LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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	19	rVB	165178	254775	7.59%	1.095%
2	1.827	19	21	74	rVB	1583428	3354753	100.00%	14.423%
3	4.901	288	290	295	rBB	168994	235107	7.01%	1.011%
4	5.336	325	328	331	rBV	1500735	1528371	45.56%	6.571%
5	6.387	416	420	422	rBV	1549980	1940075	57.83%	8.341%
6	6.513	428	431	433	rBV	1879494	1749057	52.14%	7.520%
7	6.742	449	451	453	rBV	448431	551117	16.43%	2.369%
8	6.902	463	465	467	rBB	1490927	1303456	38.85%	5.604%
9	7.313	498	501	503	rBV	1236926	1260400	37.57%	5.419%
10	8.033	561	564	566	rBV	909108	828944	24.71%	3.564%
11	8.650	616	618	620	rBB	190974	165264	4.93%	0.711%
12	9.108	655	658	661	rVB	2168587	2059881	61.40%	8.856%
13	9.508	690	693	695	rVB	215848	273956	8.17%	1.178%
14	9.782	714	717	719	rBV	1014887	938227	27.97%	4.034%
15	10.228	751	756	757	rBV	41405	57488	1.71%	0.247%
16	10.559	783	785	788	rBV2	964328	1076661	32.09%	4.629%
17	10.696	795	797	801	rBV	60881	67662	2.02%	0.291%
18	11.142	834	836	837	rBV	77263	65556	1.95%	0.282%
19	11.256	843	846	848	rBV	1078251	926525	27.62%	3.983%
20	11.325	849	852	856	rVB2	13838	34314	1.02%	0.148%
21	12.456	949	951	954	rVB	42808	36830	1.10%	0.158%
22	12.685	967	971	973	rBV2	33140	50933	1.52%	0.219%
23	12.845	982	985	987	rBV	1793477	2235615	66.64%	9.612%
24	13.748	1062	1064	1073	rBV	141479	222881	6.64%	0.958%
25	13.874	1073	1075	1078	rBV	745321	767156	22.87%	3.298%
26	14.377	1116	1119	1128	rBV	64856	128951	3.84%	0.554%
27	14.731	1148	1150	1152	rBV	45041	41804	1.25%	0.180%
28	15.257	1193	1196	1199	rBV	471170	531662	15.85%	2.286%
29	16.731	1322	1325	1330	rVB	72550	132435	3.95%	0.569%
30	17.108	1354	1358	1362	rBV2	19449	52649	1.57%	0.226%
31	17.463	1380	1389	1392	rBV4	11877	47470	1.42%	0.204%
32	17.543	1393	1396	1400	rVB4	18445	44362	1.32%	0.191%
33	17.851	1417	1423	1428	rBV2	52067	136608	4.07%	0.587%
34	17.966	1428	1433	1439	rVB9	10079	39061	1.16%	0.168%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

