LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

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-BF081616.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	1.667	6	7	16	rVV	1062067	2338337	6.87%	0.352%
2	1.793	16	18	69	rVB	13242459	33970539	99.85%	5.120%
3	4.833	282	284	291	rBV	1017020	1278709	3.76%	0.193%
4	5.279	320	323	325	rBV	5229223	6612621	19.44%	0.997%
5	6.159	395	400	405	rBV2	298993	600063	1.76%	0.090%
6	6.353	412	417	419	rBV2	8132390	16260542	47.80%	2.451%
7	6.467	422	427	430	rBV3	5876078	13894736	40.84%	2.094%
8	6.639	439	442	444	rVB	4064024	3285714	9.66%	0.495%
9	6.696	445	447	449	rBV	3978395	3628054	10.66%	0.547%
10	6.856	458	461	463	rVB	7134655	6175082	18.15%	0.931%
11	6.959	467	470	474	rBV	7103765	8998436	26.45%	1.356%
12	7.119	481	484	488	rBV2	10810496	21187495	62.28%	3.193%
13	7.267	494	497	499	rVB	5343053	5012275	14.73%	0.755%
14	7.542	517	521	523	rVB	12341119	15576387	45.78%	2.348%
15	7.610	524	527	529	rBV	7559536	7656249	22.50%	1.154%
16	7.850	545	548	550	rBV	13687676	13671185	40.18%	2.060%
17	7.930	552	555	557	rVV	12092875	15914012	46.78%	2.399%
18	8.010	557	562	564	rVV2	11003226	14912008	43.83%	2.248%
19	8.136	570	573	576	rBV	10310377	9501691	27.93%	1.432%
20	8.536	606	608	615	rBV	6066331	5433992	15.97%	0.819%
21	8.708	620	623	625	rBV	10332752	13517317	39.73%	2.037%
22	9.016	647	650	652	rVV	11340030	12691975	37.31%	1.913%
23	9.073	652	655	657	rVB	11210661	12415733	36.49%	1.871%
24	9.188	662	665	667	rVV	6816230	6738488	19.81%	1.016%
25	9.473	687	690	692	rBV	1531048	1857628	5.46%	0.280%
26	9.530	692	695	697	rVV	9391676	11437677	33.62%	1.724%
27	9.599	697	701	703	rVB	10244029	8733027	25.67%	1.316%
28	9.736	711	713	715	rBV	6457511	5744650	16.89%	0.866%
29	9.862	721	724	728	rBV	4978599	6368370	18.72%	0.960%
30	9.953	728	732	734	rVB2	18339850	34020755	100.00%	5.128%
31	10.193	748	753	755	rBV	18801789	27107637	79.68%	4.086%
32	10.296	758	762	765	rVB	21452259	31541871	92.71%	4.754%
33	10.422	769	773	775	rBV2	862829	828271	2.43%	0.125%
34	10.525	779	782	785	rBV	8282429	8600110	25.28%	1.296%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

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-BF081616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.662	792	794	799	rVB	439627	539975	1.59%	0.081%
36	10.776	801	804	806	rVV	8421226	8490656	24.96%	1.280%
37	10.845	806	810	812	rVV	16359389	24034266	70.65%	3.622%
38	11.016	823	825	831	rBV	2860783	4062067	11.94%	0.612%
39	11.211	840	842	845	rVV	5536718	5655845	16.62%	0.852%
40	11.291	846	849	852	rVB	12114765	11667211	34.29%	1.758%
41	11.771	889	891	892	rBV	2138134	2436807	7.16%	0.367%
42	11.805	892	894	896	rVB	11118040	13619893	40.03%	2.053%
43	12.022	911	913	917	rVB	360388	437399	1.29%	0.066%
44	12.422	945	948	950	rBV	11195003	11296891	33.21%	1.703%
45	12.468	950	952	957	rVB3	307327	600430	1.76%	0.090%
46	12.571	957	961	965	rBV2	626809	1303485	3.83%	0.196%
47	12.662	965	969	972	rBV	17223759	28826608	84.73%	4.345%
48	12.811	979	982	984	rBV	12927279	13205535	38.82%	1.990%
49	13.908	1074	1078	1080	rBV	15817525	32170211	94.56%	4.849%
50	13.942	1080	1081	1084	rVB	11488310	13341636	39.22%	2.011%
51	14.137	1093	1098	1102	rBV4	154455	567991	1.67%	0.086%
52	14.274	1108	1110	1117	rVB2	145910	340827	1.00%	0.051%
53	14.914	1163	1166	1168	rBV	409037	662246	1.95%	0.100%
54	15.040	1173	1177	1179	rVV	11072392	24190672	71.11%	3.646%
55	15.074	1179	1180	1183	rVV	11705567	15332328	45.07%	2.311%
56	15.177	1187	1189	1194	rVB	441269	554021	1.63%	0.084%
57	15.371	1203	1206	1209	rBV	6859350	9009923	26.48%	1.358%
58	15.428	1209	1211	1214	rVV	2988501	3384735	9.95%	0.510%
59	15.931	1252	1255	1261	rVB	310107	580391	1.71%	0.087%
60	16.788	1321	1330	1333	rBV2	9181722	30152478	88.63%	4.545%
61	16.925	1339	1342	1352	rVB3	155209	592208	1.74%	0.089%
62	17.166	1352	1363	1374	rVV	6144157	17277800	50.79%	2.604%
63	17.337	1375	1378	1384	rVB4	125129	377800	1.11%	0.057%
64	17.794	1414	1418	1423	rVB4	134582	360638	1.06%	0.054%
65	19.109	1528	1533	1544	rVB	279570	907019	2.67%	0.137%

