LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2B-CS-2(0-10FTBGS)

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-BF042716.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	4.910	245	247	256	rBV	82639	109507	3.71%	0.359%
2	5.333	282	284	287	rBV	2465149	2647363	89.67%	8.682%
3	6.384	374	376	379	rBV	2234321	2834792	96.02%	9.296%
4	6.522	385	388	390	rBV	2088775	2952217	100.00%	9.681%
5	6.750	405	408	410	rBV	1163446	1068548	36.19%	3.504%
6	6.910	419	422	424	rBV	1831970	2258071	76.49%	7.405%
7	7.322	455	458	460	rBV	1283539	1784137	60.43%	5.851%
8	7.425	464	467	474	rVB3	25262	78785	2.67%	0.258%
9	8.042	518	521	523	rBV	1153278	1354082	45.87%	4.441%
10	8.579	565	568	570	rBV2	109519	117833	3.99%	0.386%
11	8.899	593	596	603	rBV2	44648	89881	3.04%	0.295%
12	9.116	612	615	617	rBV	3436446	2922236	98.98%	9.583%
13	9.516	646	650	652	rBV2	313113	504110	17.08%	1.653%
14	9.733	666	669	671	rBV	56768	47099	1.60%	0.154%
15	9.791	671	674	676	rBV	1612043	1455995	49.32%	4.775%
16	10.225	706	712	714	rBV2	61552	113152	3.83%	0.371%
17	10.305	717	719	720	rBV	40502	34224	1.16%	0.112%
18	10.442	728	731	734	rBV2	43554	85062	2.88%	0.279%
19	10.579	740	743	745	rBV2	1153658	1581599	53.57%	5.187%
20	10.625	745	747	752	rVV	47767	119543	4.05%	0.392%
21	10.705	752	754	758	rVB	134106	178926	6.06%	0.587%
22	11.151	789	793	794	rBV	68833	71576	2.42%	0.235%
23	11.265	801	803	808	rBV2	1031691	1239008	41.97%	4.063%
24	11.345	808	810	812	rVB2	28083	36766	1.25%	0.121%
25	11.574	828	830	834	rVB	27781	34283	1.16%	0.112%
26	11.814	848	851	853	rBV	615771	619589	20.99%	2.032%
27	11.882	855	857	861	rVB	38806	72901	2.47%	0.239%
28	12.477	907	909	912	rBV	252824	244551	8.28%	0.802%
29	12.591	917	919	926	rBV2	81711	117964	4.00%	0.387%
30	12.705	926	929	931	rBV	202327	243739	8.26%	0.799%
31	12.854	940	942	947	rBV	2043508	1919555	65.02%	6.295%
32	13.037	954	958	960	rVB	18591	38832	1.32%	0.127%
33	13.094	960	963	965	rBV4	29512	59903	2.03%	0.196%
34	13.139	965	967	968	rBV	23561	33901	1.15%	0.111%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2B-CS-2(0-10FTBGS)

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-BF042716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.551	1000	1003	1006	rBV2	15384	33572	1.14%	0.110%
36	13.654	1009	1012	1013	rBV2	22319	44339	1.50%	0.145%
37	13.757	1019	1021	1028	rBV2	182660	332614	11.27%	1.091%
38	13.894	1031	1033	1041	rBV2	642985	1202487	40.73%	3.943%
39	14.408	1074	1078	1082	rBV5	36833	137790	4.67%	0.452%
40	14.637	1095	1098	1099	rBV2	41881	68957	2.34%	0.226%
41	14.660	1099	1100	1101	rBV	61111	51492	1.74%	0.169%
42	14.900	1119	1121	1126	rBV	103289	221548	7.50%	0.727%
43	15.174	1143	1145	1148	rVB	62021	98504	3.34%	0.323%
44	15.231	1148	1150	1153	rBV	61389	108764	3.68%	0.357%
45	15.288	1153	1155	1158	rBV	494695	825464	27.96%	2.707%
46	15.734	1192	1194	1196	rBV	37009	55849	1.89%	0.183%
47	16.660	1273	1275	1279	rVB	134668	242784	8.22%	0.796%

