LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

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-BF083116.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	1.735	11	13	57	rVB	2311614	5645533	84.22%	8.672%
2	4.764	275	278	297	rBV	765781	1394515	20.80%	2.142%
3	5.210	314	317	319	rBV	4047601	5175065	77.20%	7.950%
4	6.273	406	410	412	rBV	4106751	5486735	81.85%	8.428%
5	6.387	417	420	428	rVB	4746243	5575572	83.18%	8.565%
6	6.513	428	431	438	rVB3	73424	283001	4.22%	0.435%
7	6.616	438	440	447	rBV	1330241	1338144	19.96%	2.056%
8	6.776	451	454	456	rBV	3425935	4274568	63.77%	6.566%
9	7.187	486	490	492	rBV	3091891	3735192	55.72%	5.738%
10	7.610	524	527	530	rBV	93292	205386	3.06%	0.315%
11	7.896	550	552	555	rBV	1271084	1715443	25.59%	2.635%
12	8.353	589	592	594	rBV	104972	149770	2.23%	0.230%
13	8.399	594	596	601	rVB	43468	71112	1.06%	0.109%
14	8.719	622	624	627	rBV	41616	76532	1.14%	0.118%
15	8.856	634	636	641	rVB2	47769	74049	1.10%	0.114%
16	8.982	644	647	650	rVV	5402558	6120456	91.30%	9.402%
17	9.050	652	653	659	rVB	57680	92400	1.38%	0.142%
18	9.279	671	673	675	rBV	76338	77226	1.15%	0.119%
19	9.428	681	686	689	rBV	54515	90608	1.35%	0.139%
20	9.645	701	705	708	rBV	2108246	2158389	32.20%	3.316%
21	9.851	720	723	728	rBV	95985	190083	2.84%	0.292%
22	10.045	737	740	741	rBV2	135631	137251	2.05%	0.211%
23	10.079	741	743	745	rVV	68613	77580	1.16%	0.119%
24	10.148	748	749	755	rVB2	56038	89613	1.34%	0.138%
25	10.433	771	774	776	rBV	3670212	3993998	59.58%	6.135%
26	10.548	783	784	790	rVB	47321	83456	1.24%	0.128%
27	10.639	790	792	794	rBV	242755	216470	3.23%	0.333%
28	10.993	819	823	826	rBV3	62007	130499	1.95%	0.200%
29	11.119	829	834	836	rBV	2480877	2504368	37.36%	3.847%
30	11.165	836	838	843	rVB2	58138	97600	1.46%	0.150%
31	11.291	846	849	852	rBV	42013	73958	1.10%	0.114%