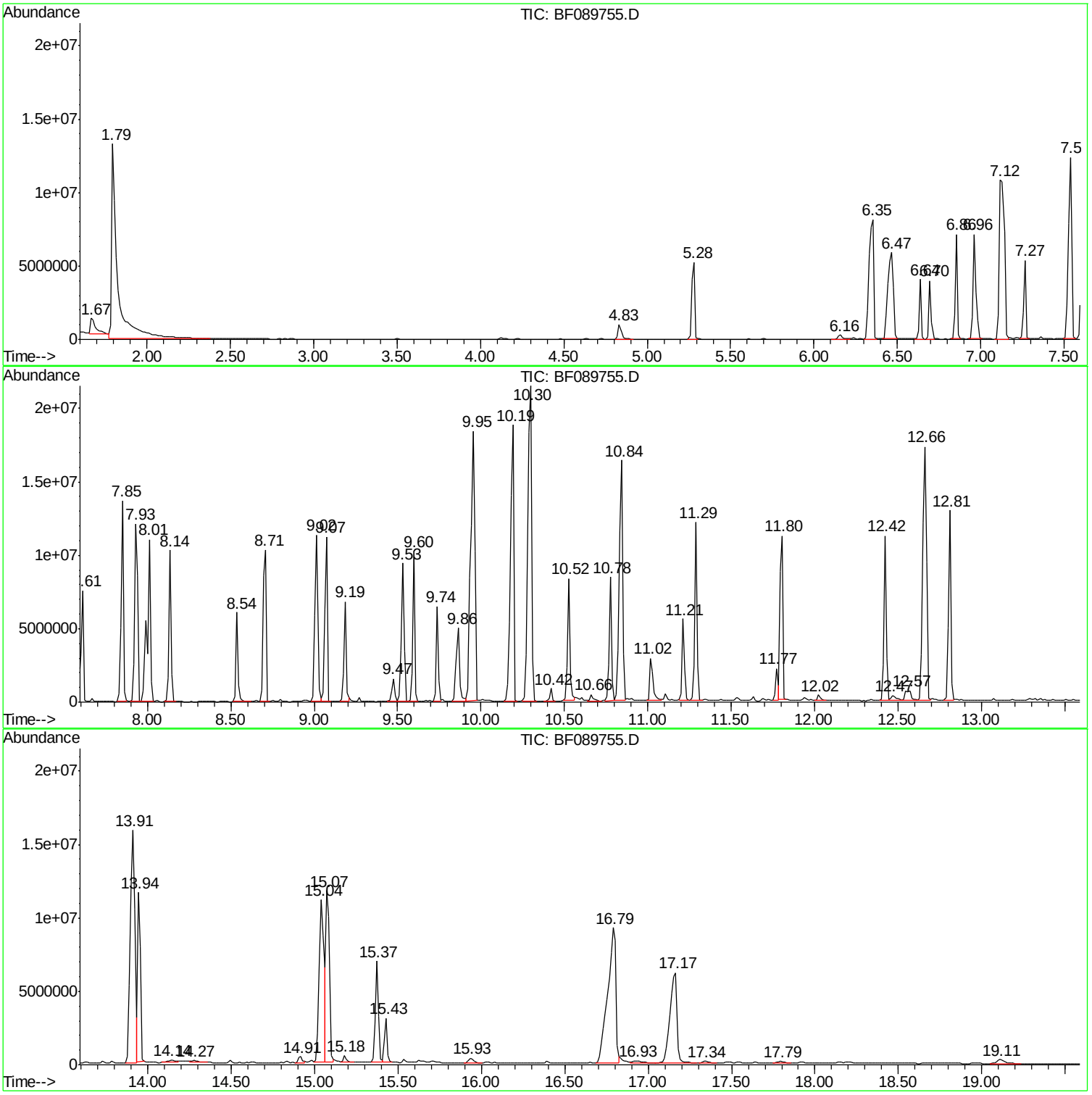
Sum of corrected areas: 663491628

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

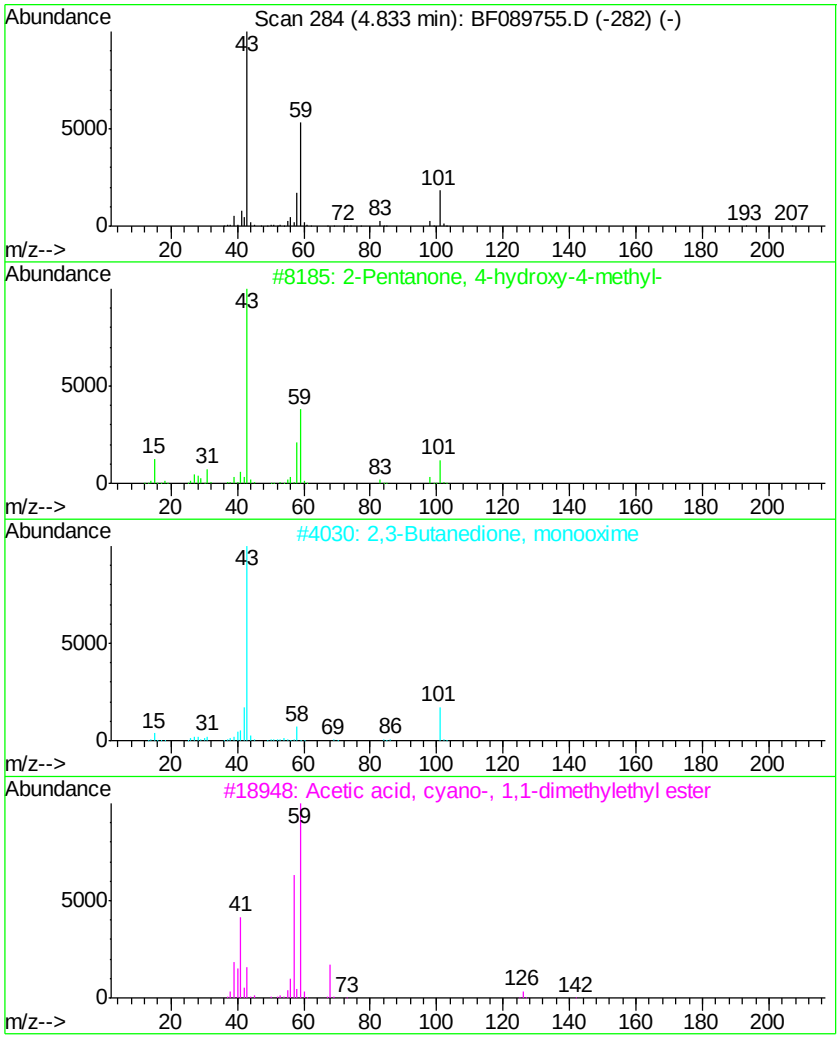
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

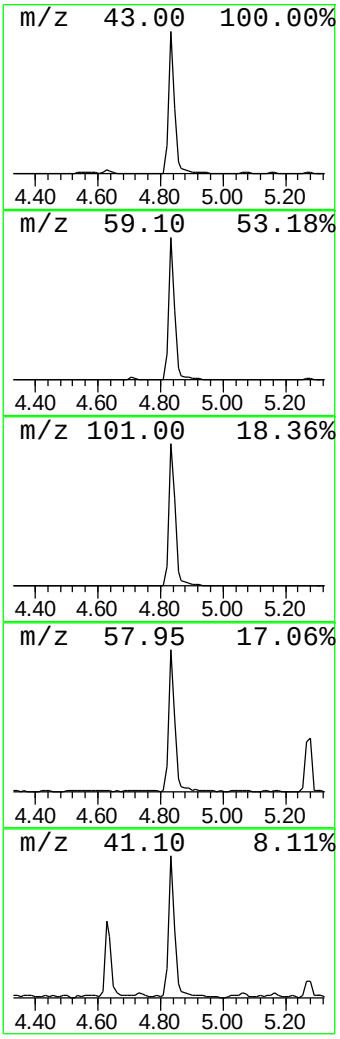
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	7.05 ng	1278710	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