Sum of corrected areas: 30493894

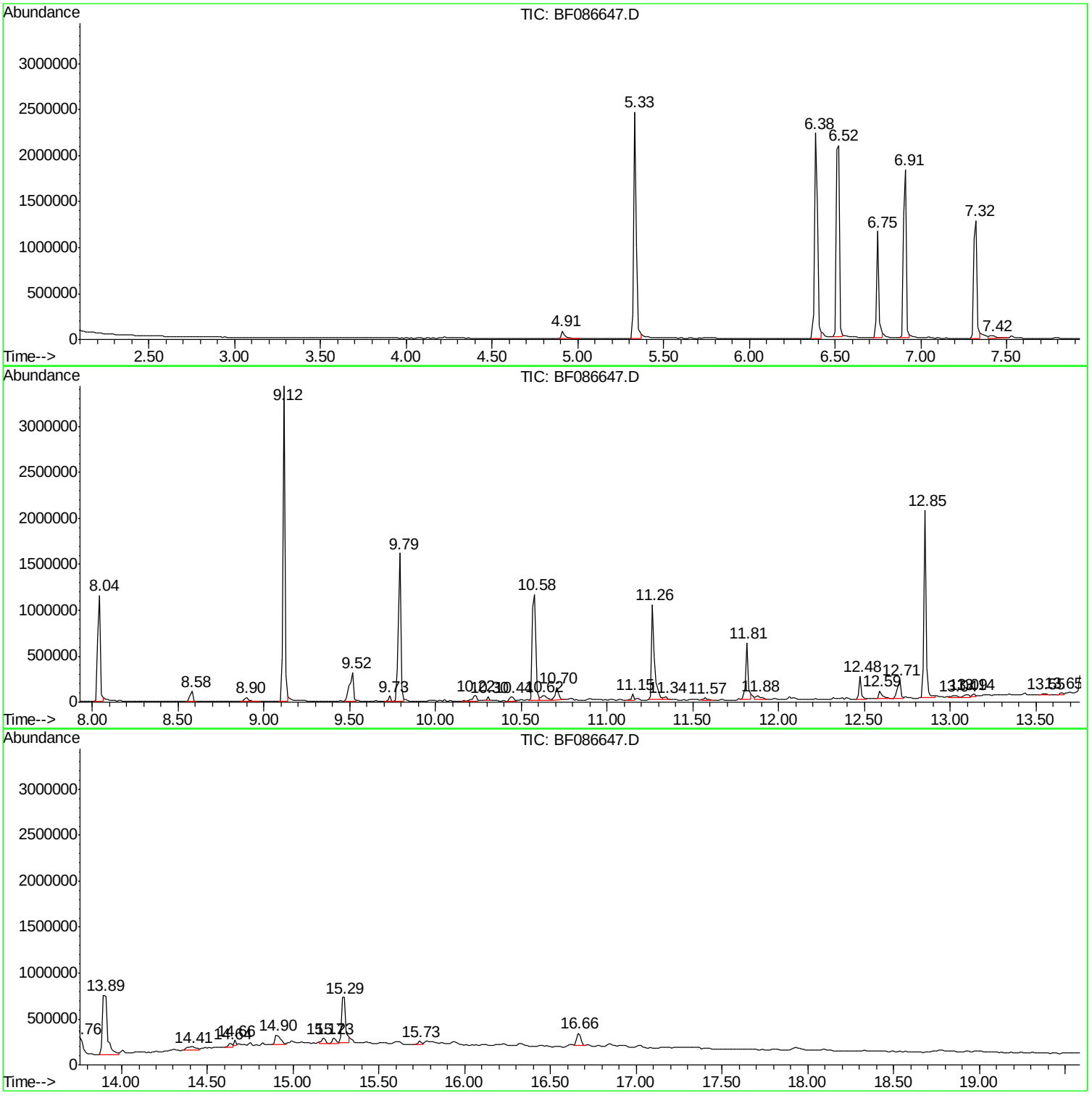
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2B-CS-2(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2B-CS-2(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

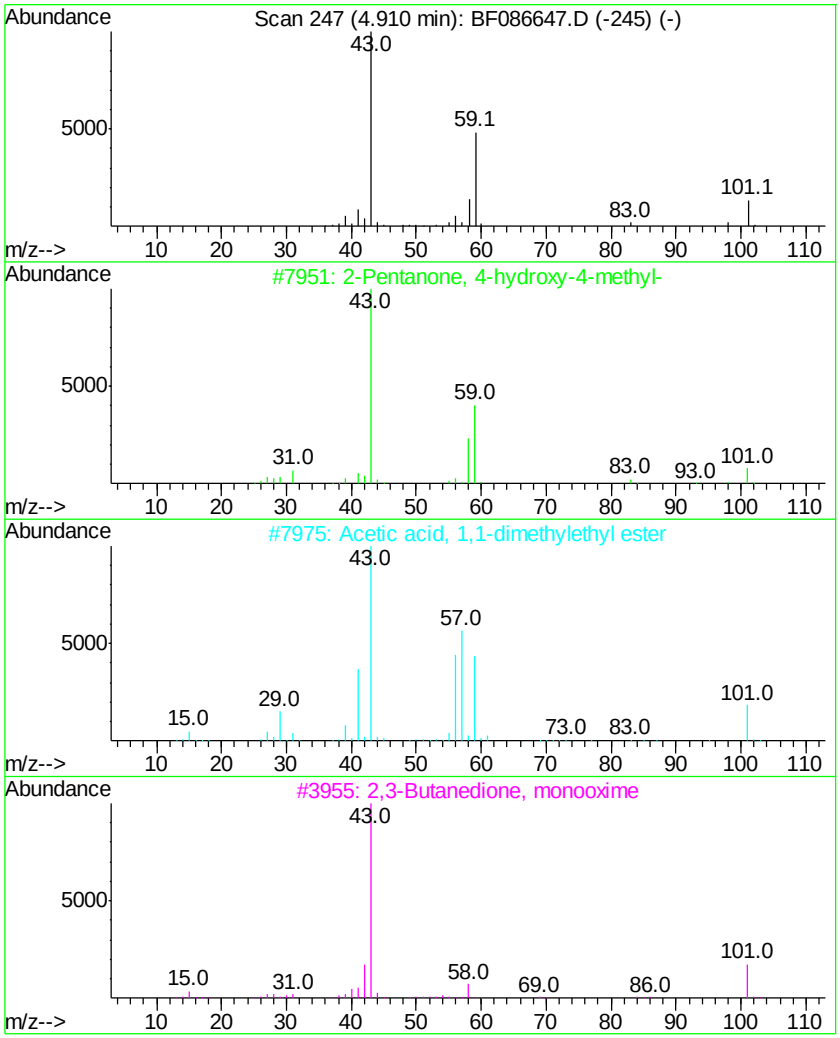
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