32	11.359	852	855	860	rBV	68966	115065	1.72%	0.177%
33	11.519	867	869	872	rVB	156752	154062	2.30%	0.237%
34	11.656	879	881	882	rBV	254334	267241	3.99%	0.411%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

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-BF083116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.908	901	903	907	rVB	240753	270857	4.04%	0.416%
36	12.171	923	926	929	rBV	51010	86685	1.29%	0.133%
37	12.434	947	949	955	rBV	121642	214097	3.19%	0.329%
38	12.548	955	959	961	rVB2	63273	97274	1.45%	0.149%
39	12.605	961	964	967	rVB2	77439	139284	2.08%	0.214%
40	12.708	969	973	975	rBV	5207370	6703405	100.00%	10.297%
41	13.245	1017	1020	1021	rBV	161256	202565	3.02%	0.311%
42	13.279	1021	1023	1028	rVB2	82231	175277	2.61%	0.269%
43	13.599	1049	1051	1055	rVB2	55792	96732	1.44%	0.149%
44	13.725	1060	1062	1065	rBV	2002137	2310633	34.47%	3.549%
45	13.919	1076	1079	1084	rVB	66203	91288	1.36%	0.140%
46	14.228	1103	1106	1110	rBV	46701	84823	1.27%	0.130%
47	14.365	1117	1118	1121	rVB	79781	121876	1.82%	0.187%
48	14.514	1127	1131	1134	rBV	58843	99647	1.49%	0.153%
49	14.582	1134	1137	1140	rBV	249871	385104	5.74%	0.592%
50	14.811	1154	1157	1160	rBV	67900	98858	1.47%	0.152%
51	15.074	1177	1180	1183	rBV	1546504	1728553	25.79%	2.655%
52	15.131	1183	1185	1190	rVB	82421	132475	1.98%	0.203%
53	15.497	1215	1217	1220	rBV	65294	90773	1.35%	0.139%
54	15.920	1250	1254	1259	rVB	49947	97750	1.46%	0.150%

Sum of corrected areas: 65098896

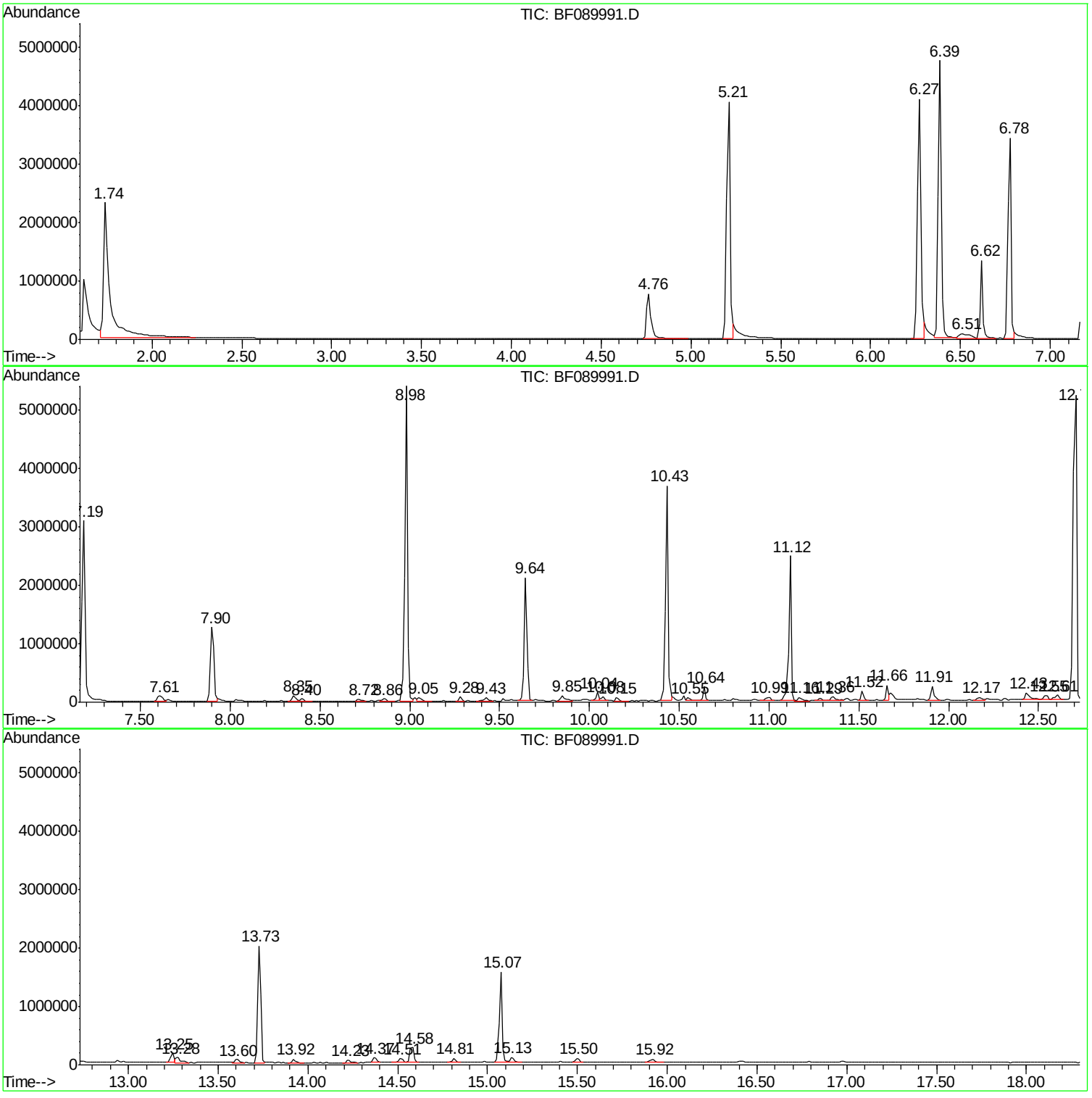
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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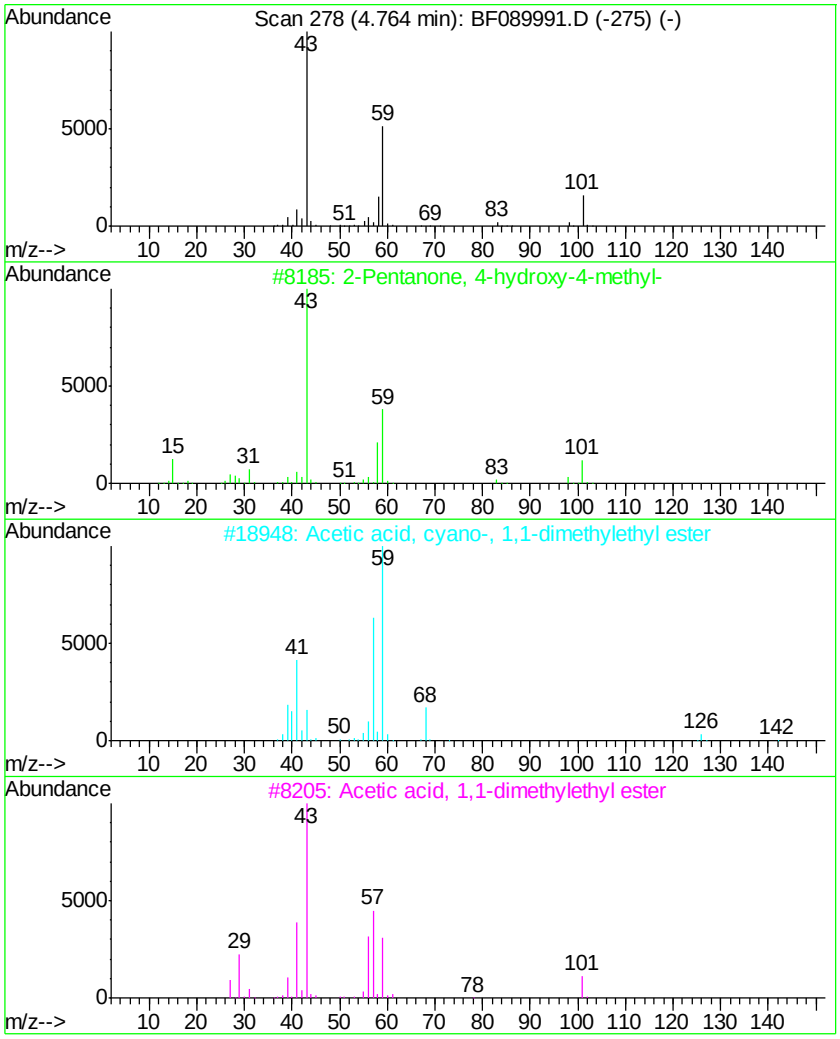
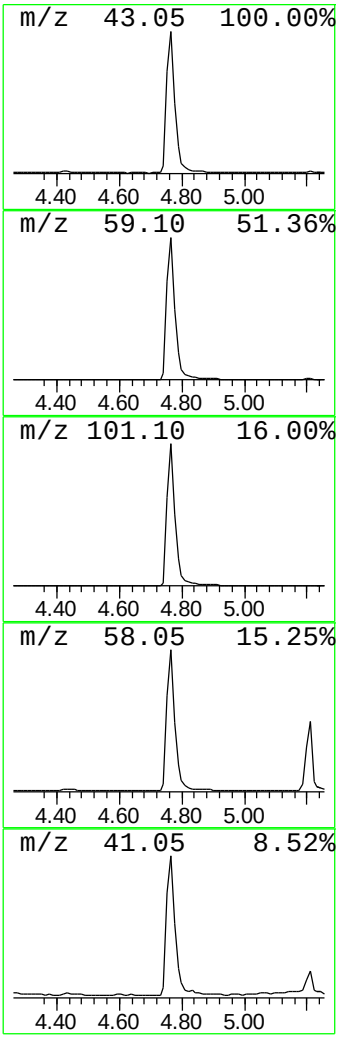
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	20.84 ng	1394520	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