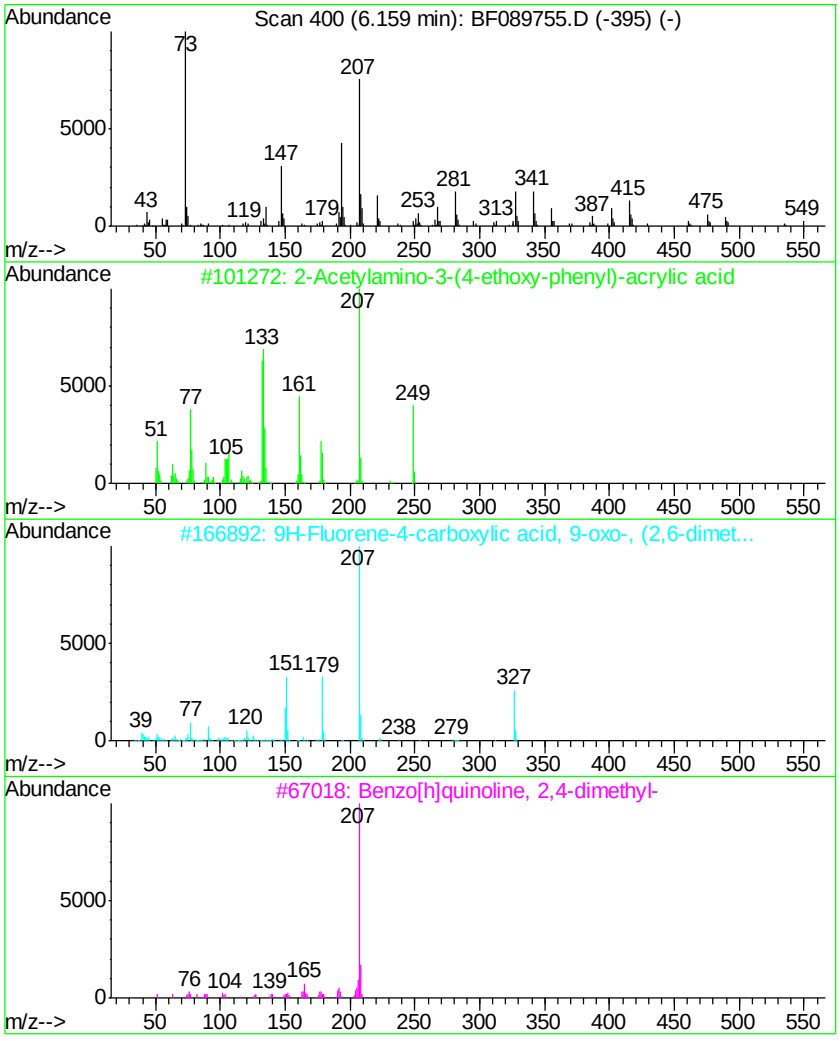
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