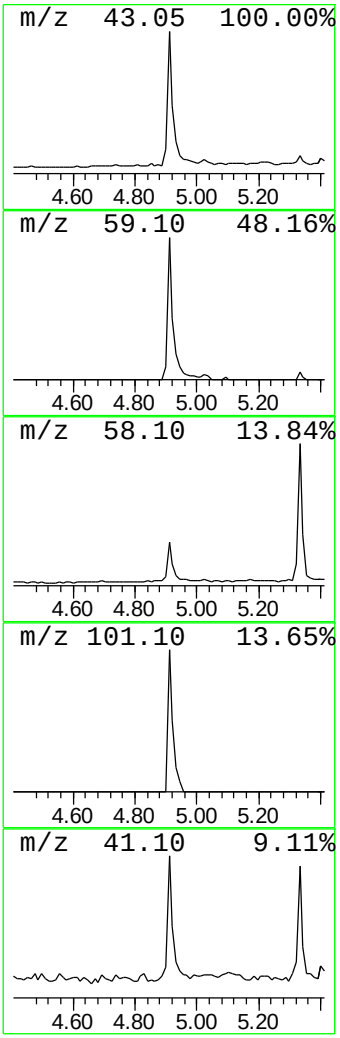
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.05 ng	109507	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
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Instrument : BNA_F
ClientSampleId : 26WARD-2B-CS-2(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

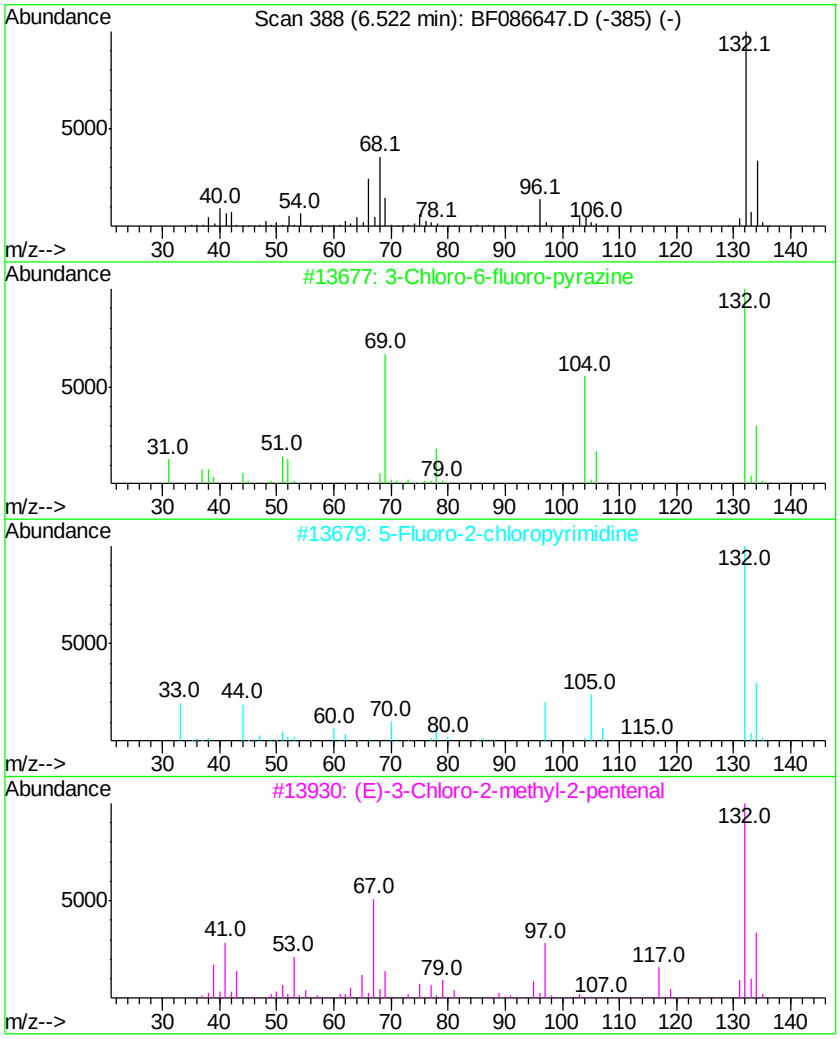
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