35	19.017	1514	1525	1544	rVB9	15087	119416	3.56%	0.513%

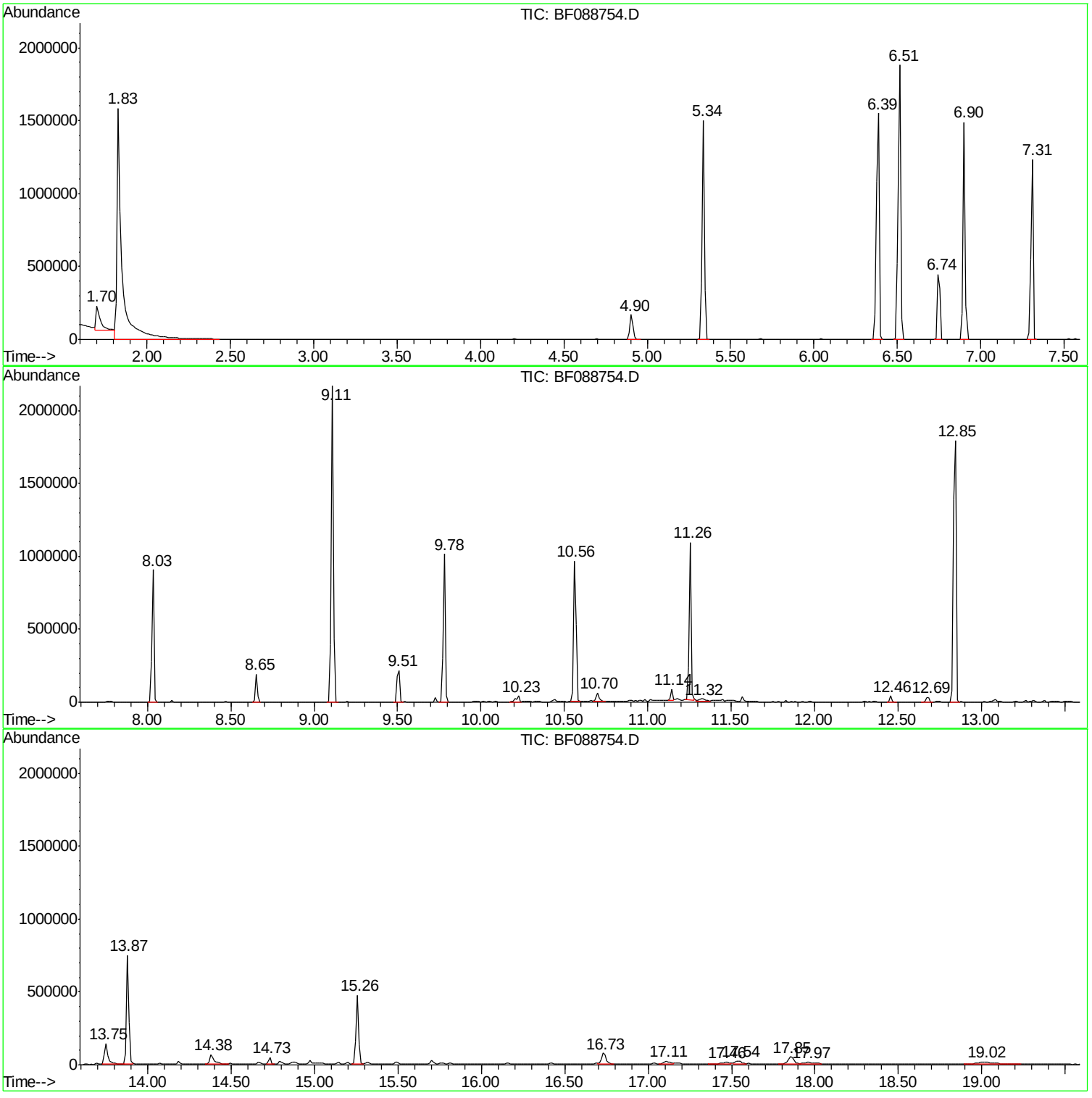
Sum of corrected areas: 23259422

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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 : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

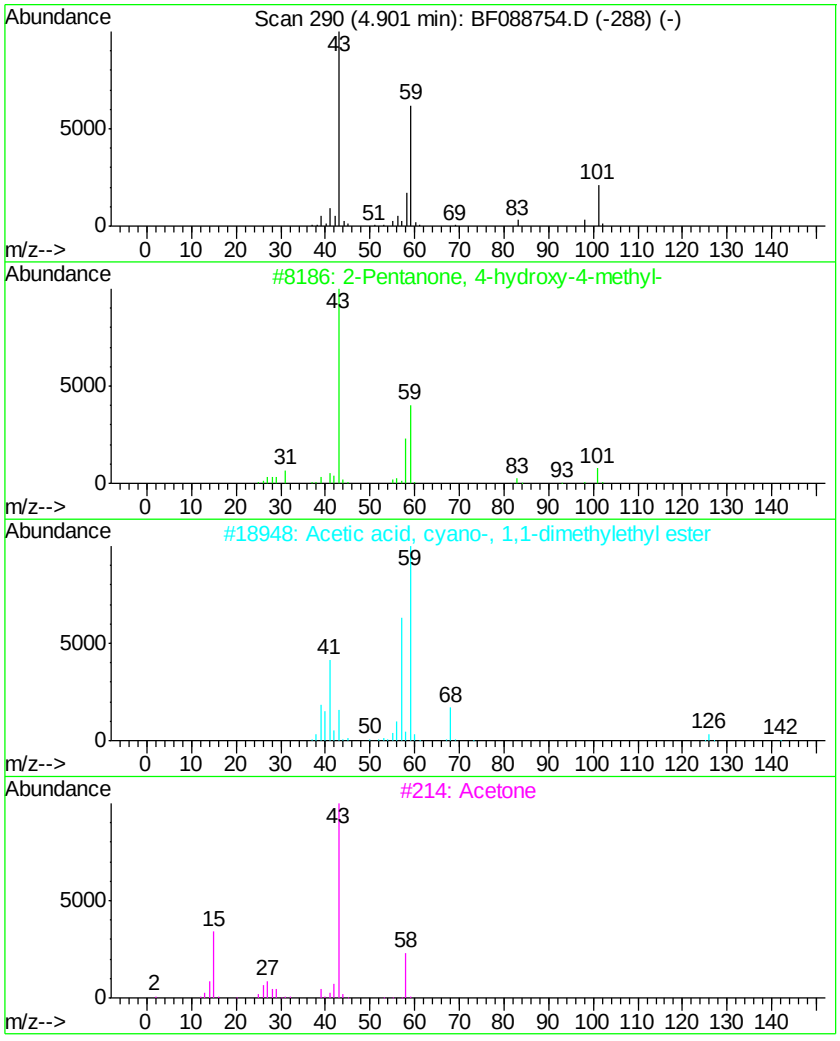
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