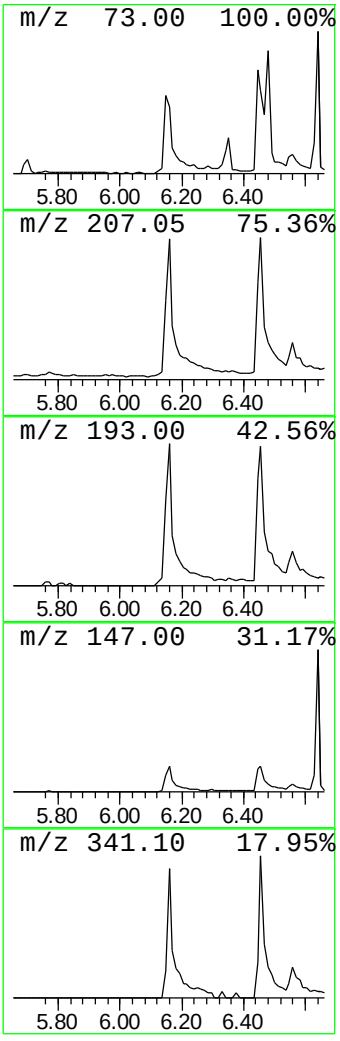
****

Peak Number 4 2-Acetylamino-3-(4-ethoxy-p... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	3.31 ng	600063	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Acetylamino-3-(4-ethoxy-phenyl...	249	C13H15NO4	325482-56-2	50
2	9H-Fluorene-4-carboxylic acid, 9...	327	C22H17NO2	1000304-78-2	38
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	38
4	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	38
5	Tris(tert-butyldimethylsilyloxy)...	468	C18H45AsO3Si3	1000366-57-5	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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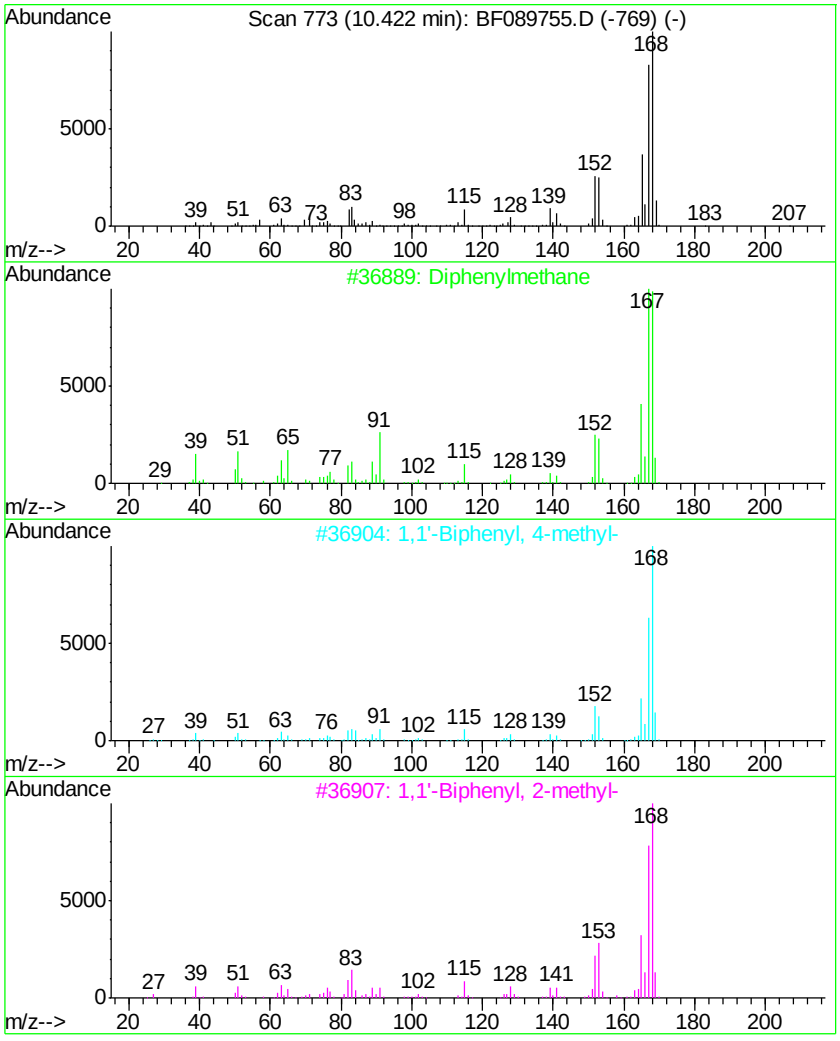
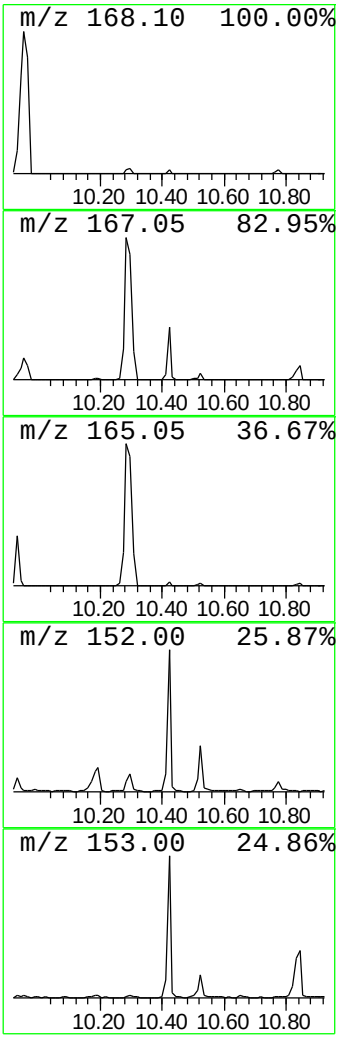
Peak Number 6 Diphenylmethane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	2.88 ng	828271	Acenaphthene-d10	9.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenylmethane	168	C13H12	000101-81-5	93
2	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	93
3	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	93
4	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	83
5	Nordiphenamid	225	C15H15NO	000954-21-2	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

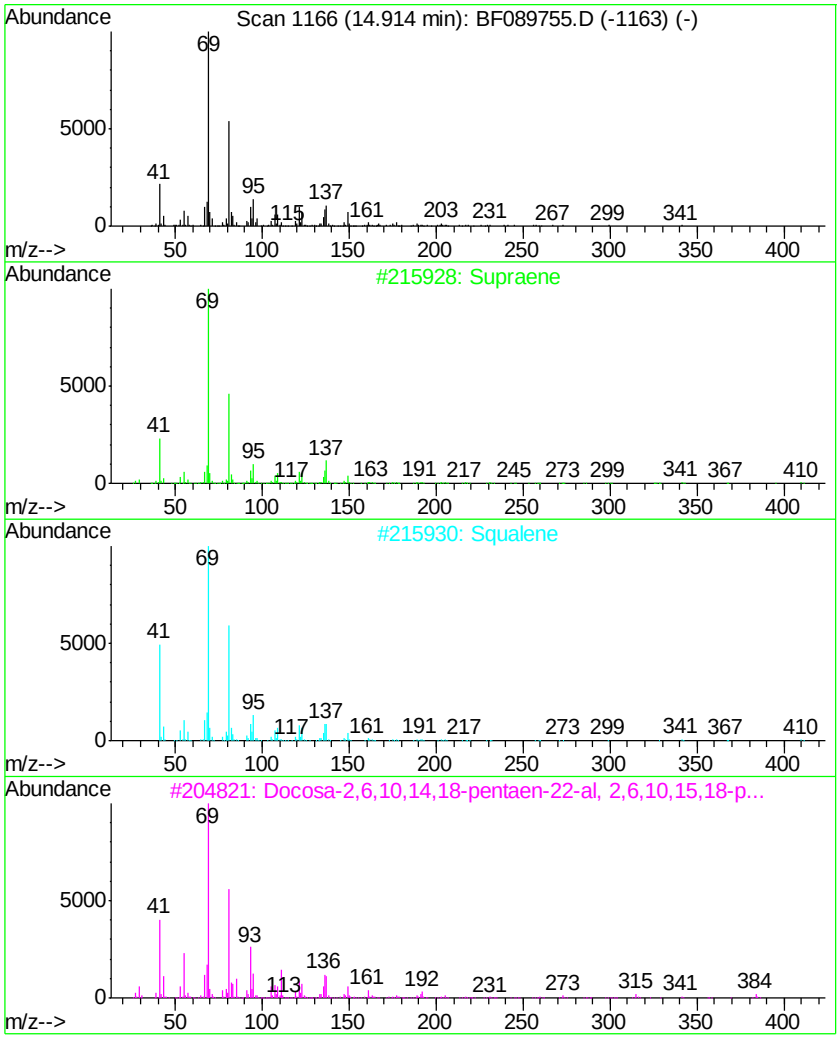
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

