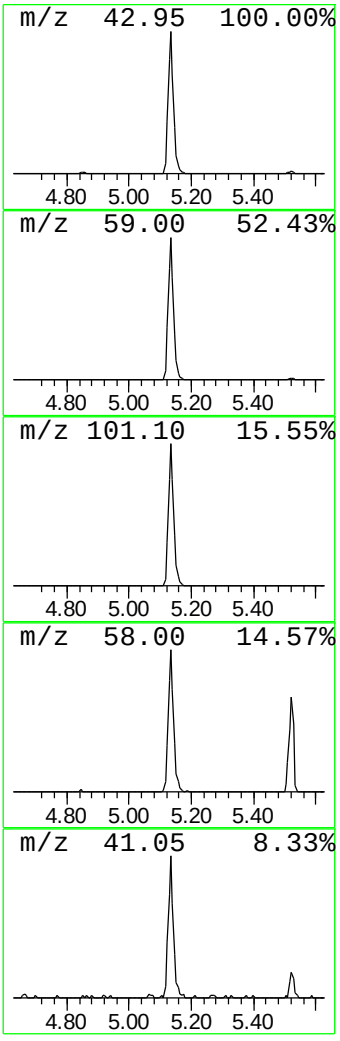
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	10.97 ng	548736	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Library Search Compound Report

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Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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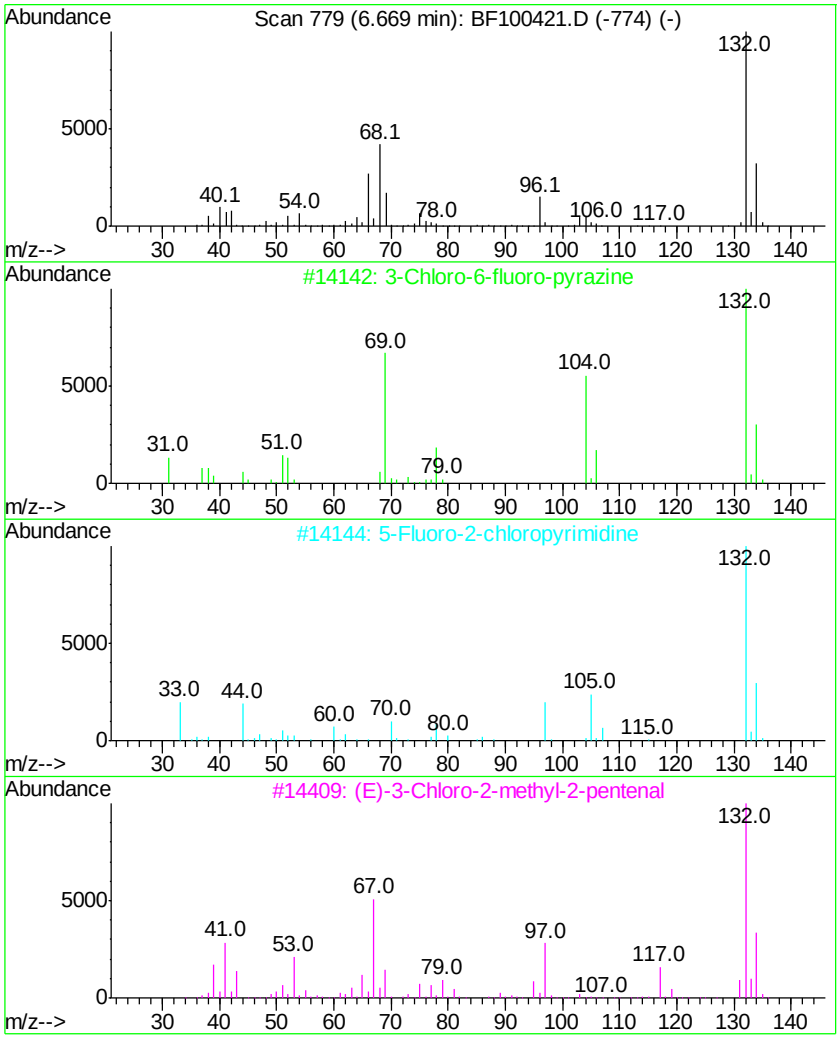
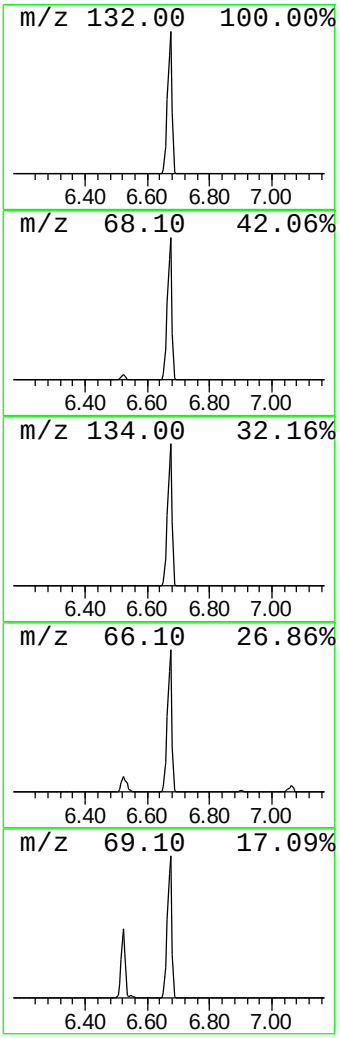
Peak Number 2 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	89.42 ng	4470770	1,4-Dichlorobenzene-d4	6.90

