

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070815\
 Data File : BF080390.D
 Acq On : 8 Jul 2015 16:23
 Operator : TP/UM
 Sample : G2905-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB3

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.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	2.190	4	9	24	rVV2	257351	442001	29.25%	4.251%
2	2.395	24	27	30	rVB	528101	812390	53.76%	7.812%
3	3.356	108	111	115	rVB	9844	16638	1.10%	0.160%
4	4.807	237	238	242	rVB	29100	30967	2.05%	0.298%
5	5.401	288	290	298	rVB	124200	150663	9.97%	1.449%
6	5.813	324	326	328	rBV	253794	282637	18.70%	2.718%
7	6.213	359	361	363	rVB	45440	37301	2.47%	0.359%
8	6.442	379	381	384	rBV	10474	15629	1.03%	0.150%
9	6.807	411	413	417	rVB	181191	185859	12.30%	1.787%
10	6.967	425	427	430	rBV	702605	626615	41.47%	6.026%
11	7.207	446	448	450	rBV	293778	243371	16.10%	2.340%
12	7.367	460	462	464	rVB	819273	724507	47.94%	6.967%
13	7.767	494	497	499	rBV	478848	515260	34.10%	4.955%
14	8.499	558	561	563	rBV	370132	316619	20.95%	3.045%
15	9.448	642	644	648	rBV	17130	20926	1.38%	0.201%
16	9.573	652	655	657	rBV	1620334	1304946	86.35%	12.549%
17	9.962	687	689	691	rBV	224888	176096	11.65%	1.693%
18	10.259	713	715	718	rBV2	312818	364263	24.10%	3.503%
19	10.682	749	752	753	rVB2	21169	31187	2.06%	0.300%
20	10.888	768	770	773	rBV2	23551	29065	1.92%	0.280%
21	10.968	773	777	780	rVB2	24175	35644	2.36%	0.343%
22	11.059	783	785	787	rBV	633674	645518	42.72%	6.208%
23	11.162	792	794	799	rVB	18192	33376	2.21%	0.321%
24	11.768	845	847	850	rBV	405252	403854	26.72%	3.884%
25	12.008	864	868	871	rBV	12166	18447	1.22%	0.177%