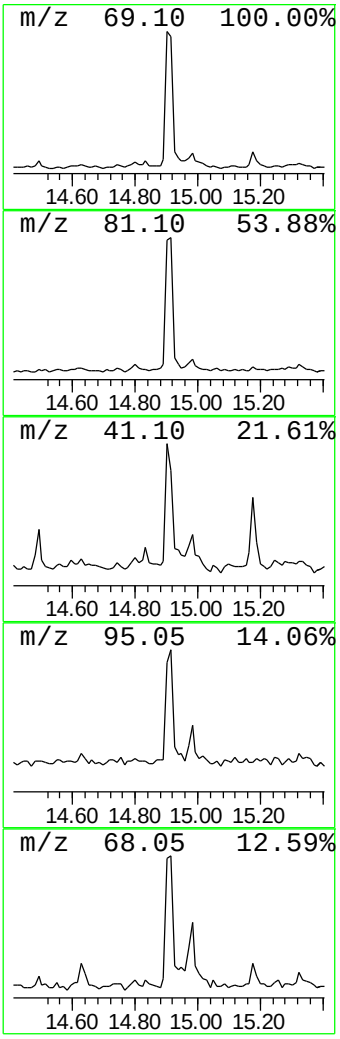
****

Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	3.91 ng	662246	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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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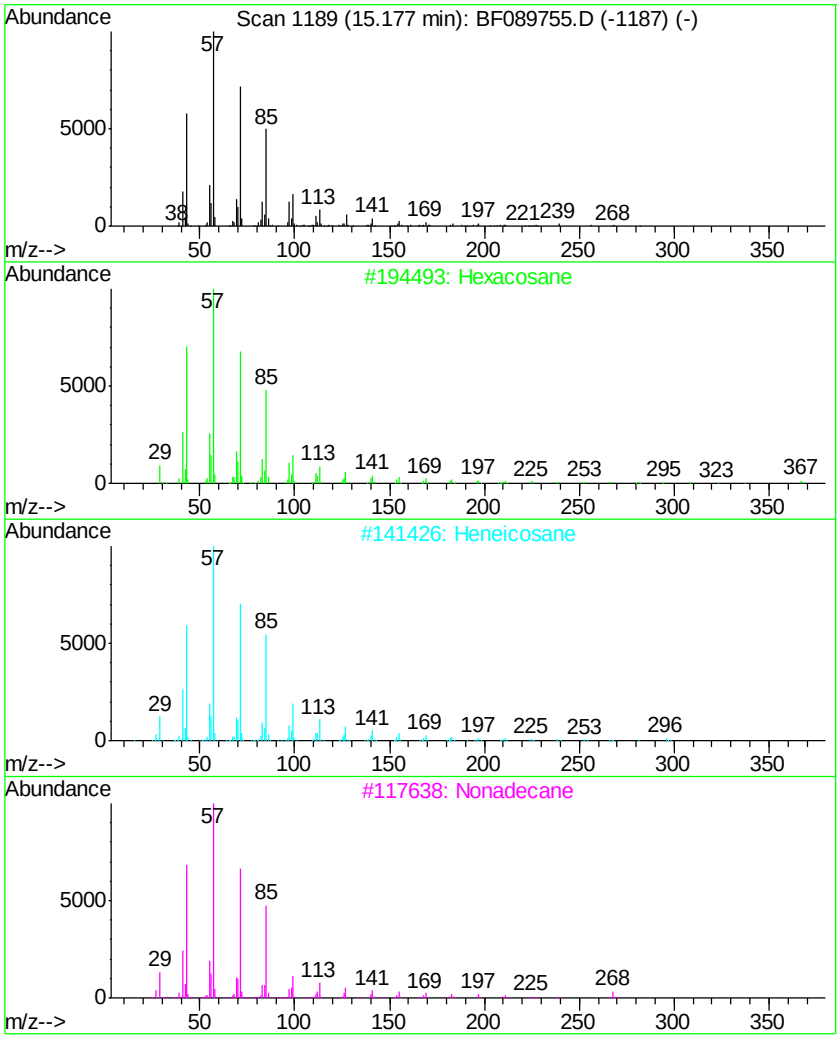
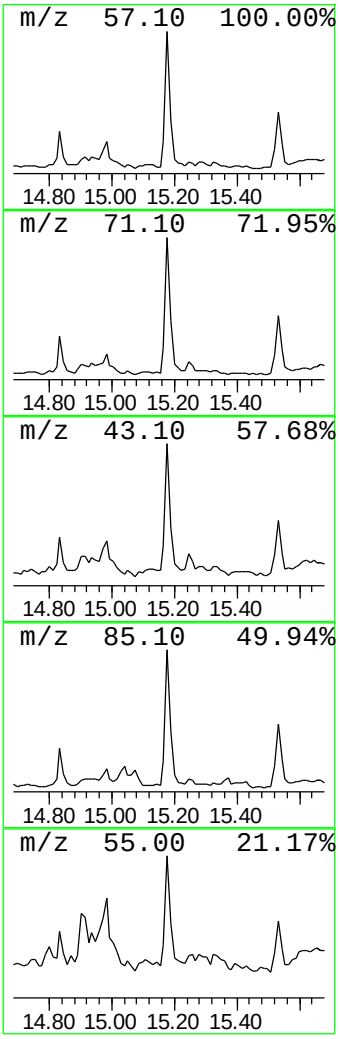
Peak Number 8 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	3.27 ng	554021	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Nonadecane	268	C19H40	000629-92-5	90
4	Hexadecane	226	C16H34	000544-76-3	86
5	Pentacosane	352	C25H52	000629-99-2	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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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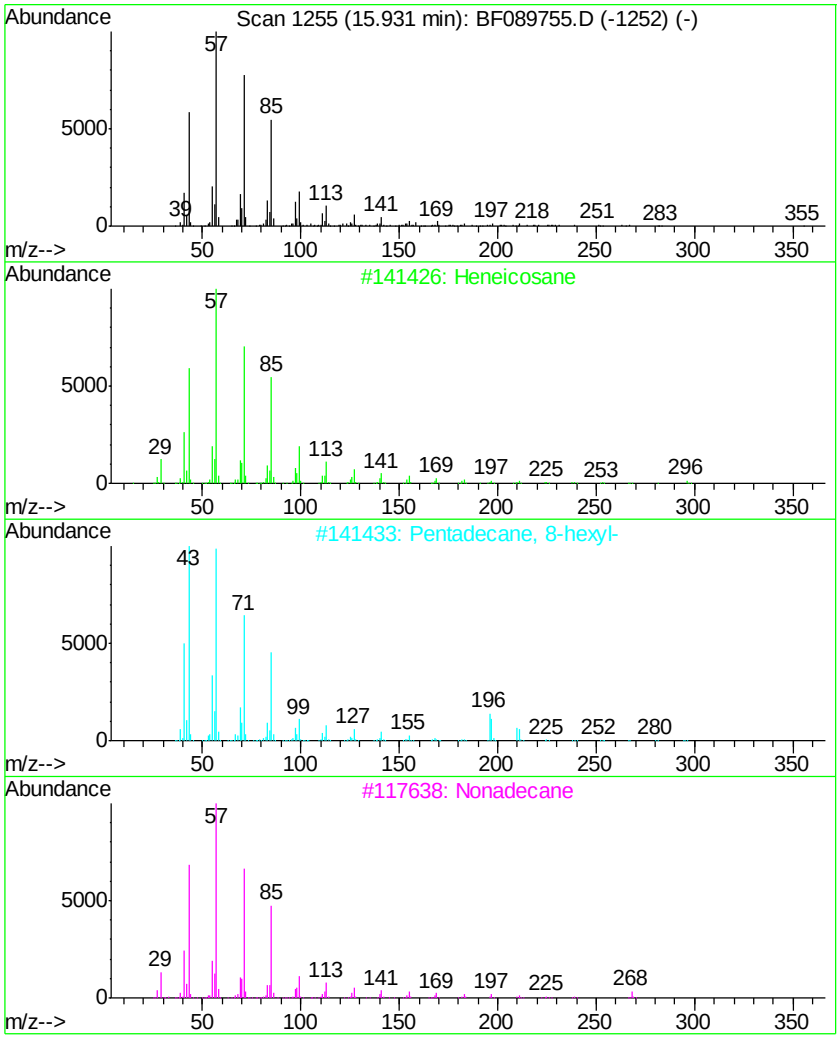
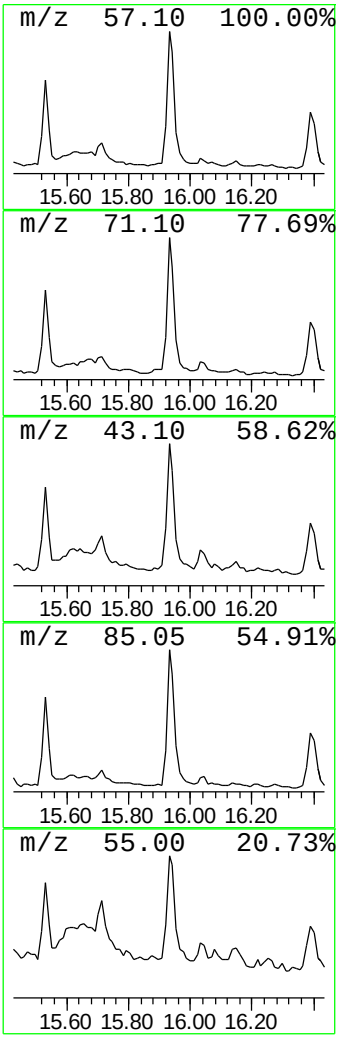
Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.43 ng	580391	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Hexadecane	226	C16H34	000544-76-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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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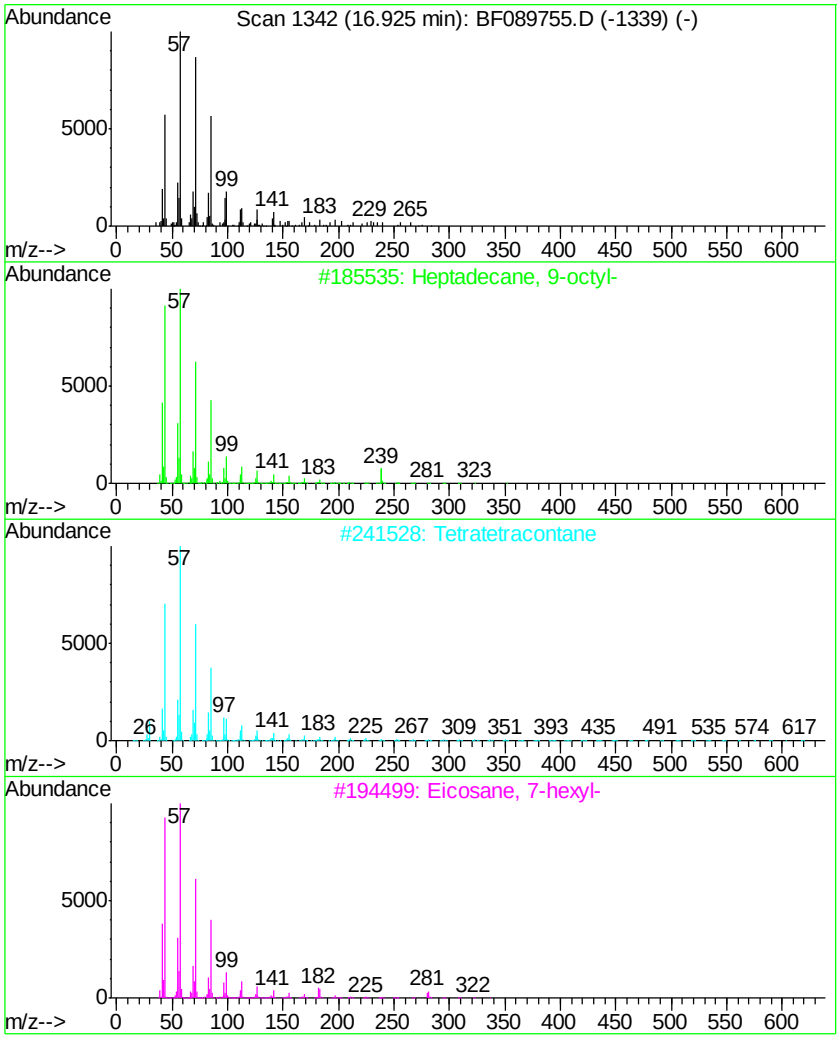
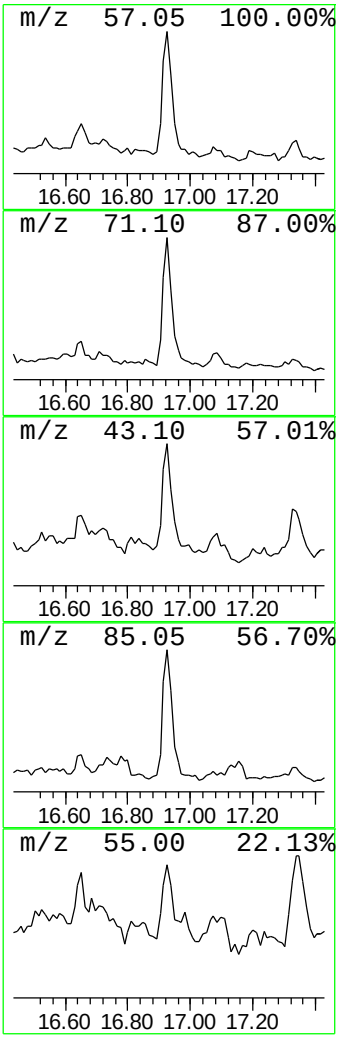
Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	3.50 ng	592208	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