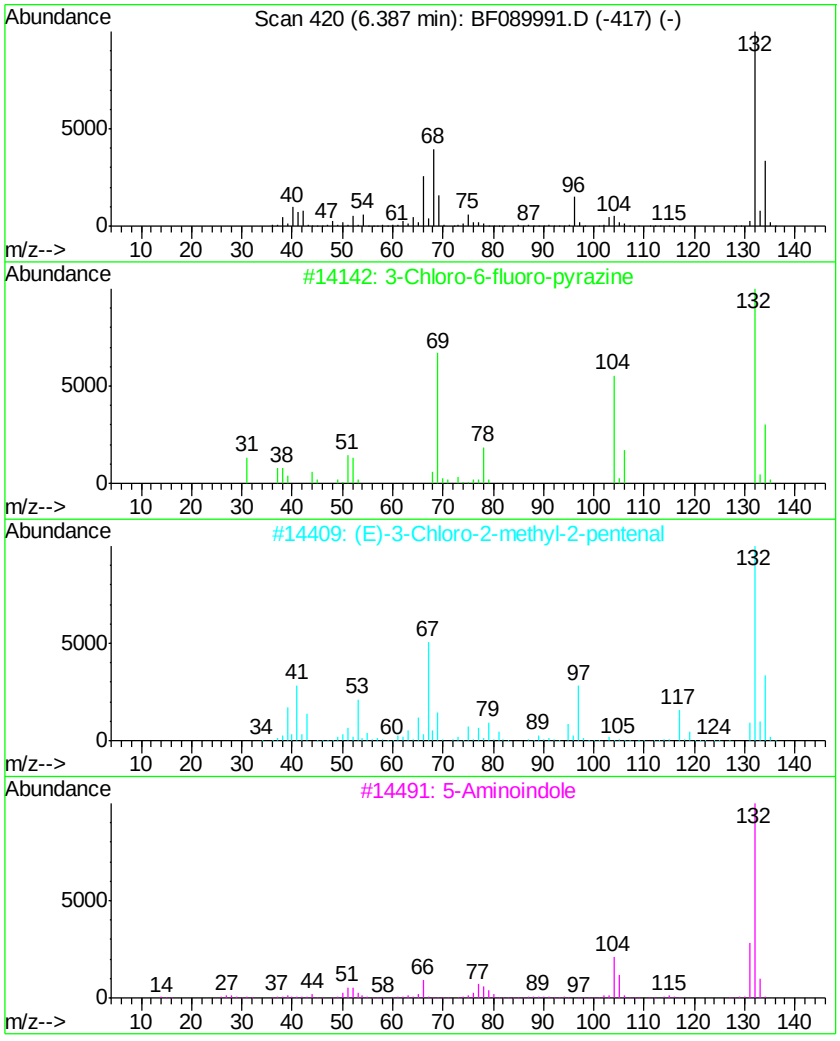
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

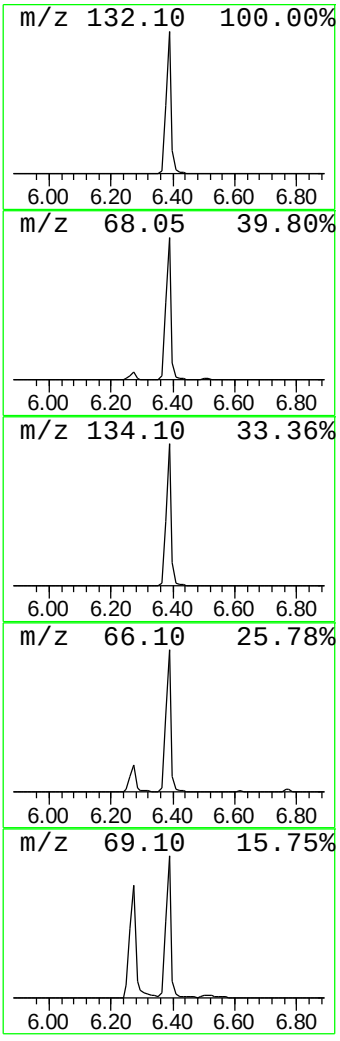
****

Peak Number 3 unknown6.39 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	83.33 ng	5575570	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
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\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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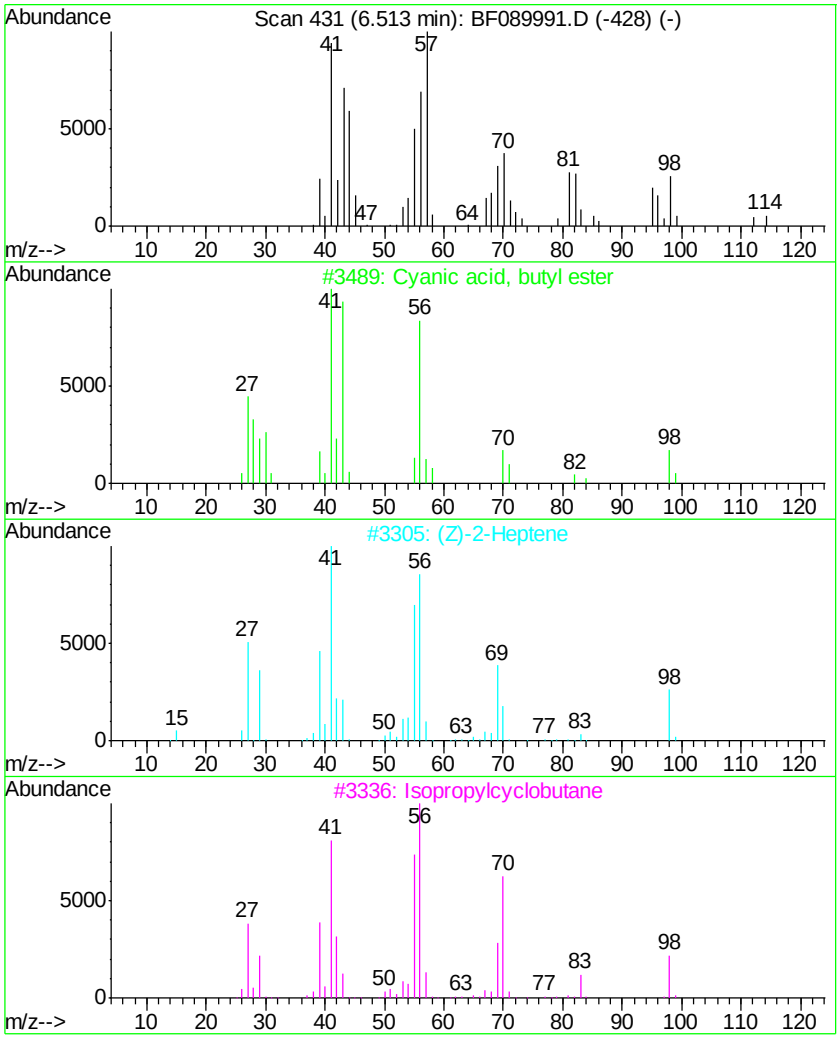
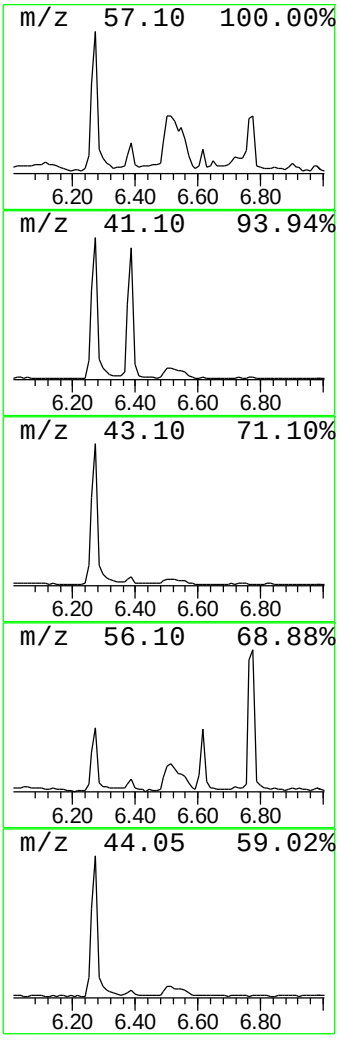
Peak Number 4 unknown6.51 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	4.23 ng	283001	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyanic acid, butyl ester	99	C5H9NO	001768-24-7	38
2	(Z)-2-Heptene	98	C7H14	006443-92-1	38
3	Isopropylcyclobutane	98	C7H14	000872-56-0	35
4	1-Heptene	98	C7H14	000592-76-7	35