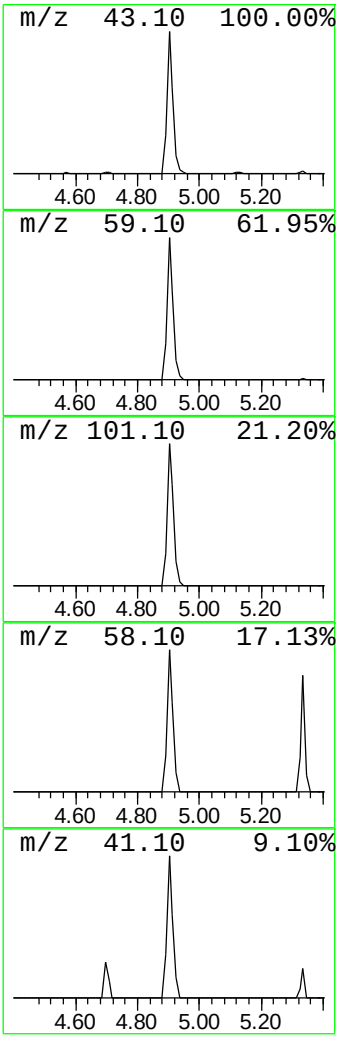
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	8.53 ng	235107	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	23
3	Acetone	58	C3H6O	000067-64-1	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

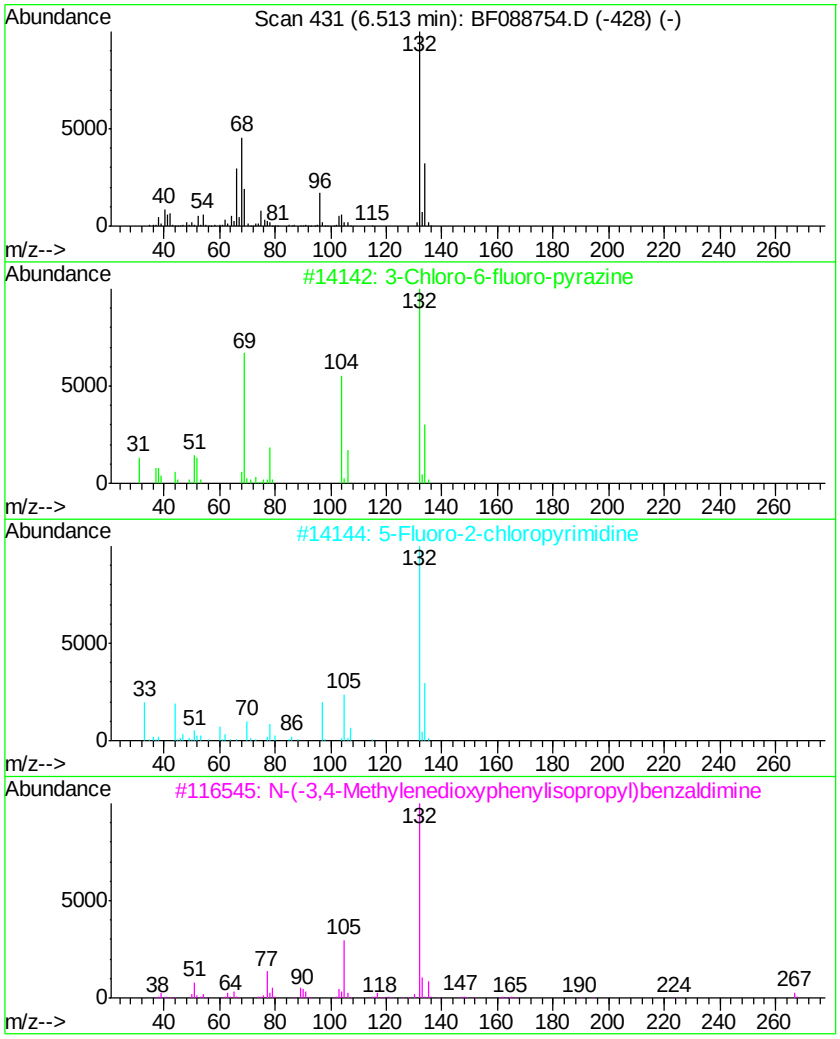
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