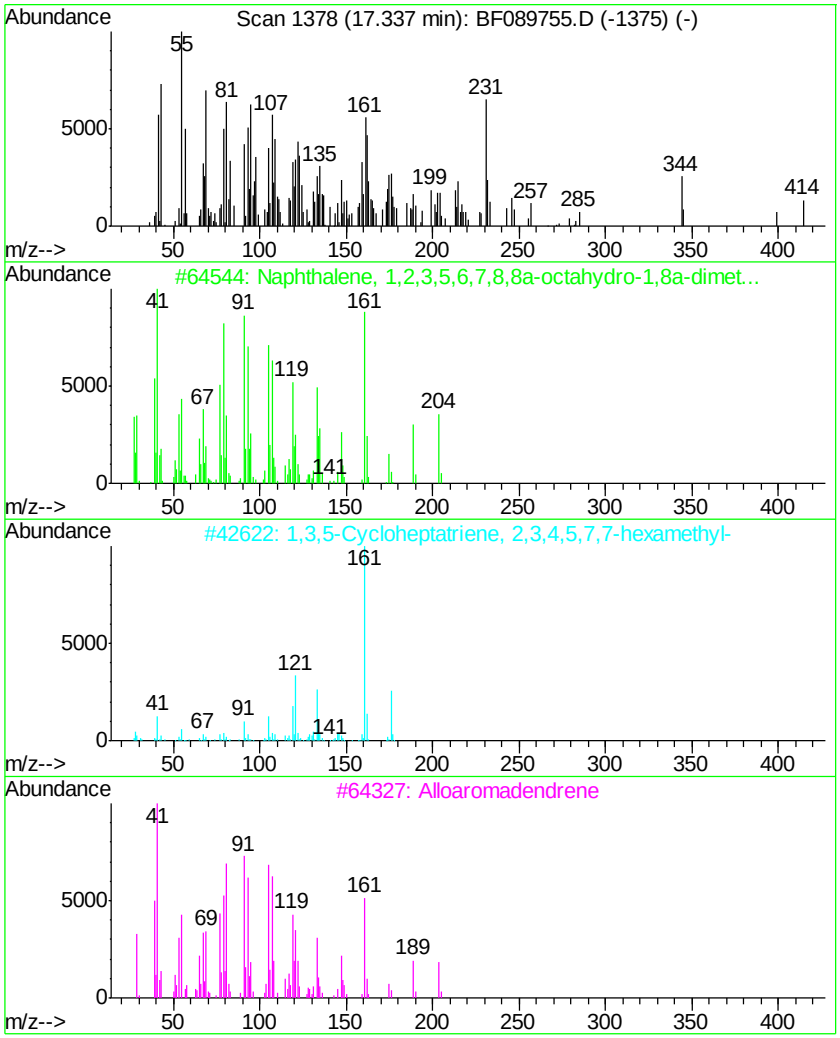
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