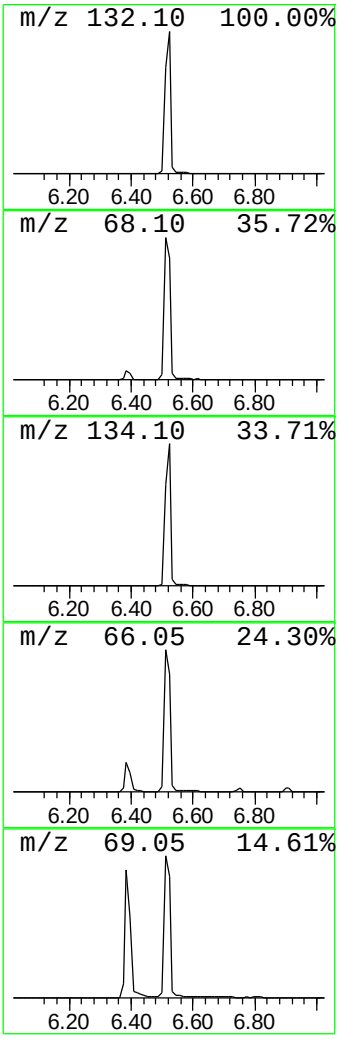
****

Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	55.26 ng	2952220	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	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2B-CS-2(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

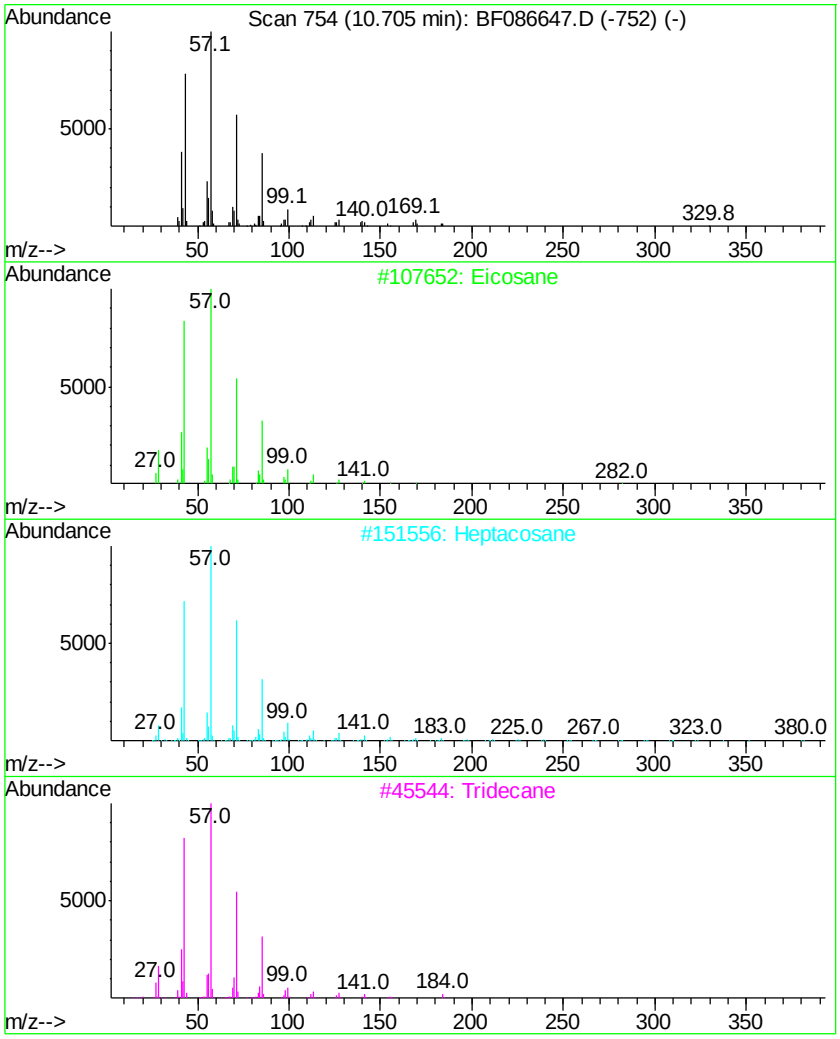
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