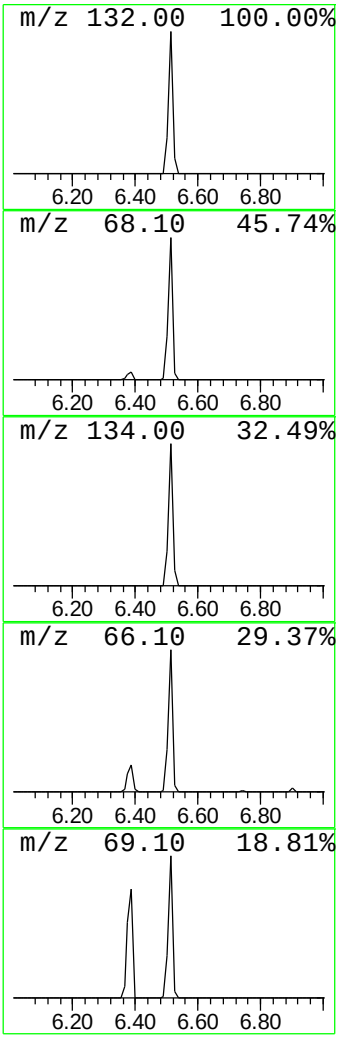
****

Peak Number 4 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	63.47 ng	1749060	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	16
3	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

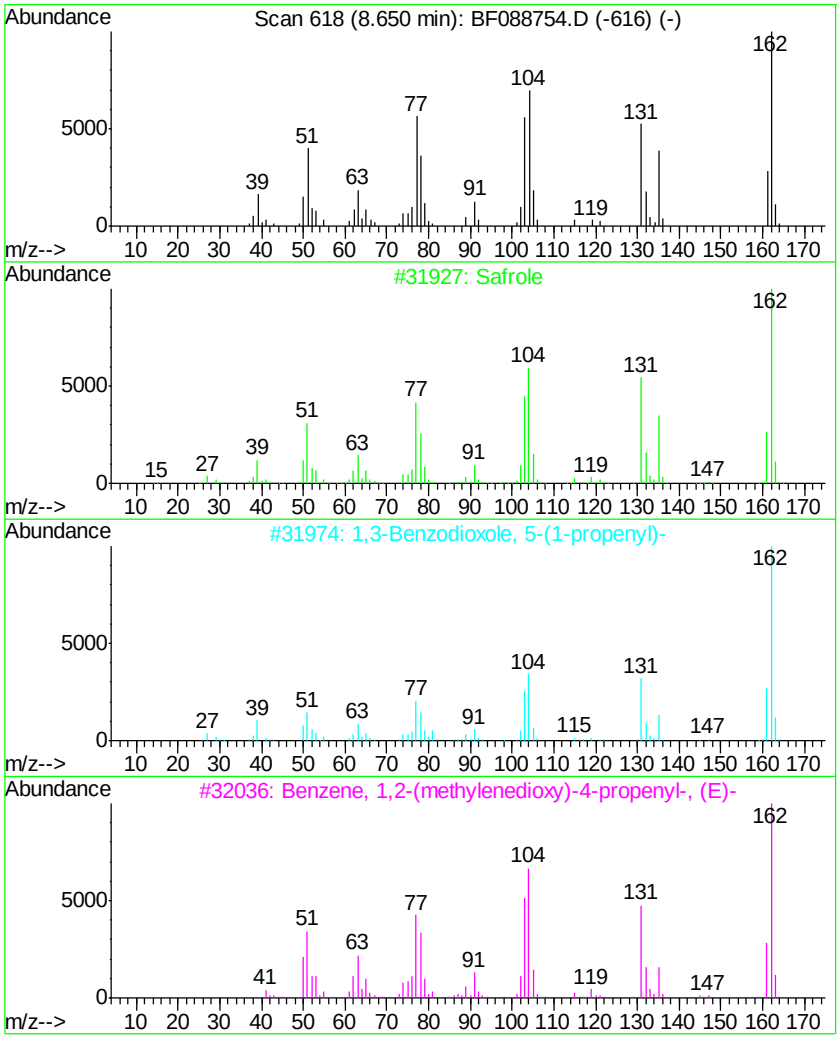
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

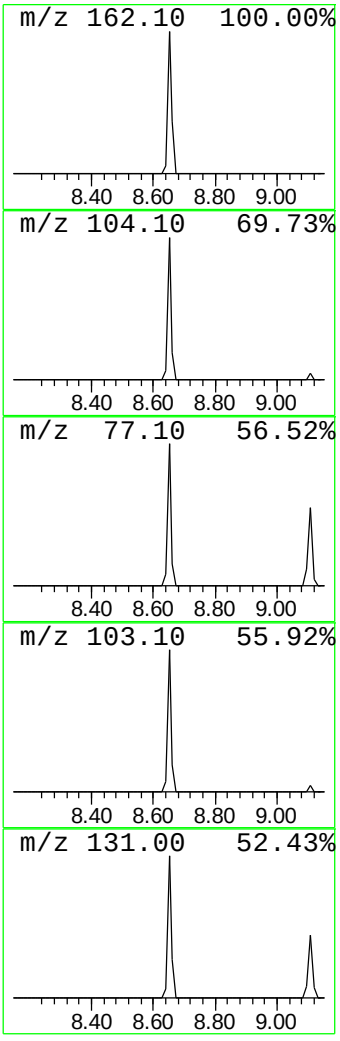
****

Peak Number 6 Safrole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	3.99 ng	165264	Naphthalene-d8	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	99
2	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	98
3	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	98
4	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	96
5	Sydnone, 3-phenyl-	162	C8H6N2O2	000120-06-9	60