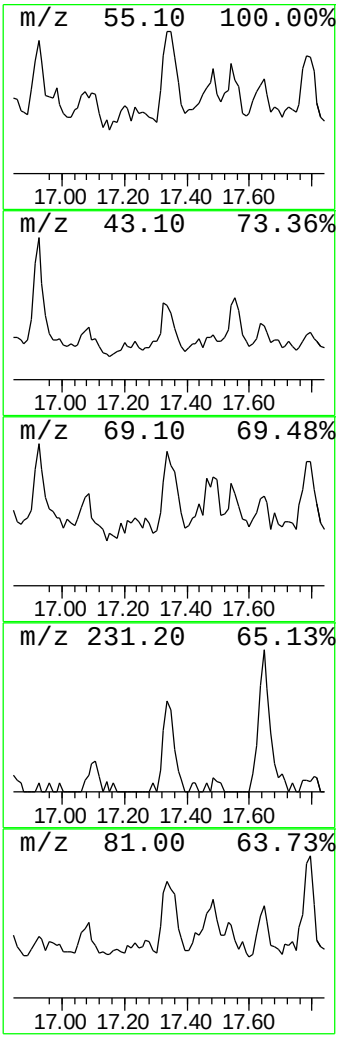
****

Peak Number 11 unknown17.34 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.34	2.23 ng	377800	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	45
2	1,3,5-Cycloheptatriene, 2,3,4,5,...	176	C13H20	074779-68-3	27
3	Alloaromadendrene	204	C15H24	025246-27-9	25
4	Longifolene	204	C15H24	000475-20-7	22
5	1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	22





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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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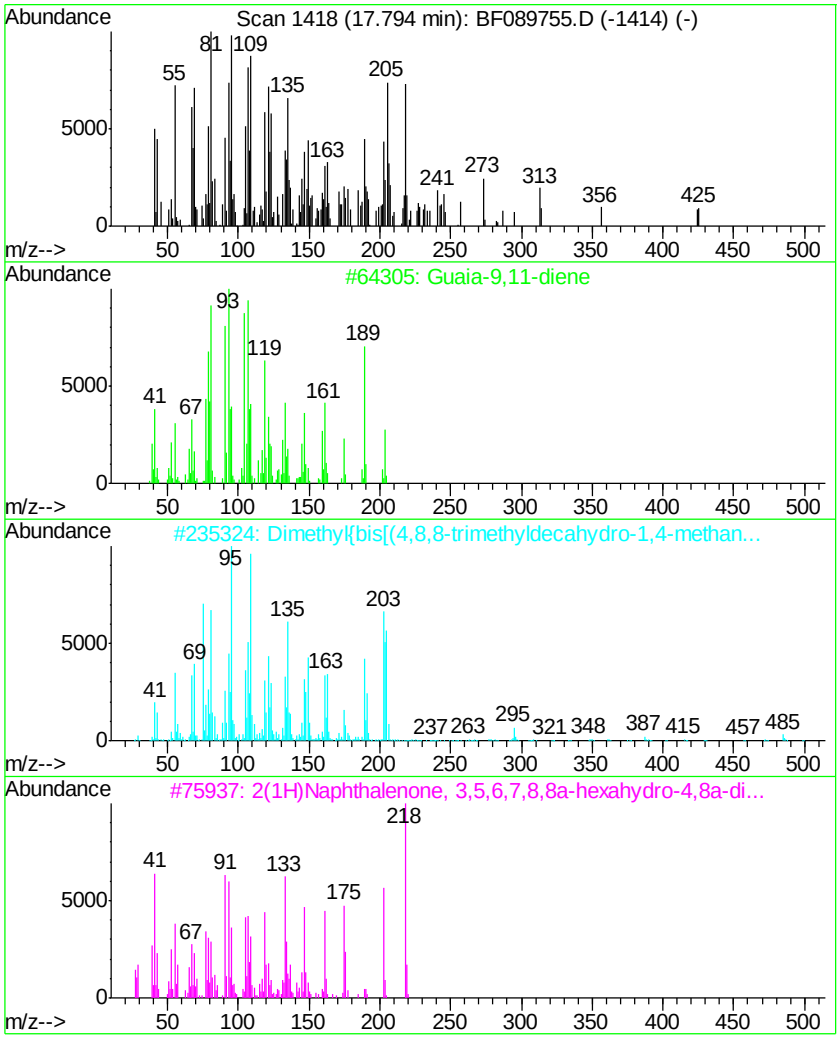
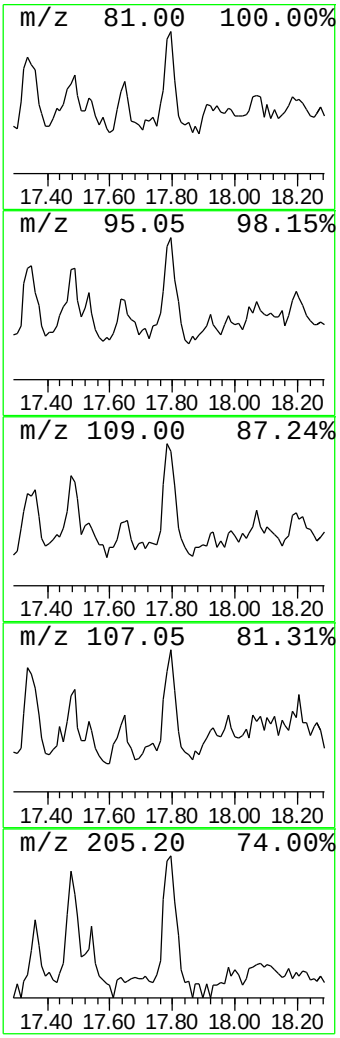
Peak Number 12 Guaia-9,11-diene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.79	2.13 ng	360638	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guaia-9,11-diene	204	C15H24	1000374-19-8	62
2	Dimethyl{bis[(4,8,8-trimethyldec...	500	C32H56O2Si	1000364-69-0	49
3	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	45
4	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	43
5	Sesquirosefuran	218	C15H22O	039007-93-7	41