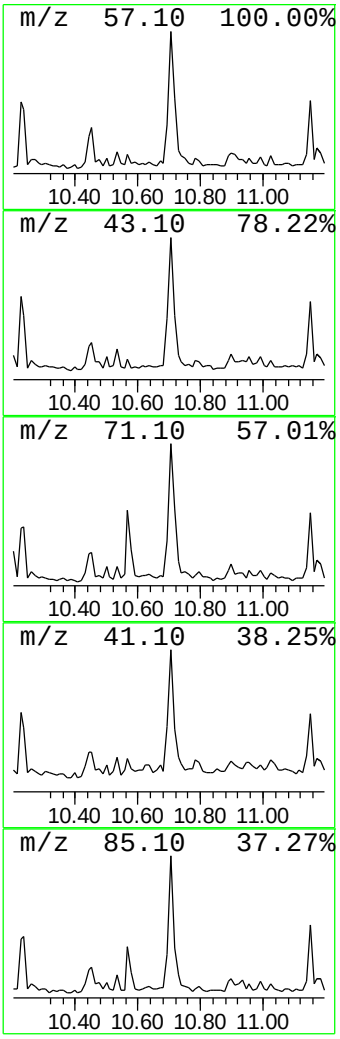
****

Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.89 ng	178926	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptacosane	380	C27H56	000593-49-7	90
3	Tridecane	184	C13H28	000629-50-5	87
4	Hexadecane	226	C16H34	000544-76-3	86
5	Undecane, 2-methyl-	170	C12H26	007045-71-8	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2B-CS-2(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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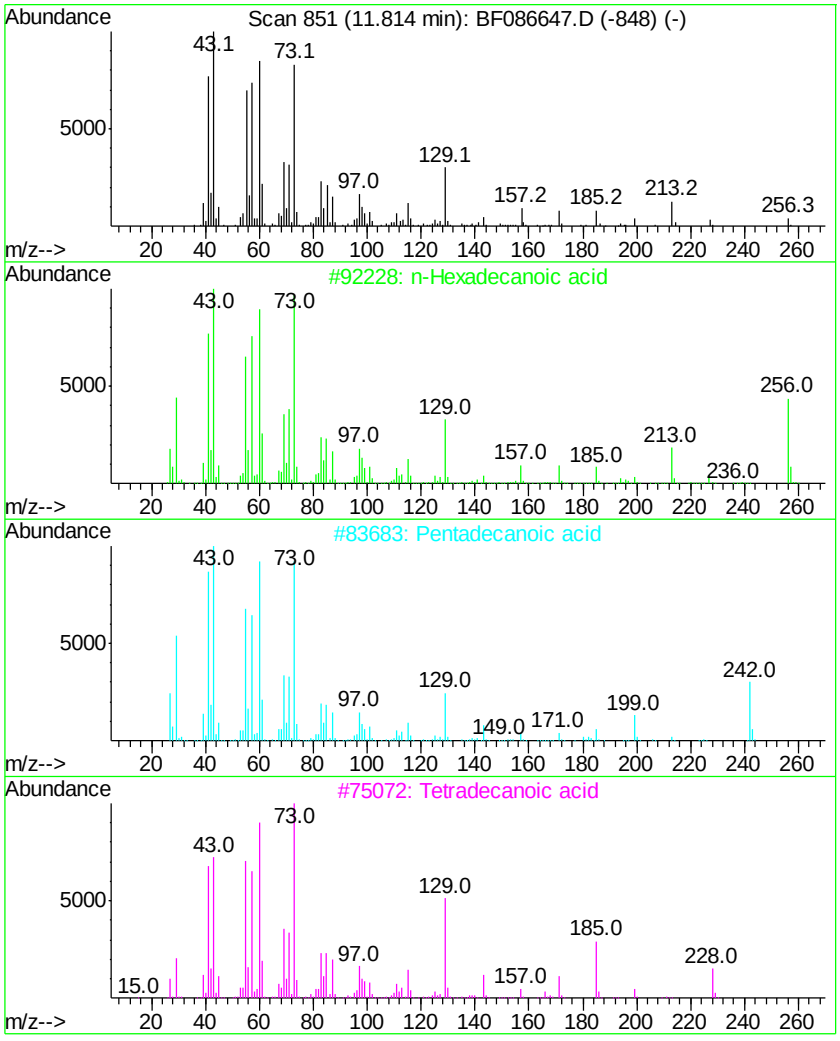
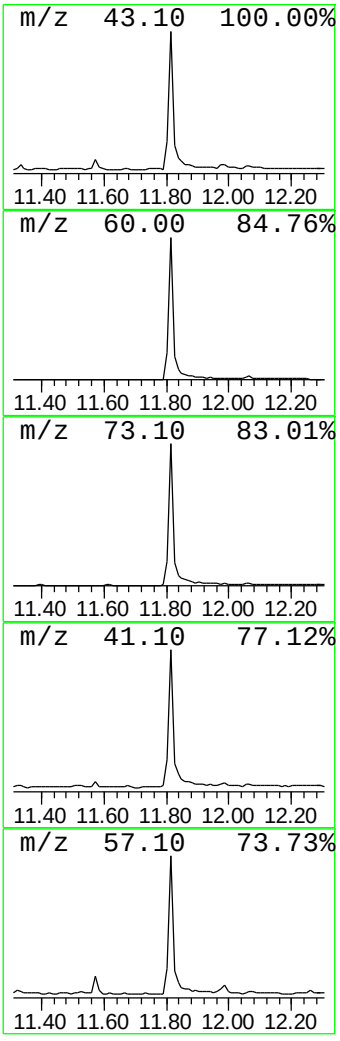
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.81	10.00 ng	619589	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2B-CS-2(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