26	12.339	895	897	900	rBV	18525	18261	1.21%	0.176%
27	13.071	959	961	963	rBV	23761	21075	1.39%	0.203%
28	13.334	980	984	985	rBV2	25695	37191	2.46%	0.358%
29	13.482	995	997	1000	rBV	1336374	1511159	100.00%	14.532%
30	14.042	1044	1046	1050	rVB	22060	21983	1.45%	0.211%
31	14.122	1050	1053	1055	rBV	18530	22577	1.49%	0.217%
32	14.168	1055	1057	1058	rVV	13744	15881	1.05%	0.153%
33	14.511	1081	1087	1089	rBV	9176	16764	1.11%	0.161%
34	14.579	1089	1093	1100	rBV3	72982	207272	13.72%	1.993%

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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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.774	1105	1110	1112	rBV	347137	552863	36.59%	5.317%
36	14.991	1126	1129	1132	rBV	16911	20644	1.37%	0.199%
37	15.402	1162	1165	1168	rBV	15281	22244	1.47%	0.214%
38	15.905	1207	1209	1212	rBV	34012	48584	3.22%	0.467%
39	16.111	1224	1227	1228	rBV	9977	15656	1.04%	0.151%
40	16.625	1269	1272	1275	rBV	305727	402723	26.65%	3.873%

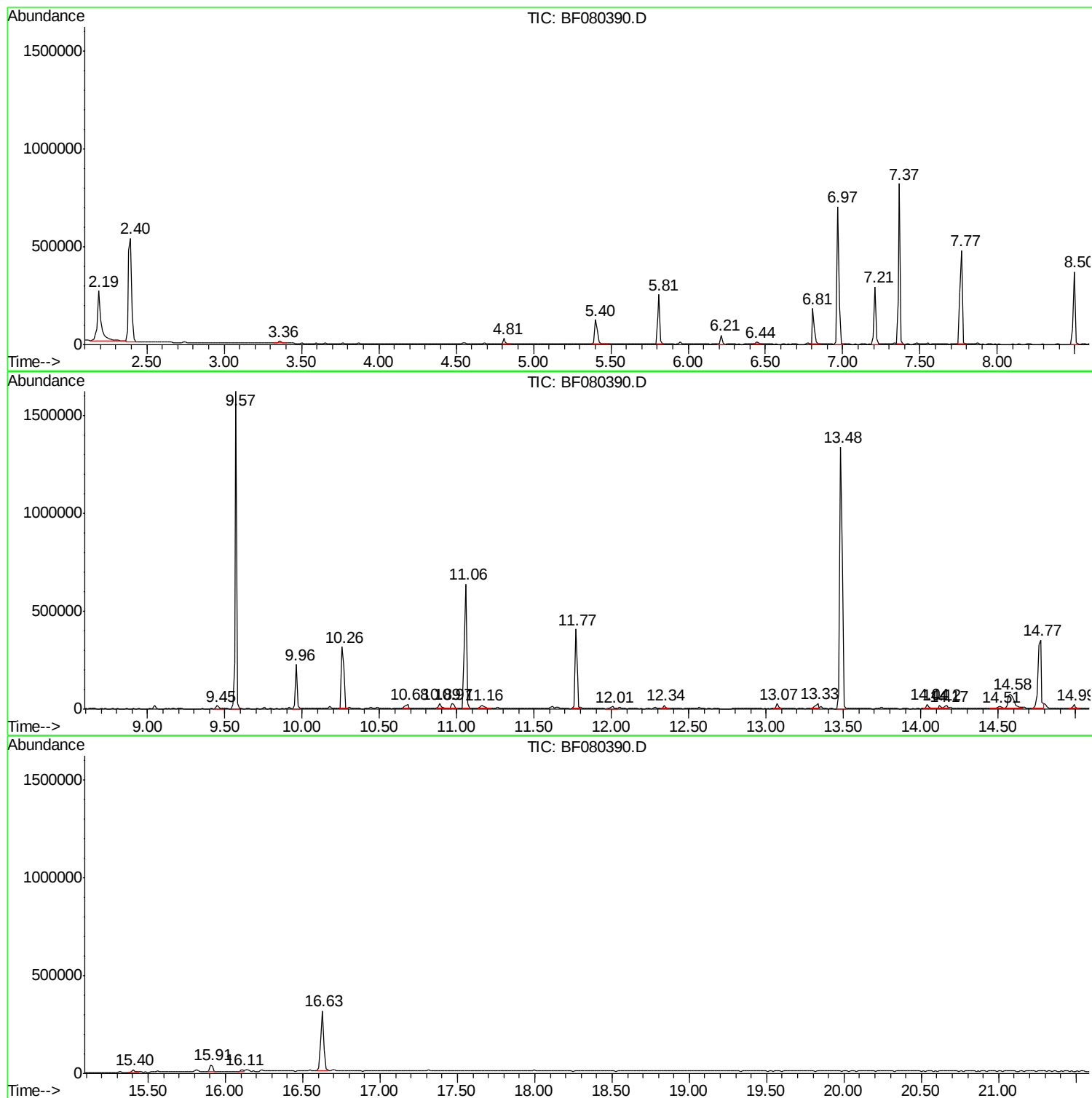
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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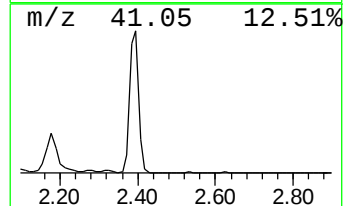
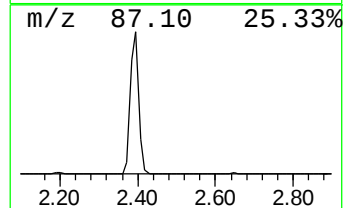
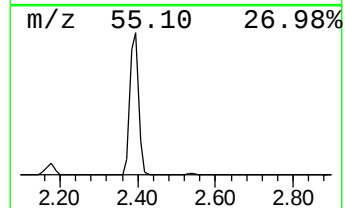
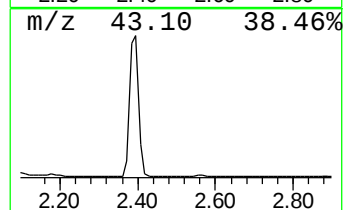
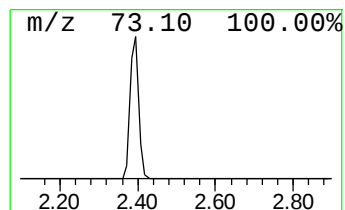
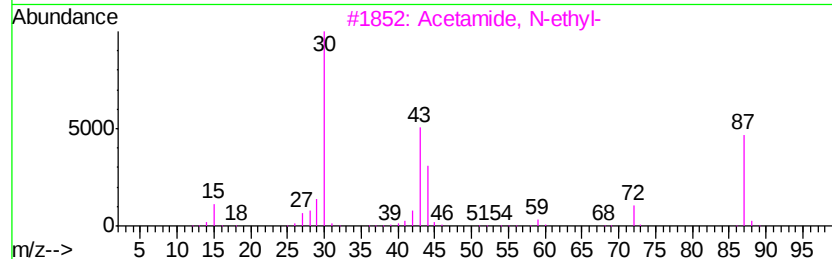
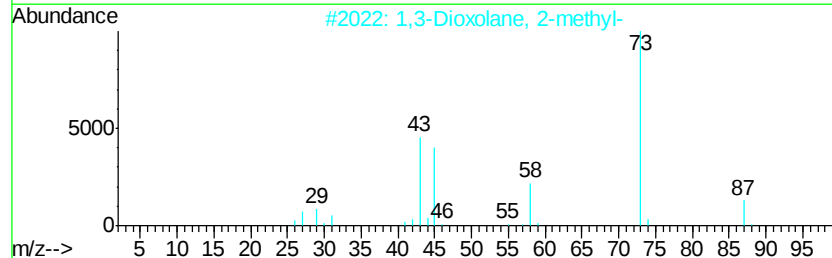
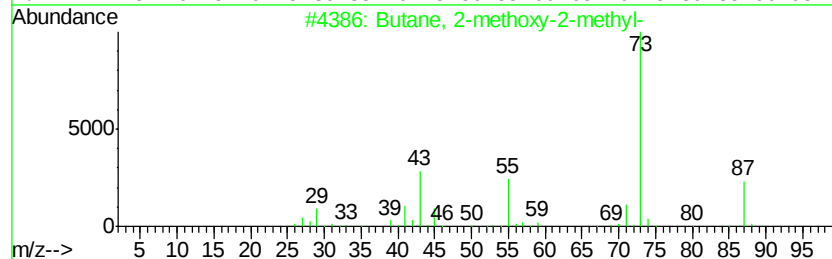
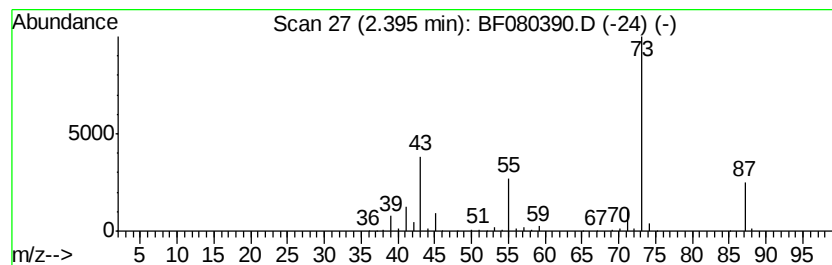