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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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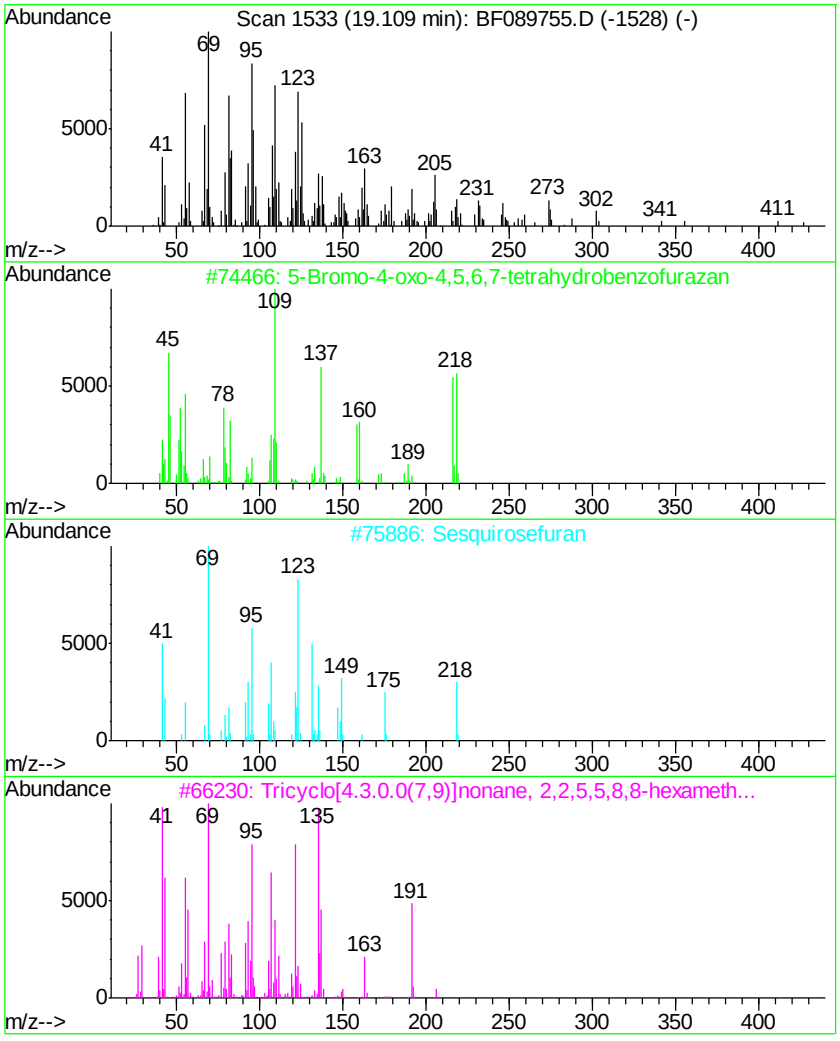
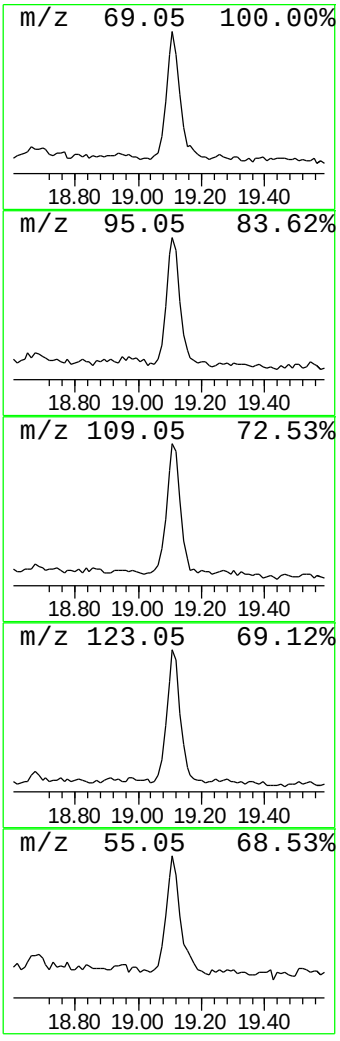
Peak Number 13 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.11	5.36 ng	907019	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	53
2	Sesquirosefuran	218	C15H22O	039007-93-7	50
3	Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	45
4	7-Tetradecyne	194	C14H26	035216-11-6	42
5	2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081616\
Data File : BF089755.D
Acq On : 17 Aug 2016 10:52
Operator : UM/SJ
Sample : H4145-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 9524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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...	4.83	7.0	ng	1278710	1	6.70	3628050	20.0
2-Acetylamino-3-(...	6.16	3.3	ng	600063	1	6.70	3628050	20.0
Diphenylmethane	10.42	2.9	ng	828271	3	9.74	5744650	20.0
Supraene	14.91	3.9	ng	662246	6	15.43	3384740	20.0
Hexacosane	15.18	3.3	ng	554021	6	15.43	3384740	20.0
Heneicosane	15.93	3.4	ng	580391	6	15.43	3384740	20.0
Heptadecane, 9-oc...	16.93	3.5	ng	592208	6	15.43	3384740	20.0
unknown17.34	17.34	2.2	ng	377800	6	15.43	3384740	20.0
Guaia-9,11-diene	17.79	2.1	ng	360638	6	15.43	3384740	20.0
5-Bromo-4-oxo-4,5...	19.11	5.4	ng	907019	6	15.43	3384740	20.0