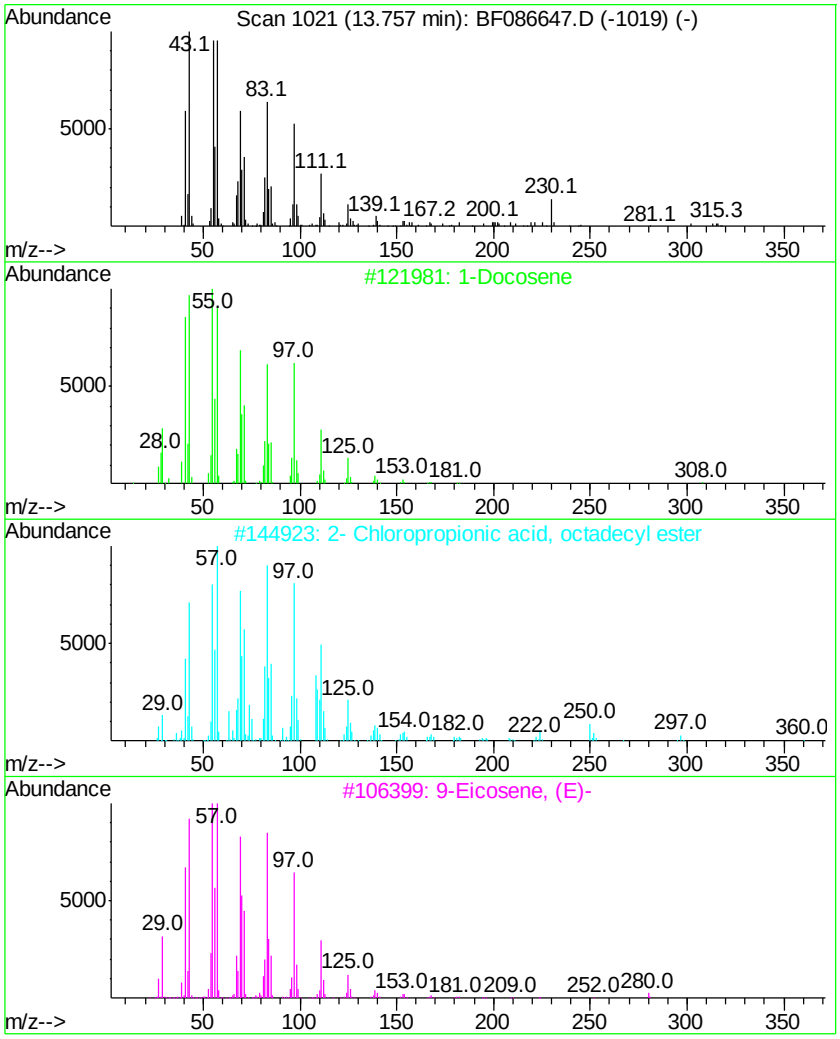
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

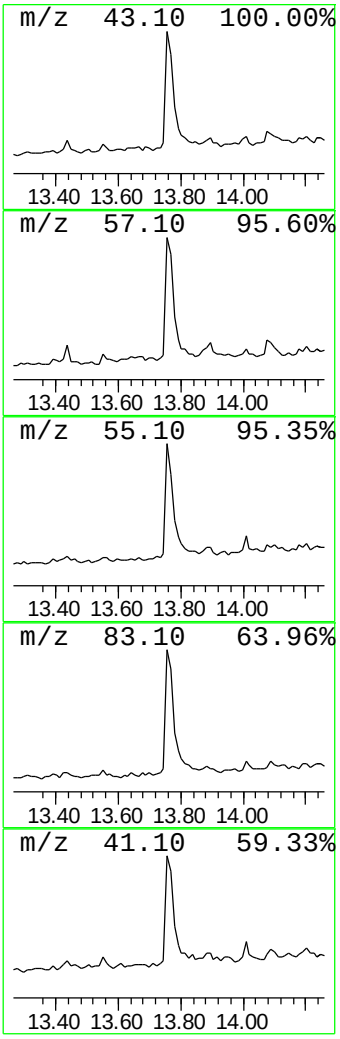
****

Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	5.53 ng	332614	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	90





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Misc :
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BNA_F
ClientSampleId :
26WARD-2B-CS-2(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