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	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Data File : BF100421.D
Acq On : 11 Nov 2017 5:16
Operator : SJ/JU
Sample : I6355-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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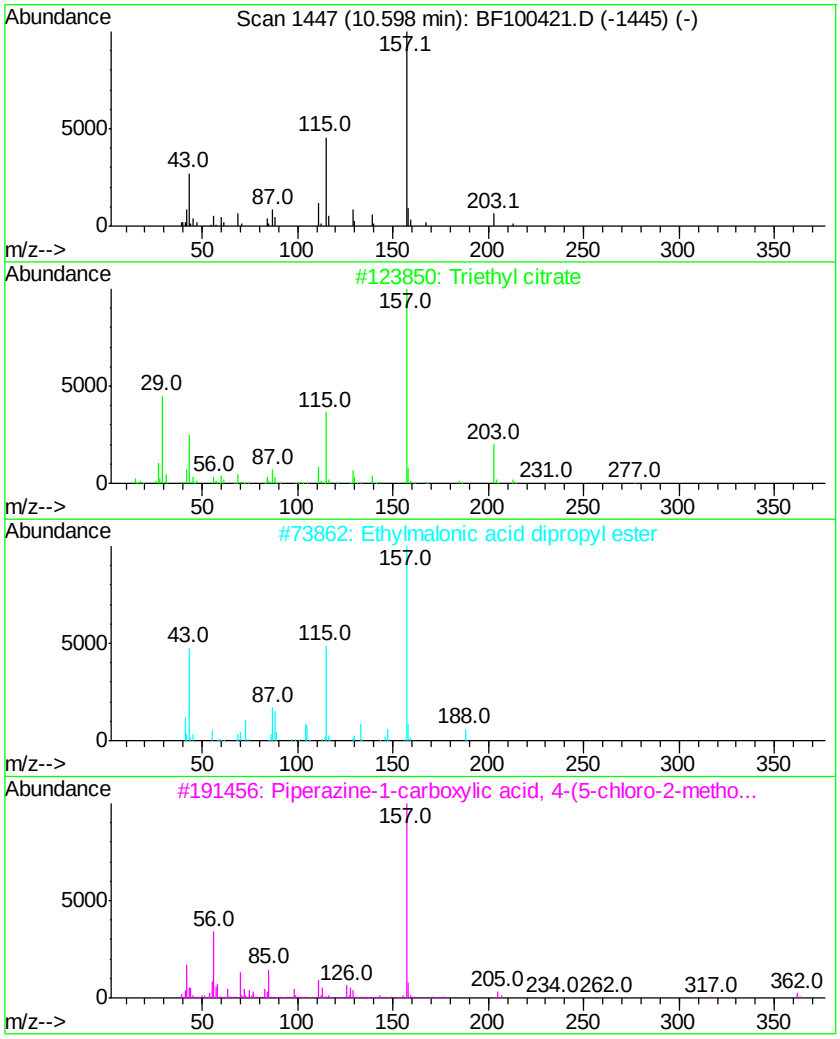
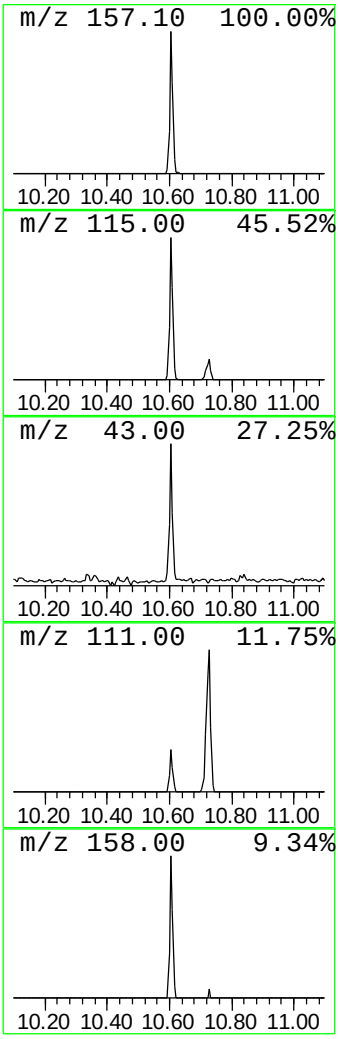
Peak Number 4 Triethyl citrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.20 ng	134961	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	40