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.40	66.76 ng	812390	1,4-Dichlorobenzene-d4	7.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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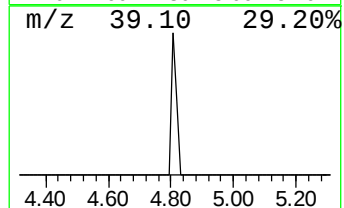
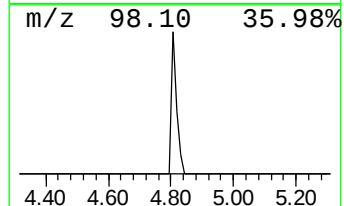
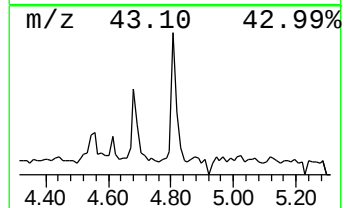
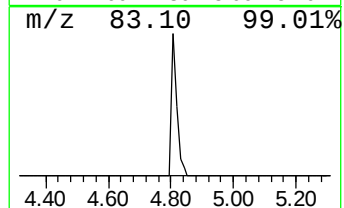
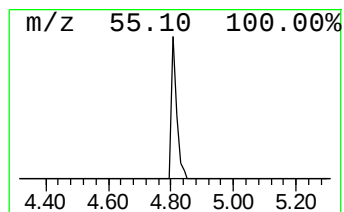
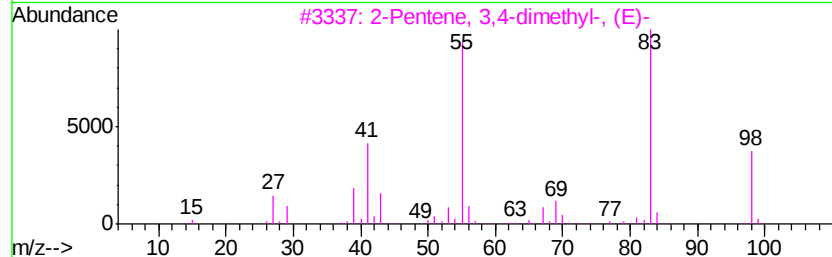
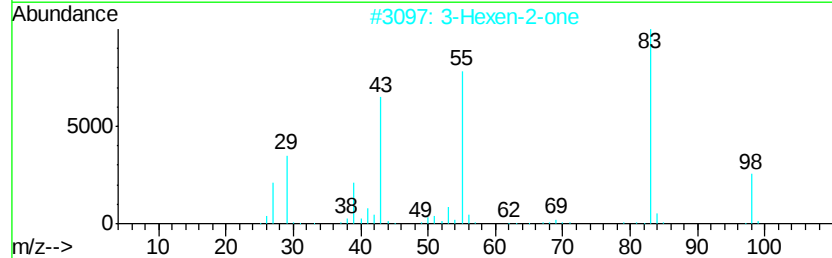
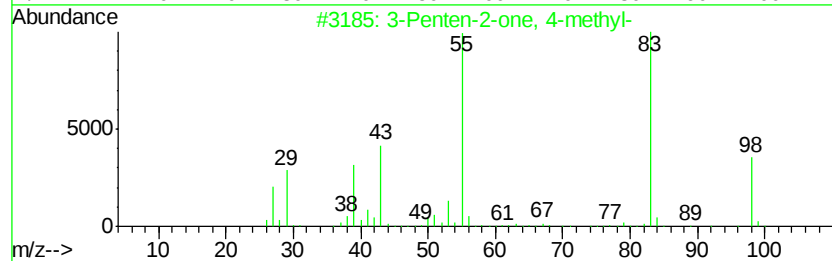
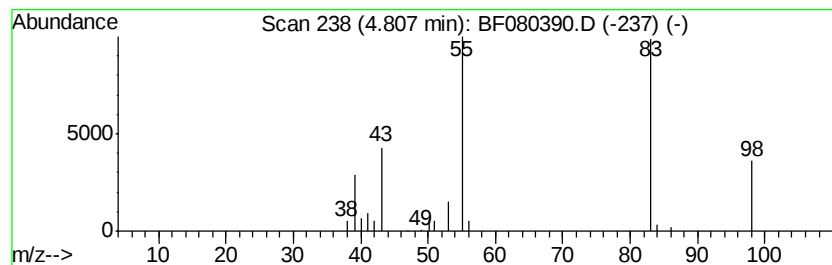
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	2.54 ng	30967	1,4-Dichlorobenzene-d4	7.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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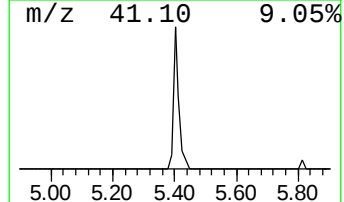
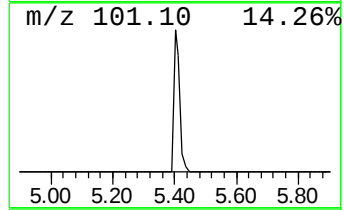
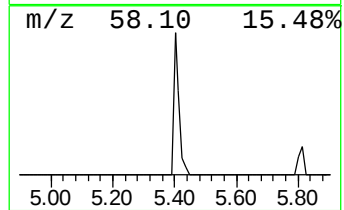