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

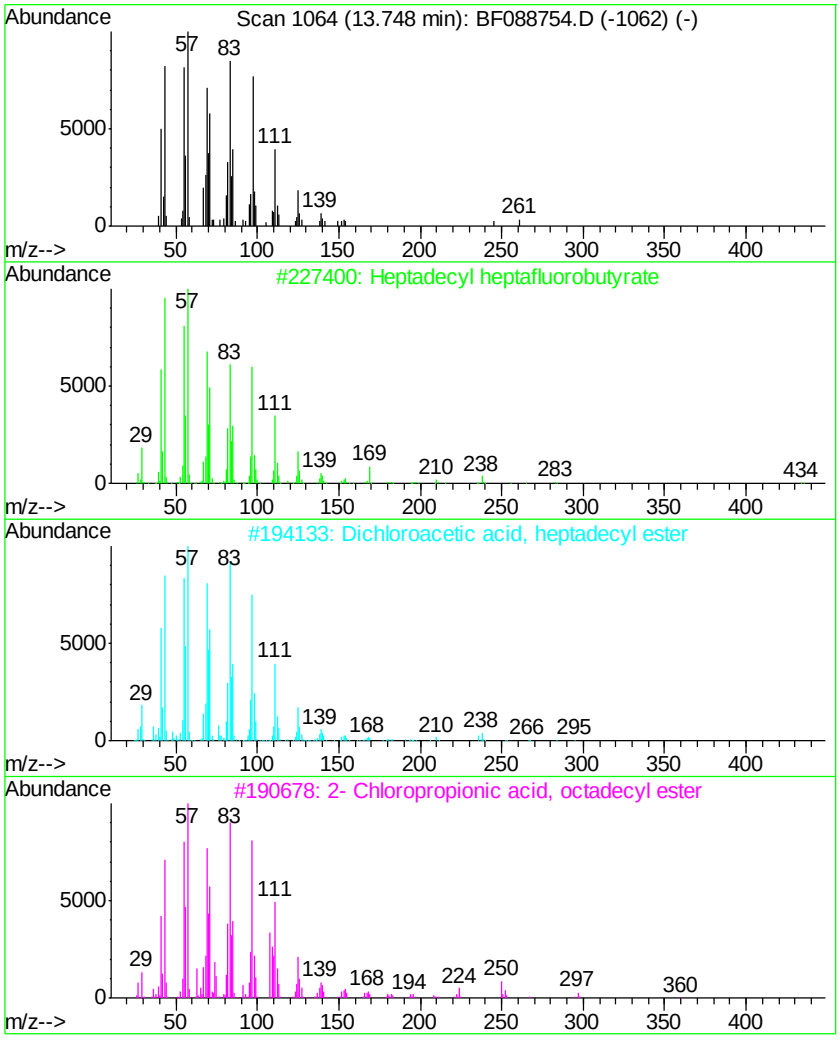
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

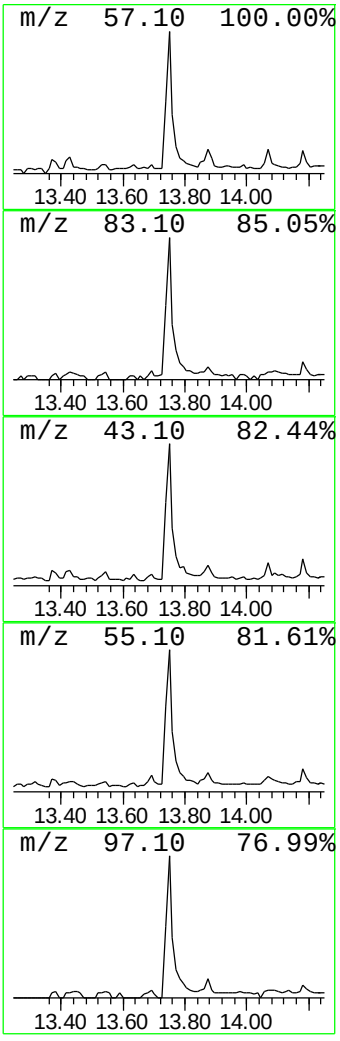
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	5.81 ng	222881	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