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	36
5	2-Chlorobenzoic acid, tetradecyl...	352	C21H33ClO2	1000292-42-9	33





Library Search Compound Report

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Operator : SJ/JU
Sample : I6355-11
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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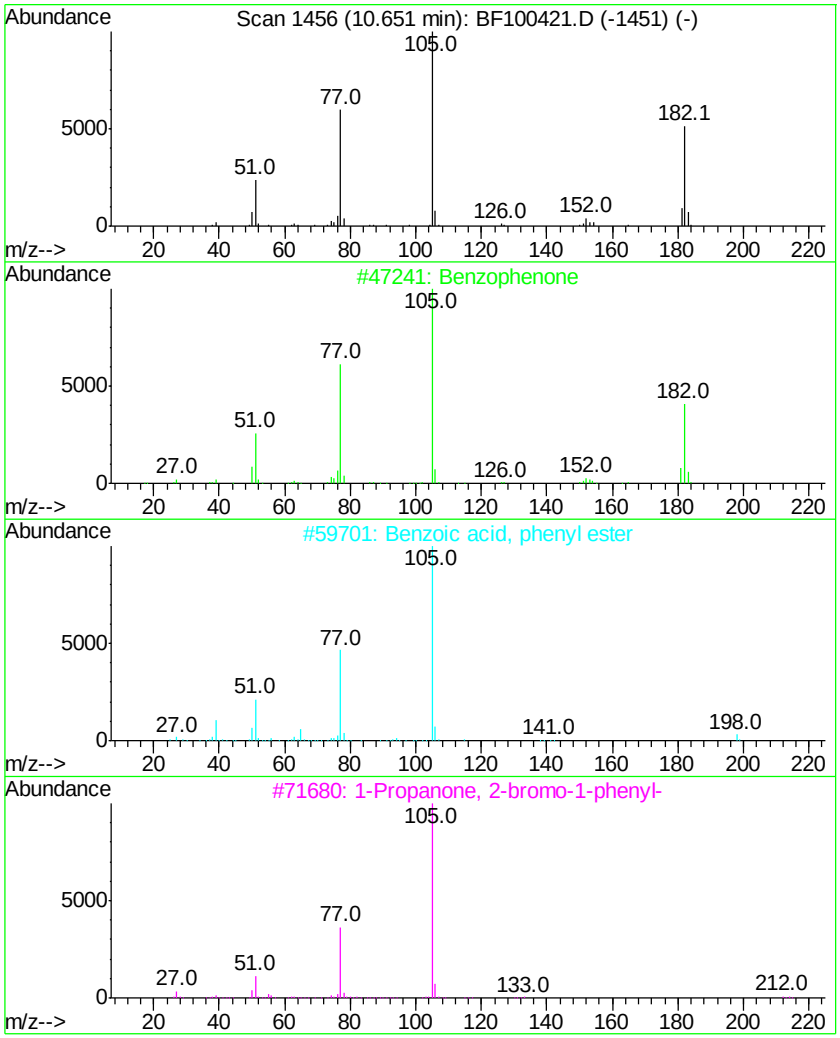
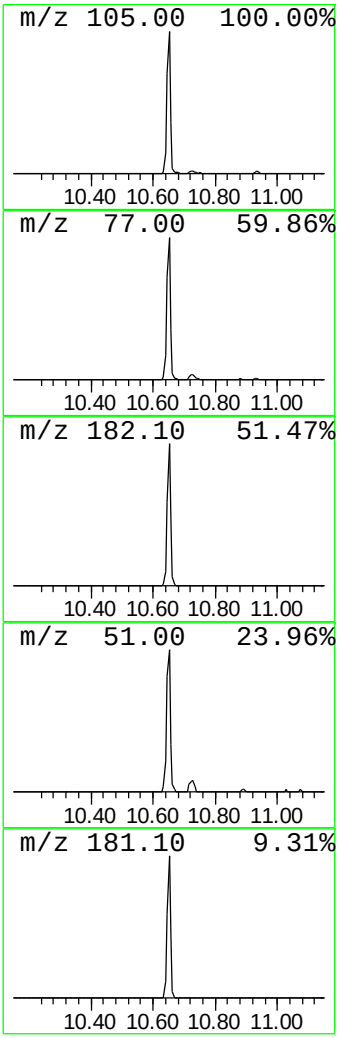
Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	3.12 ng	191255	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