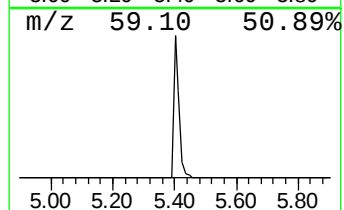
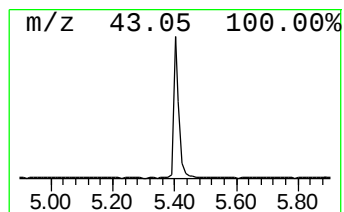
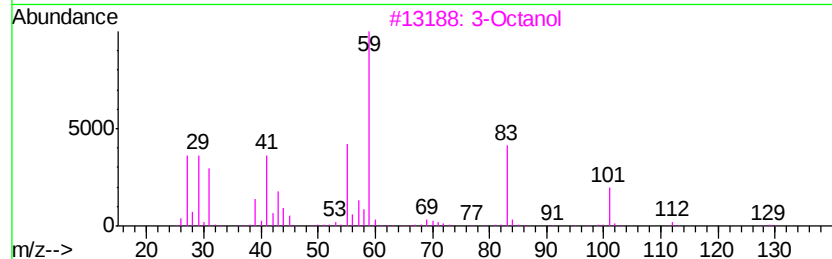
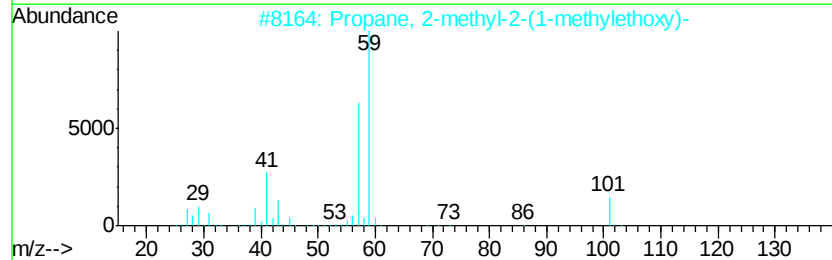
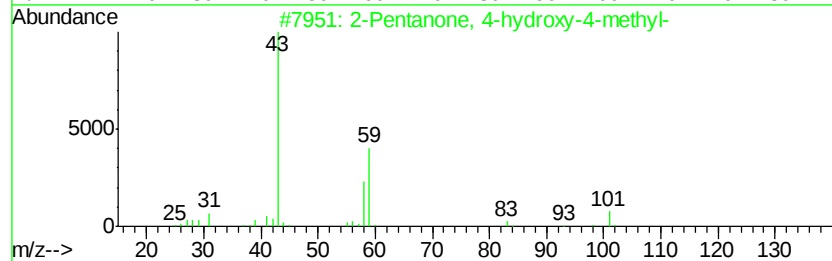
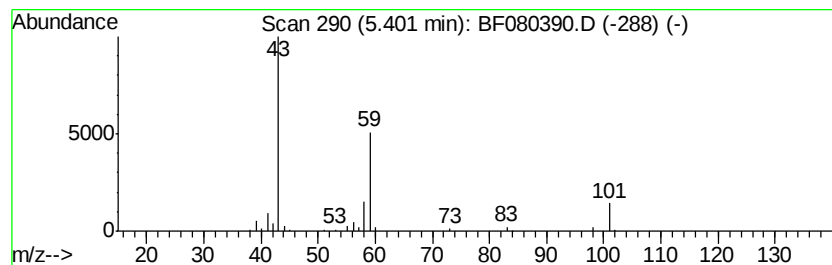
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.40	12.38 ng	150663	1,4-Dichlorobenzene-d4	7.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Octanol	130	C8H18O	000589-98-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28



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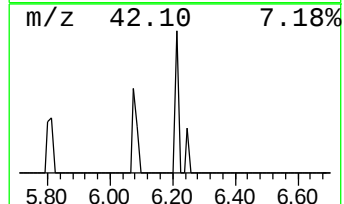
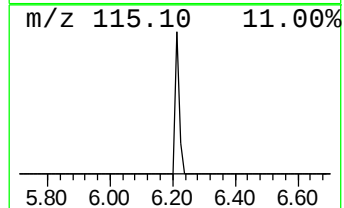
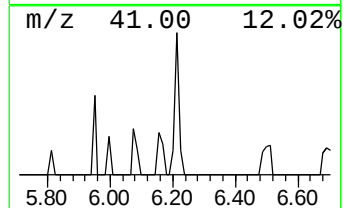
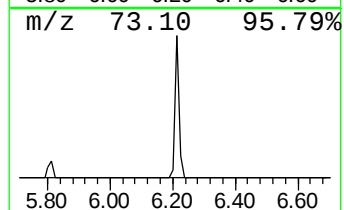
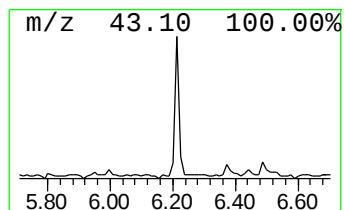
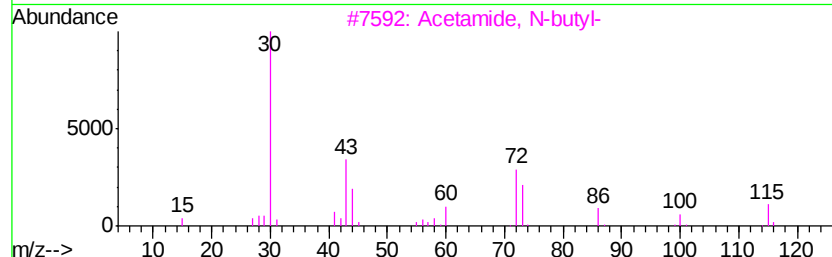