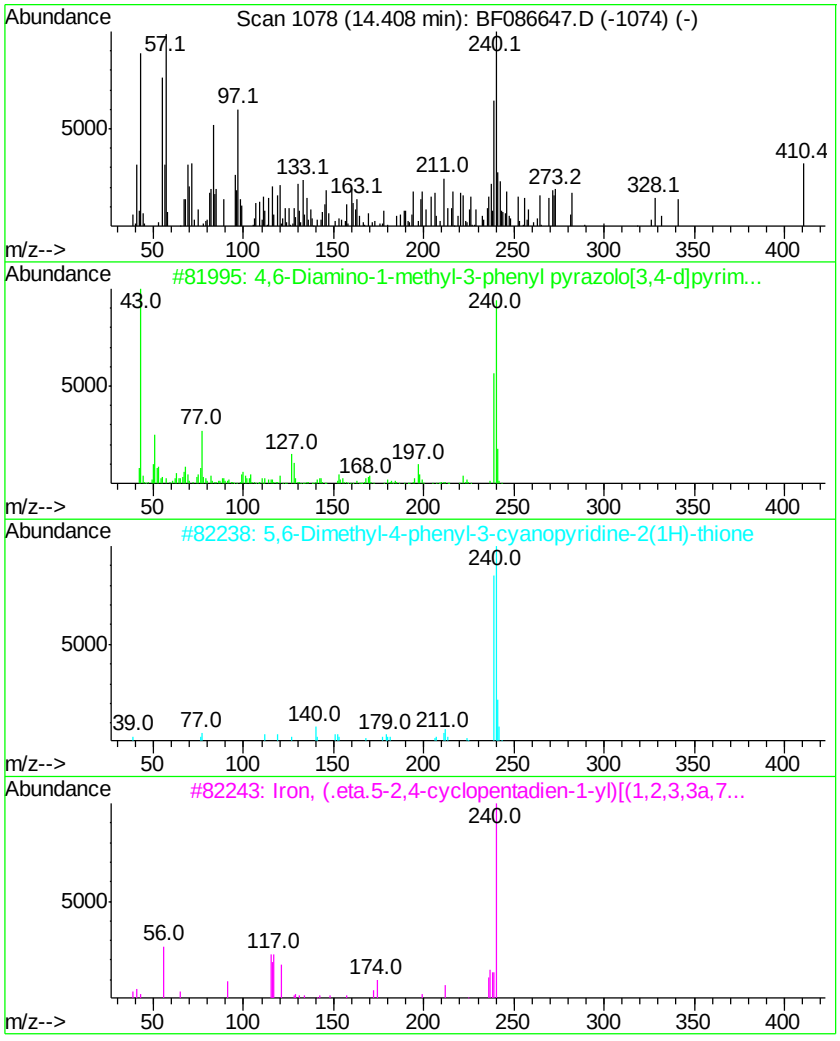
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

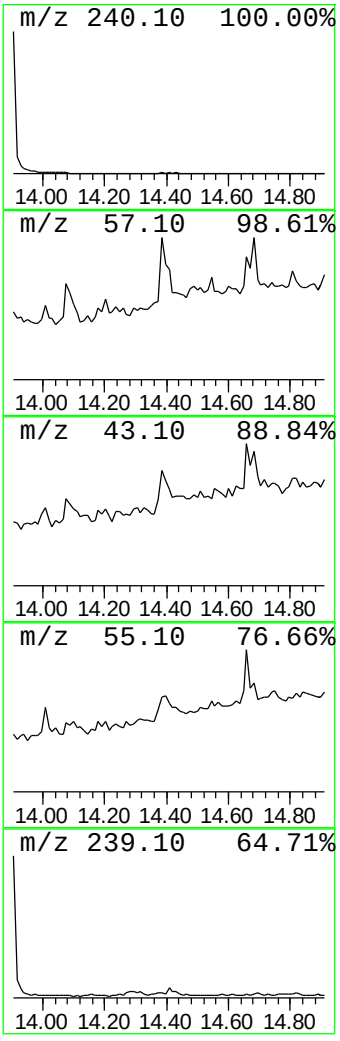
****

Peak Number 7 unknown14.41 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	2.29 ng	137790	Chrysene-d12	13.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6-Diamino-1-methyl-3-phenyl py...	240	C12H12N6	058791-67-6	35
2	5,6-Dimethyl-4-phenyl-3-cyanopyr...	240	C14H12N2S	094639-18-6	35
3	Iron, (.eta.5-2,4-cyclopentadien...	240	C14H16Fe	033039-67-7	27
4	2-Benzothiazolamine, N-(phenylme...	240	C14H12N2S	021816-82-0	22
5	Triphenylene, 1,2,3,4,5,6,7,8,9,...	240	C18H24	001610-39-5	18