5	Benzoyl bromide	184	C7H5BrO	000618-32-6	47





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 110317-SIDI-E-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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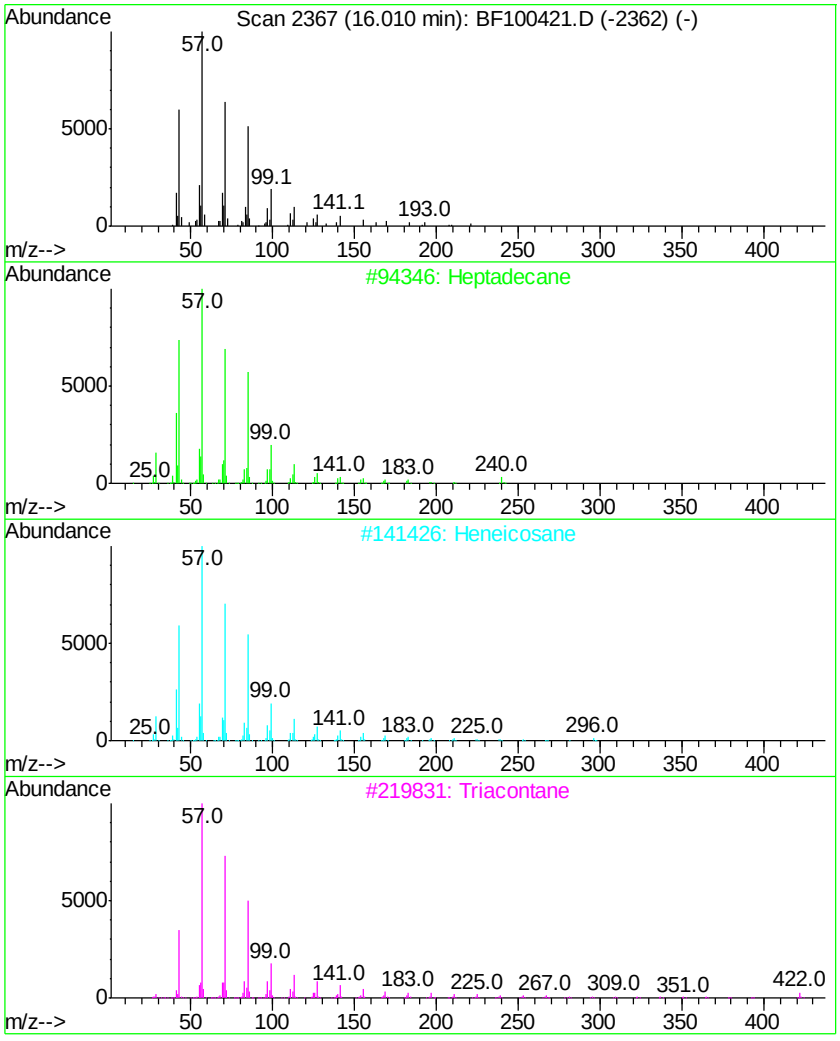
TIC Integration Parameters: LSCINT.P

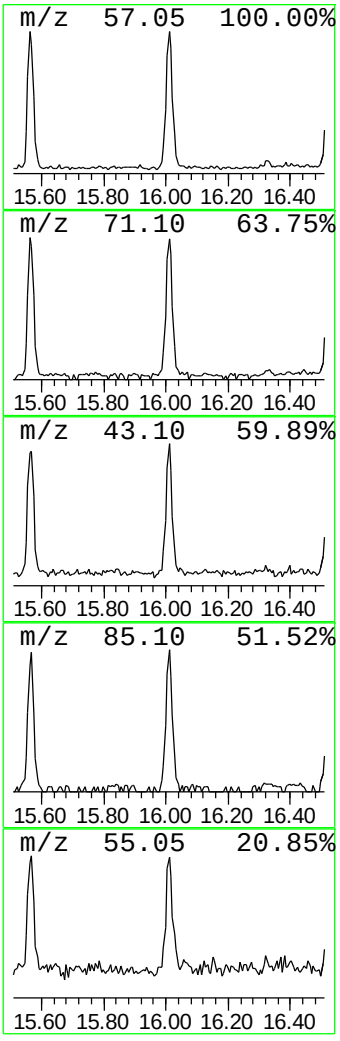
****

Peak Number 6 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	3.34 ng	128884	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heneicosane	296	C21H44	000629-94-7	86