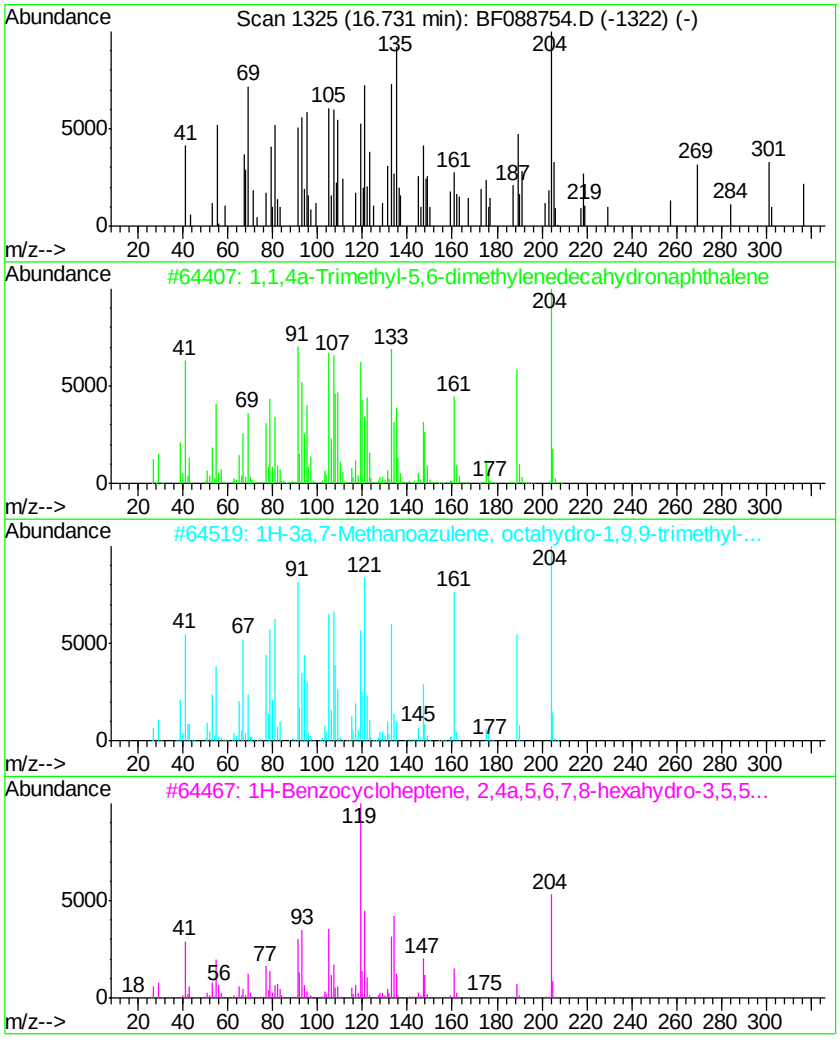
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

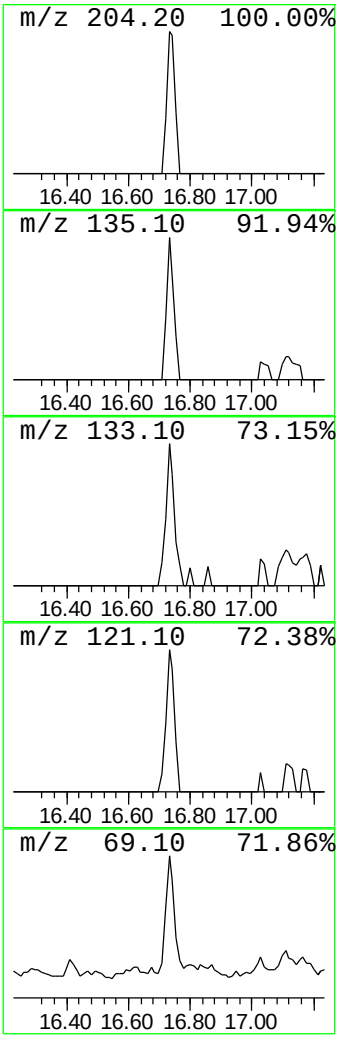
****

Peak Number 9 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	4.98 ng	132435	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	62
2	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	52
3	1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	001461-03-6	50
4	cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	49
5	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	49