5	2-Heptene	98	C7H14	000592-77-8	30





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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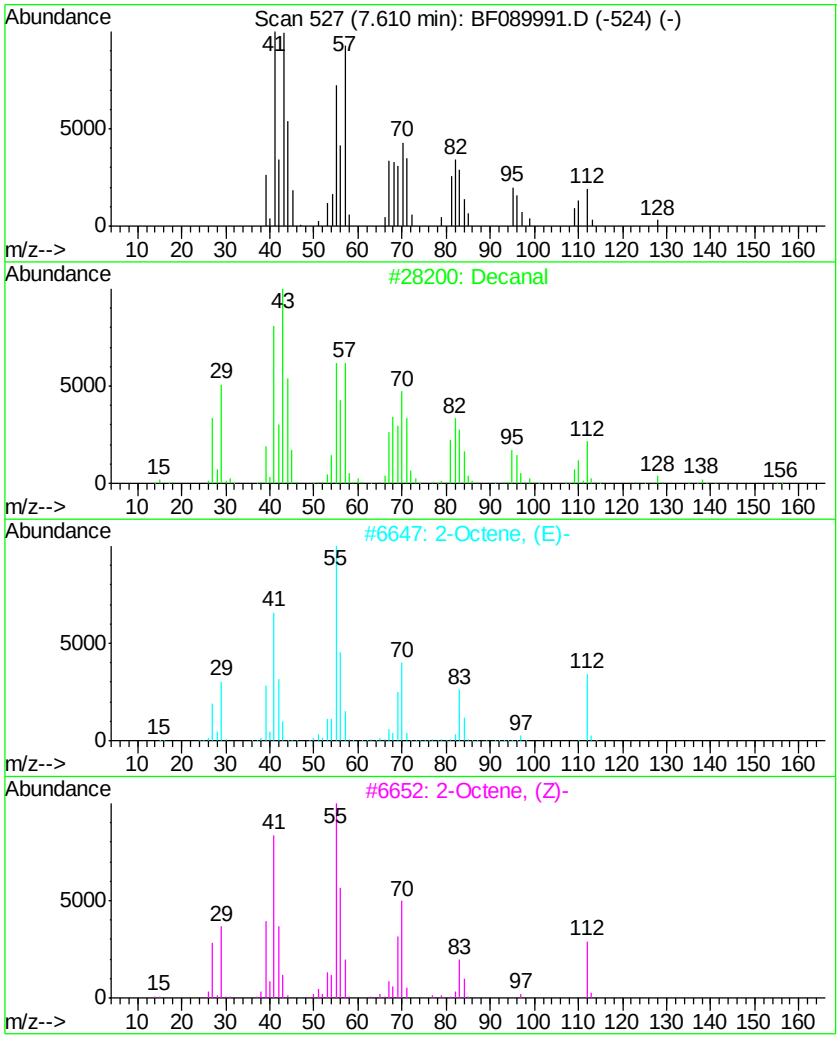
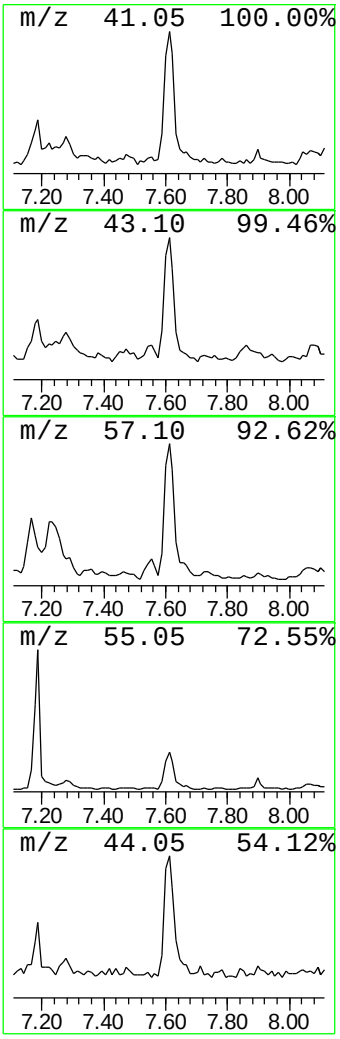
Peak Number 6 Decanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	2.39 ng	205386	Naphthalene-d8	7.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanal	156	C10H20O	000112-31-2	91
2	2-Octene, (E)-	112	C8H16	013389-42-9	53
3	2-Octene, (Z)-	112	C8H16	007642-04-8	50
4	1,2-Cyclohexanedione	112	C6H8O2	000765-87-7	49
5	4-Octene, (E)-	112	C8H16	014850-23-8	46





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

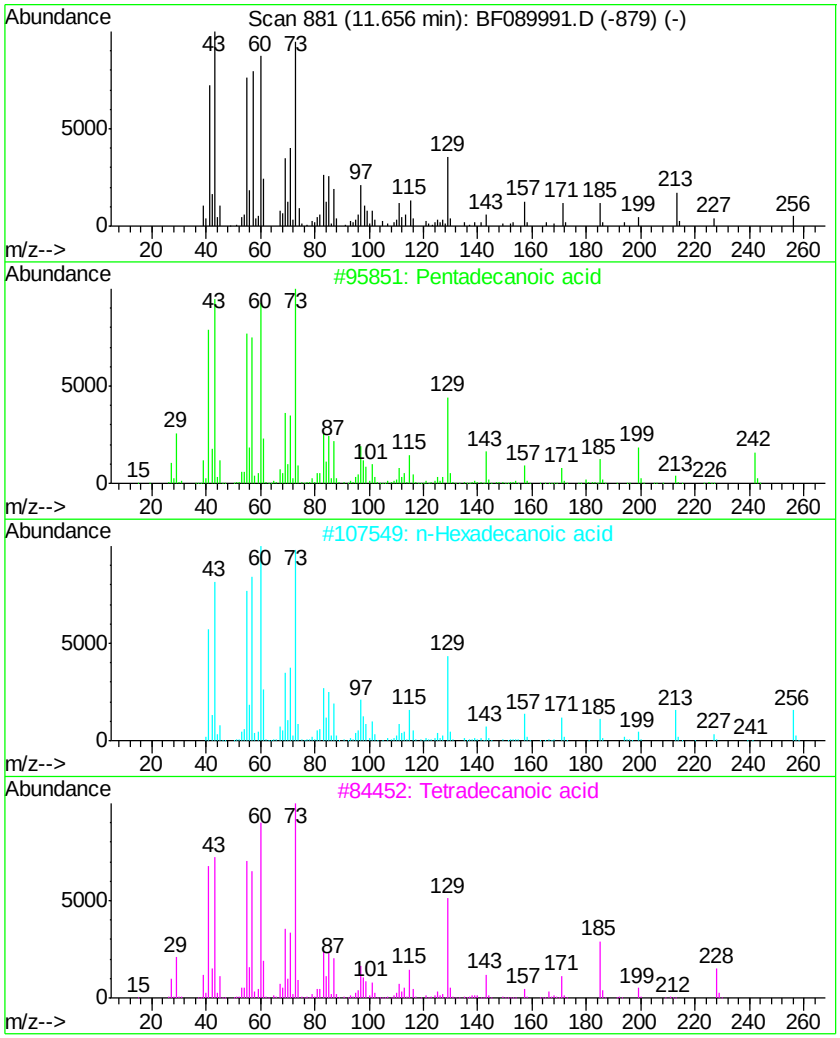
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

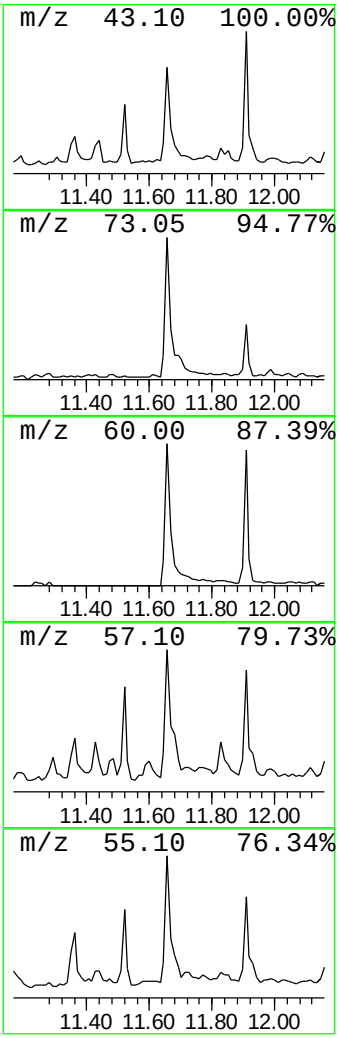
****

Peak Number 7 Pentadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	2.13 ng	267241	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	35