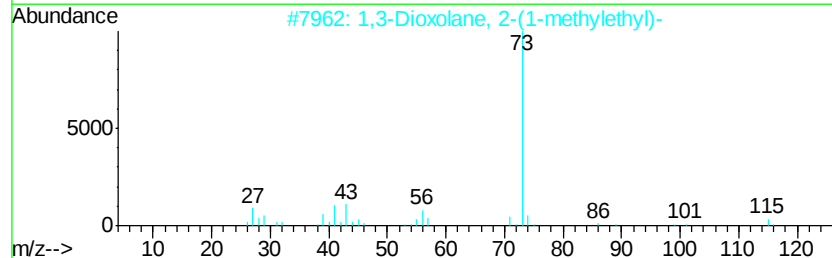
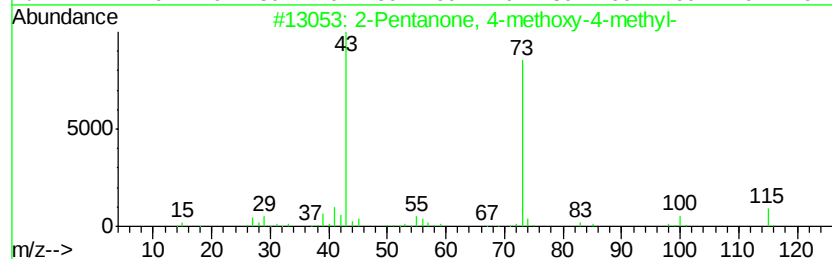
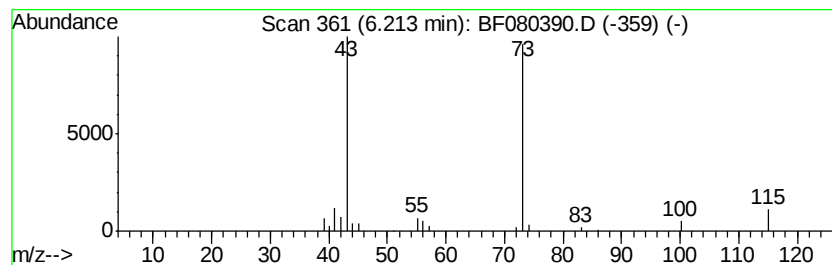
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Peak Number 5 unknown6.21 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	3.07 ng	37301	1,4-Dichlorobenzene-d4	7.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	17
3		Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9



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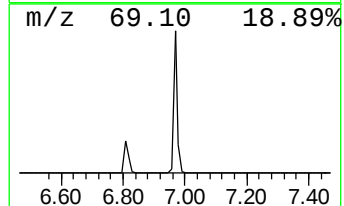
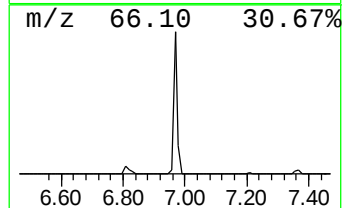
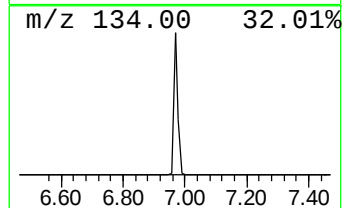
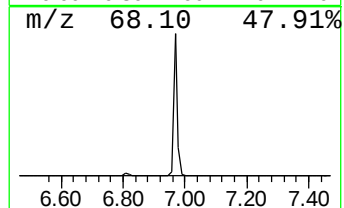
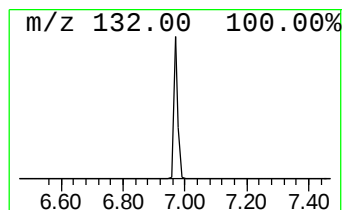
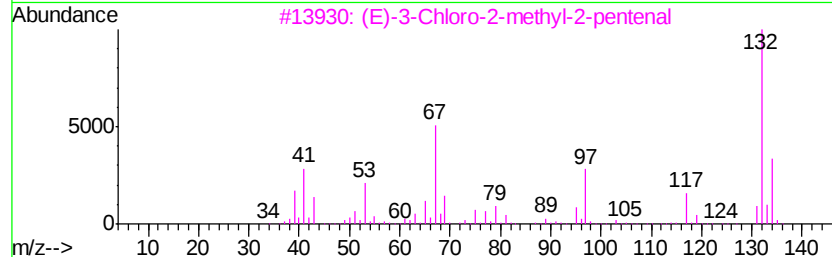
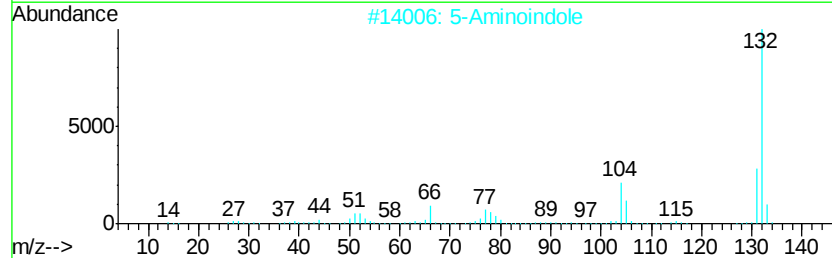
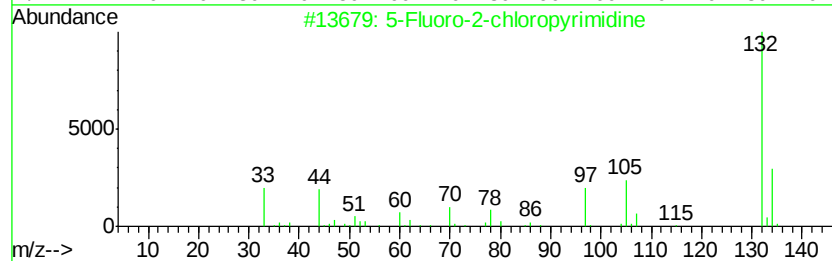