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

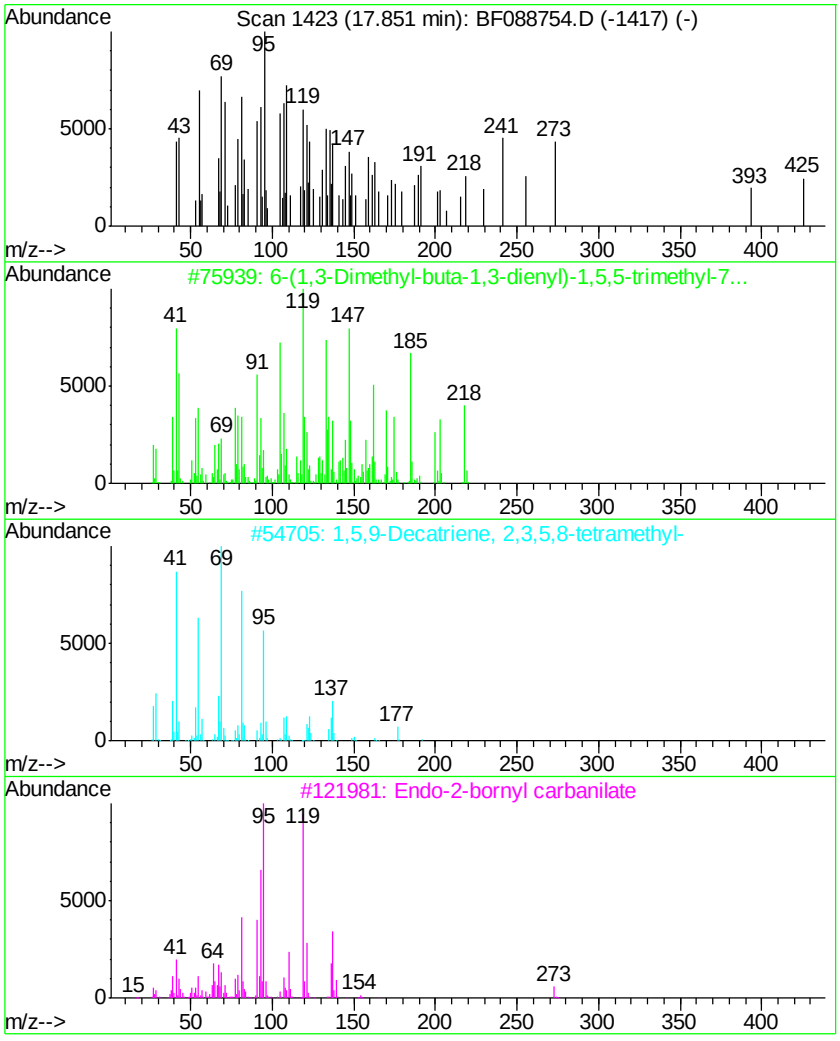
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

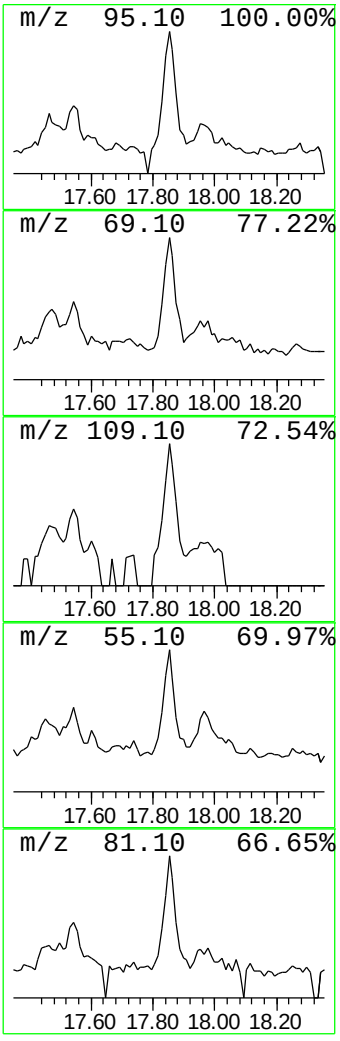
****

Peak Number 10 6-(1,3-Dimethyl-buta-1,3-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	5.14 ng	136608	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(1,3-Dimethyl-buta-1,3-dienyl)...	218	C15H22O	1000189-26-4	56
2	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	22
3	Endo-2-bornyl carbanilate	273	C17H23NO2	006907-15-9	22
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	22
5	1,6-Dihydropyridazine-3-carboxyl...	273	C13H8FN3O3	1000304-05-0	14





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070616\
Data File : BF088754.D
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Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