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Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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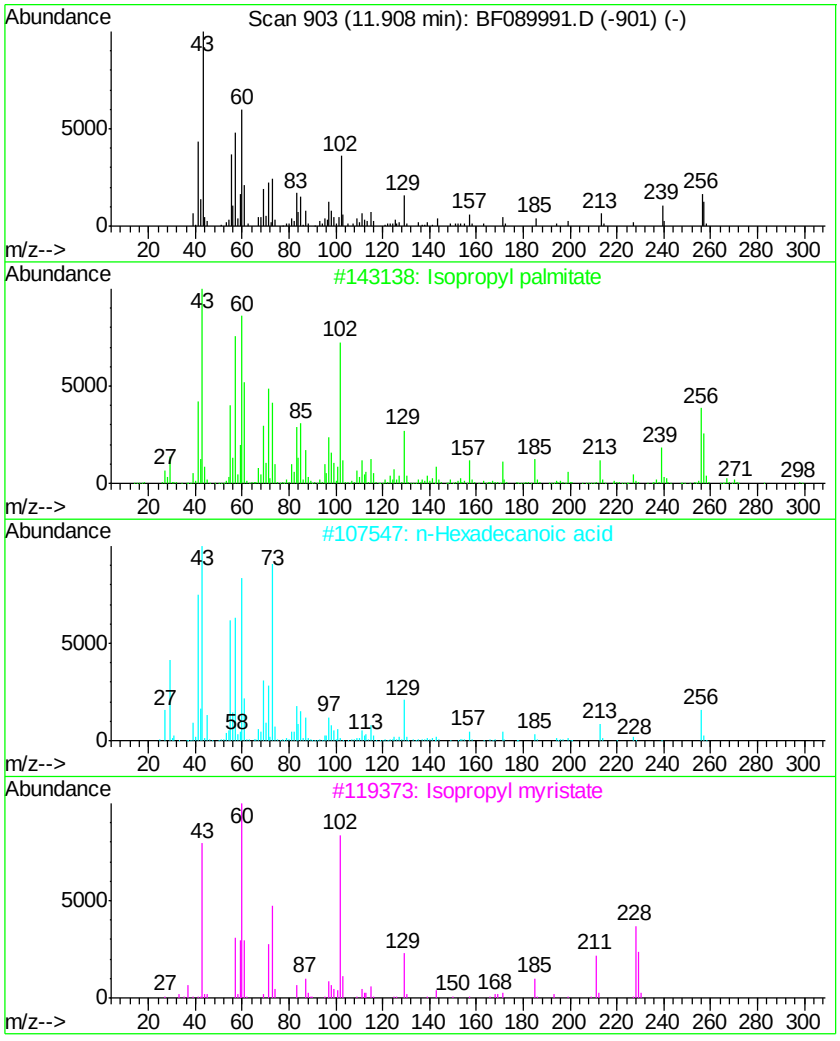
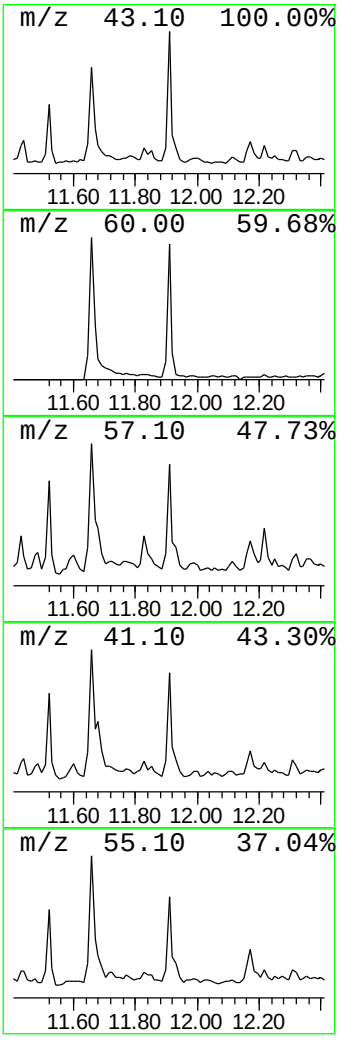
Peak Number 8 Isopropyl palmitate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.16 ng	270857	Phenanthrene-d10	11.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl palmitate	298	C19H38O2	000142-91-6	68
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
3	Isopropyl myristate	270	C17H34O2	000110-27-0	52
4	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	52
5	Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	50





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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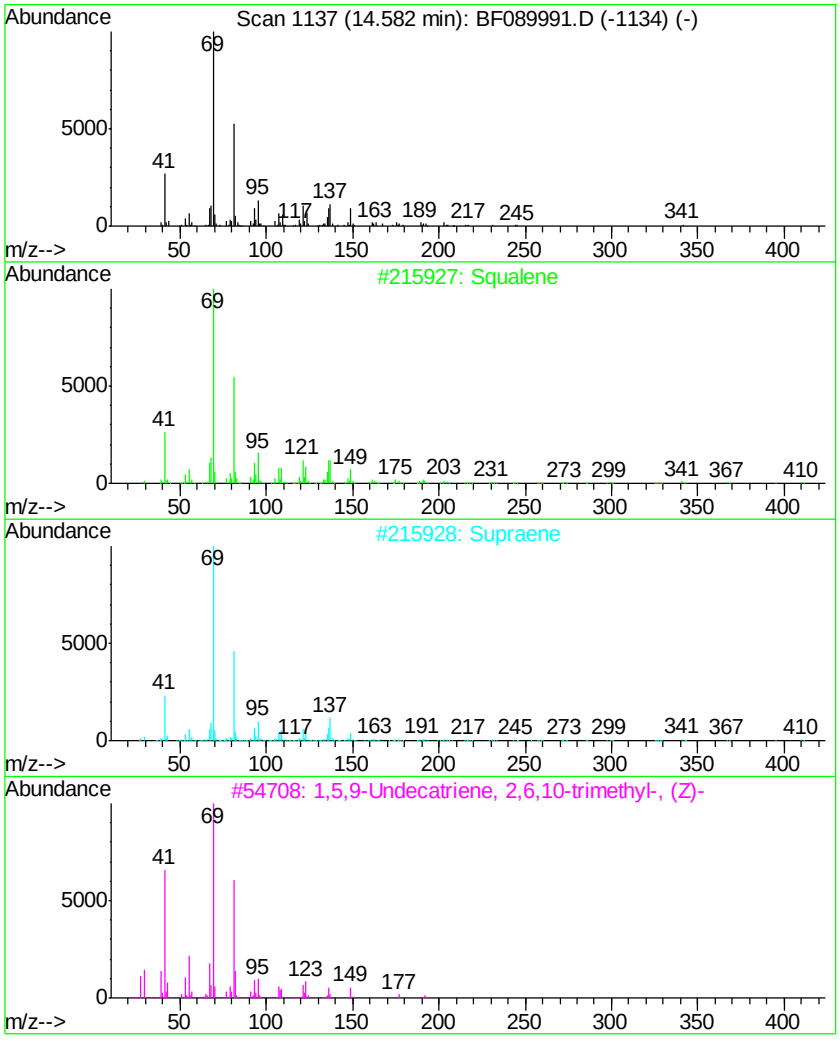