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

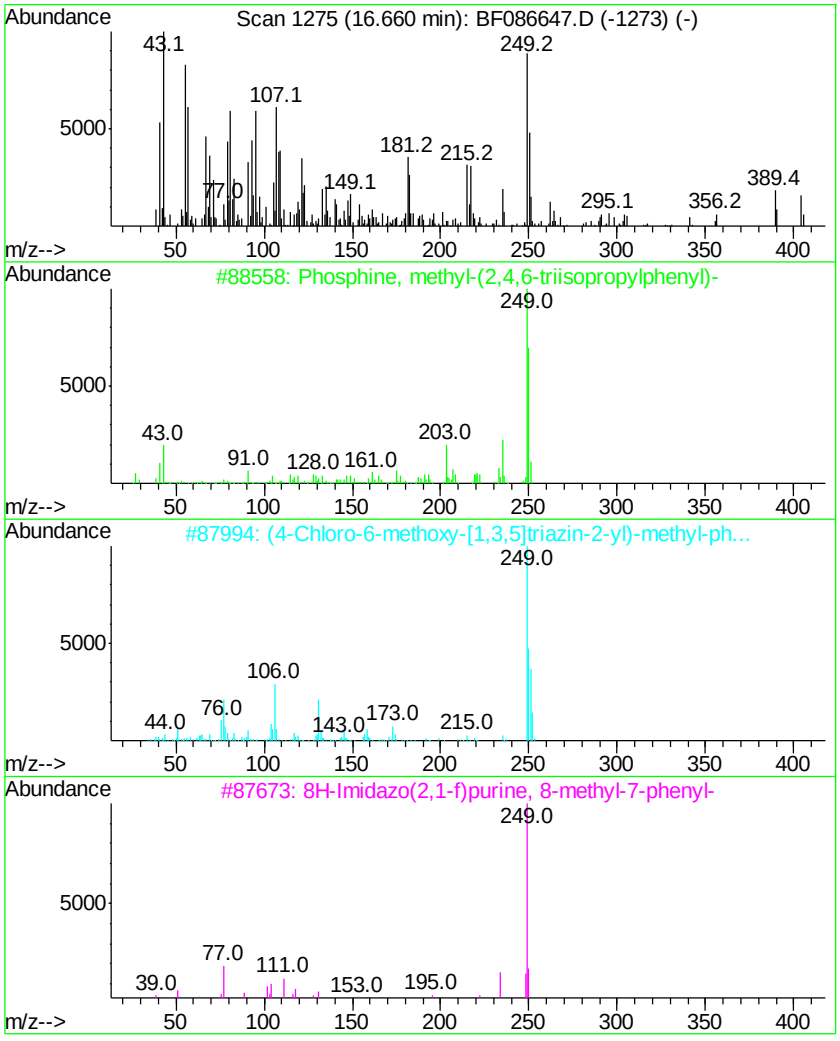
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

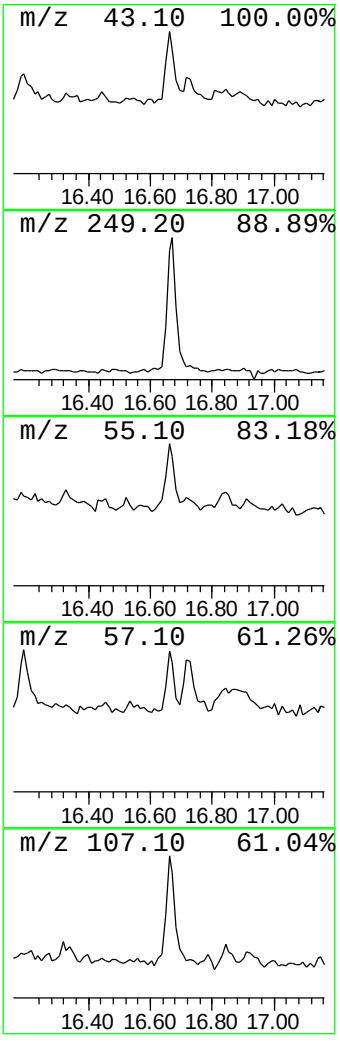
****

Peak Number 9 unknown16.66 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.66	5.88 ng	242784	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	38
2	(4-Chloro-6-methoxy-[1,3,5]triaz...	250	C11H11ClN4O	059881-58-2	27
3	8H-Imidazo(2,1-f)purine, 8-methy...	249	C14H11N5	076063-86-0	20
4	12H-Benzo[a]phenothiazine	249	C16H11NS	000225-83-2	18
5	7H-Benzo(c)phenothiazine	249	C16H11NS	000226-06-2	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050316\
Data File : BF086647.D
Acq On : 3 May 2016 16:28
Operator : UM/SJ
Sample : H2685-05 2X
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2B-CS-2(0-10FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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	2.0	ng	109507	1	6.75	1068550	20.0
unknown6.52	6.52	55.3	ng	2952220	1	6.75	1068550	20.0
Eicosane	10.70	2.9	ng	178926	4	11.27	1239010	20.0
n-Hexadecanoic acid	11.81	10.0	ng	619589	4	11.27	1239010	20.0
1-Docosene	13.76	5.5	ng	332614	5	13.91	1202490	20.0
unknown14.41	14.41	2.3	ng	137790	5	13.91	1202490	20.0
unknown16.66	16.66	5.9	ng	242784	6	15.30	825464	20.0