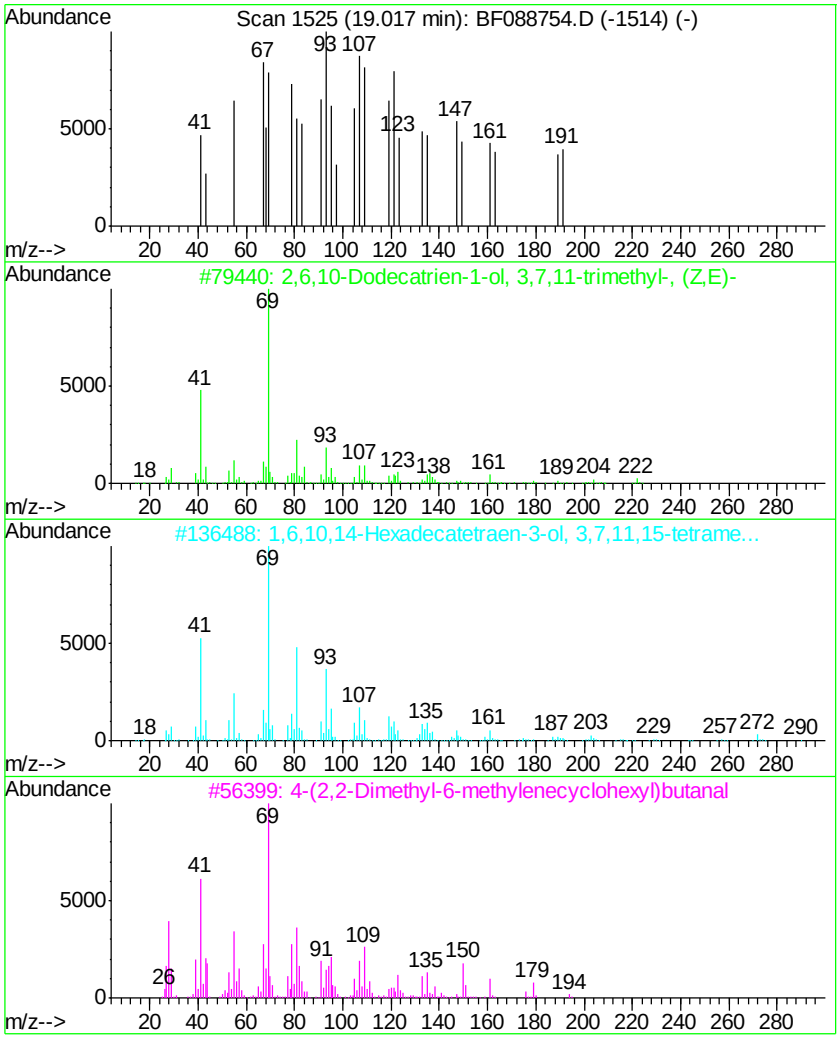
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

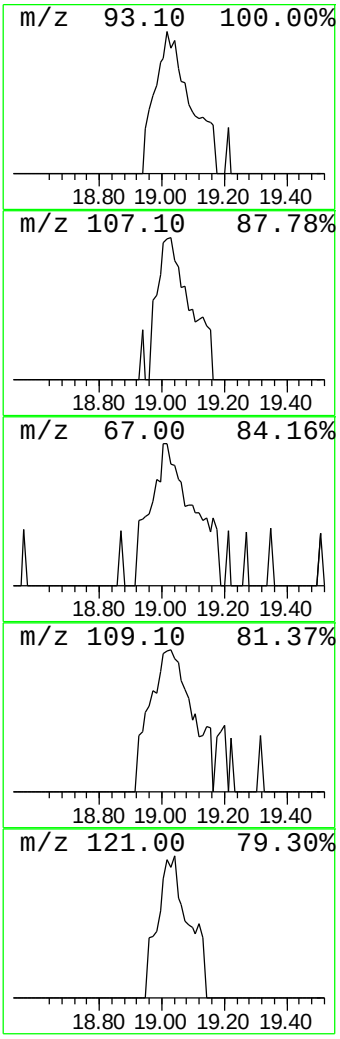
****

Peak Number 11 unknown19.02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	4.49 ng	119416	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	46
2	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	43
3	4-(2,2-Dimethyl-6-methylenecyclo...	194	C13H22O	095452-13-4	37
4	4,7-Methanobenzofuran, 2,2'-oxyb...	374	C24H38O3	087248-50-8	23
5	1,6,10-Dodecatrien-3-ol, 3,7,11-...	222	C15H26O	007212-44-4	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070616\
Data File : BF088754.D
Acq On : 7 Jul 2016 00:54
Operator : UM/SJ
Sample : H3879-18
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C2.1-02

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	8.5	ng	235107	1	6.75	551117	20.0
unknown6.51	6.51	63.5	ng	1749060	1	6.75	551117	20.0
Safrole	8.65	4.0	ng	165264	2	8.03	828944	20.0
Heptadecyl heptaf...	13.75	5.8	ng	222881	5	13.87	767156	20.0
1,1,4a-Trimethyl-...	16.73	5.0	ng	132435	6	15.26	531662	20.0
6-(1,3-Dimethyl-b...	17.85	5.1	ng	136608	6	15.26	531662	20.0
unknown19.02	19.02	4.5	ng	119416	6	15.26	531662	20.0