3	Triacontane	422	C30H62	000638-68-6	86
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Heptacosane	380	C27H56	000593-49-7	74





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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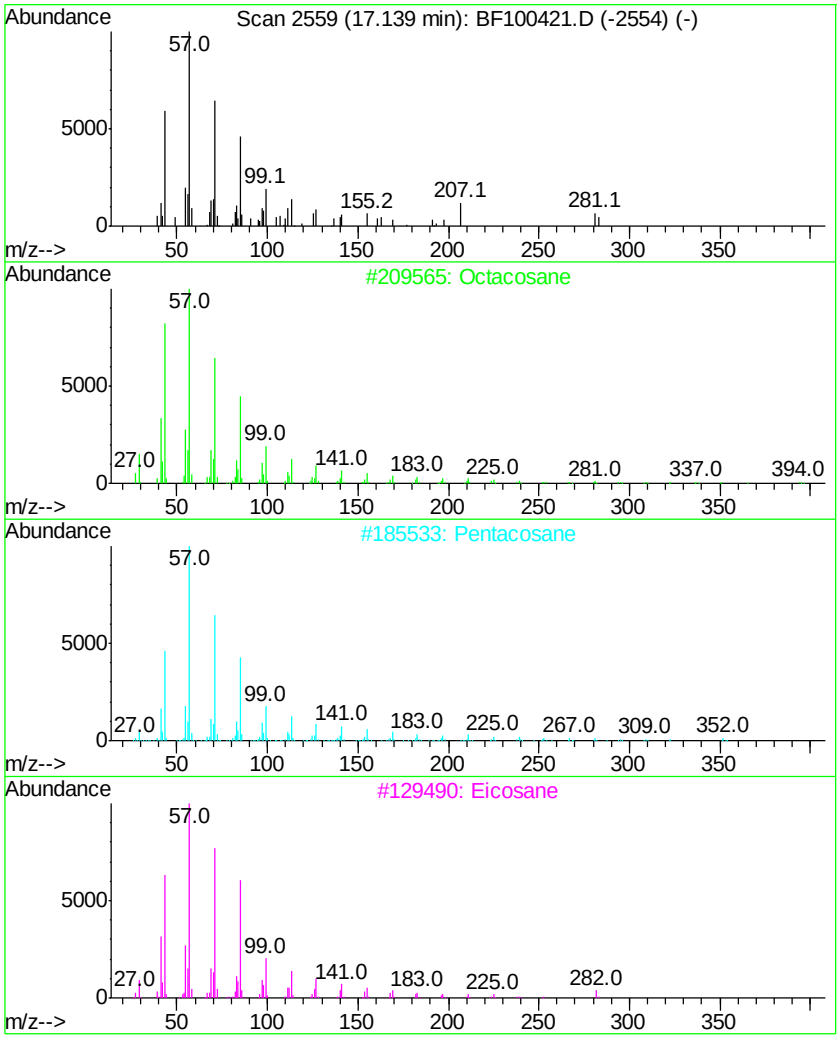
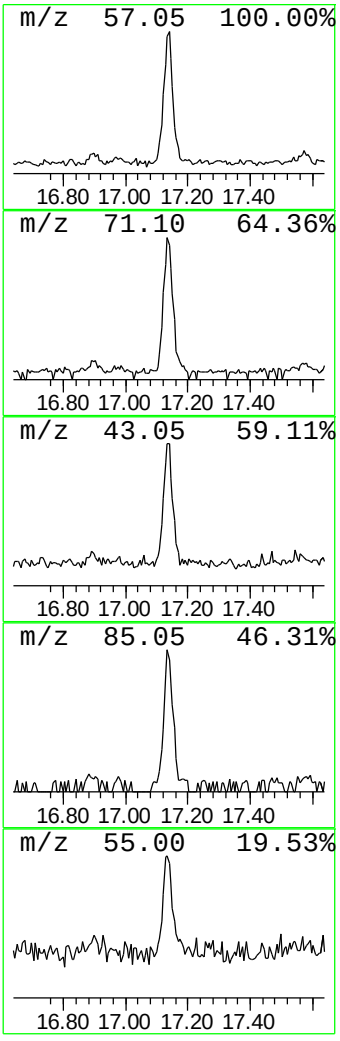
Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	2.48 ng	95938	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Pentacosane	352	C25H52	000629-99-2	83
3	Eicosane	282	C20H42	000112-95-8	80
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
5	Triacontane	422	C30H62	000638-68-6	80





Tentatively Identified Compound (LSC) summary

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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...	5.13	11.0	ng	548736	1	6.90	1000000	20.0
unknown6.67	6.67	89.4	ng	4470770	1	6.90	1000000	20.0
Triethyl citrate	10.60	2.2	ng	134961	3	9.94	1227010	20.0
Benzophenone	10.65	3.1	ng	191255	3	9.94	1227010	20.0
Heptadecane	16.01	3.3	ng	128884	6	15.54	772387	20.0
Octacosane	17.14	2.5	ng	95938	6	15.54	772387	20.0