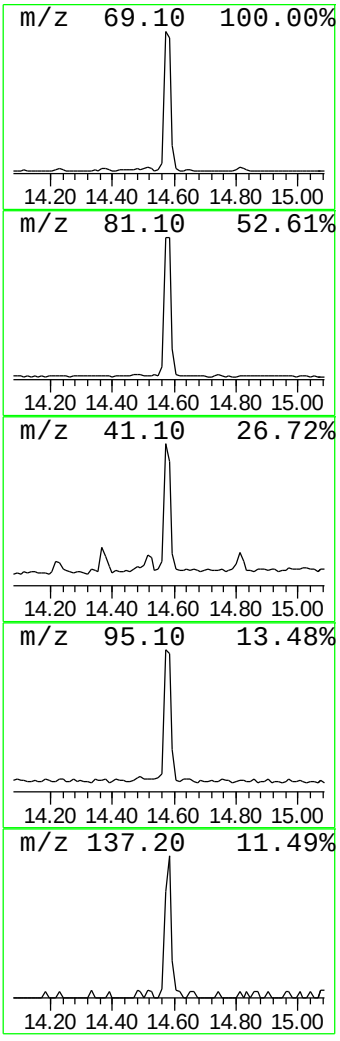
Peak Number 9 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	4.46 ng	385104	Perylene-d12	15.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
4	trans-Farnesol	222	C15H26O	000106-28-5	59
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090616\
Data File : BF089991.D
Acq On : 6 Sep 2016 16:37
Operator : UM/SJ
Sample : PB93246BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB93246BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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...	4.76	20.8	ng	1394520	1	6.62	1338140	20.0
unknown6.39	6.39	83.3	ng	5575570	1	6.62	1338140	20.0
unknown6.51	6.51	4.2	ng	283001	1	6.62	1338140	20.0
Decanal	7.61	2.4	ng	205386	2	7.90	1715440	20.0
Pentadecanoic acid	11.66	2.1	ng	267241	4	11.12	2504370	20.0
Isopropyl palmitate	11.91	2.2	ng	270857	4	11.12	2504370	20.0
Squalene	14.58	4.5	ng	385104	6	15.07	1728550	20.0