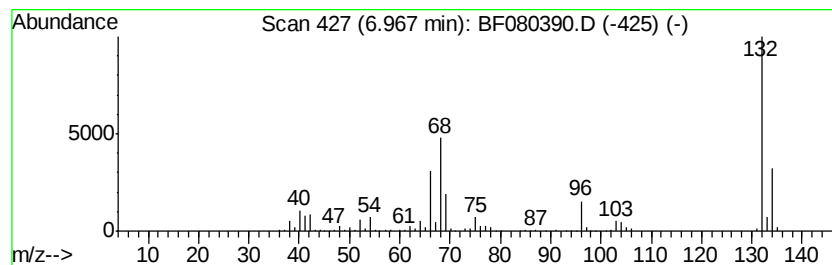
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Peak Number 6 unknown6.97 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.97	51.49 ng	626615	1,4-Dichlorobenzene-d4	7.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	10
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070815\
Data File : BF080390.D
Acq On : 8 Jul 2015 16:23
Operator : TP/UM
Sample : G2905-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

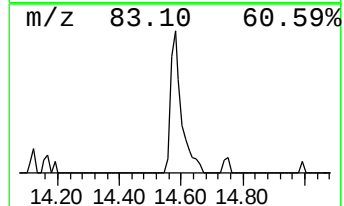
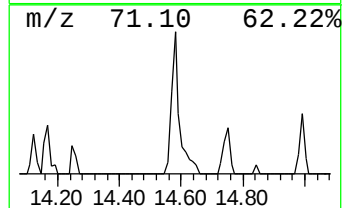
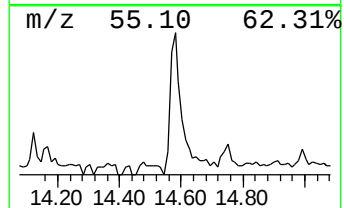
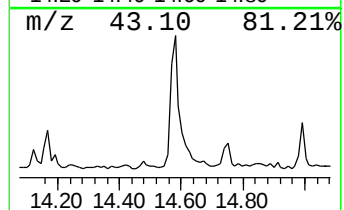
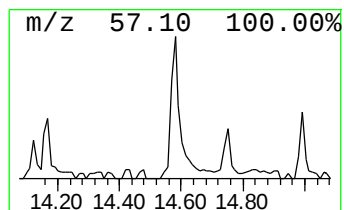
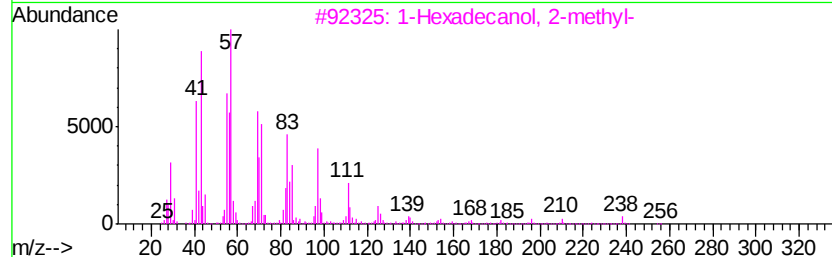
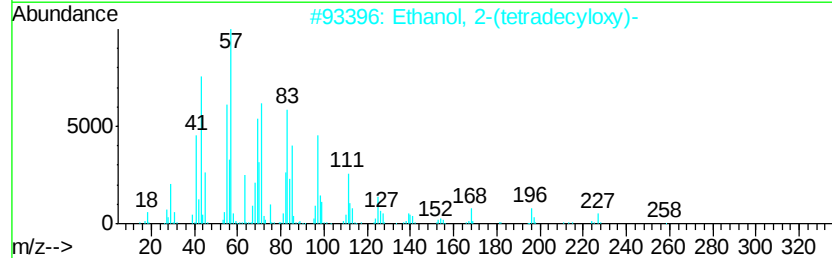
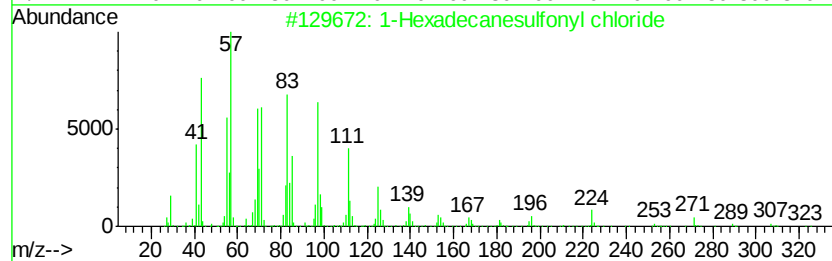
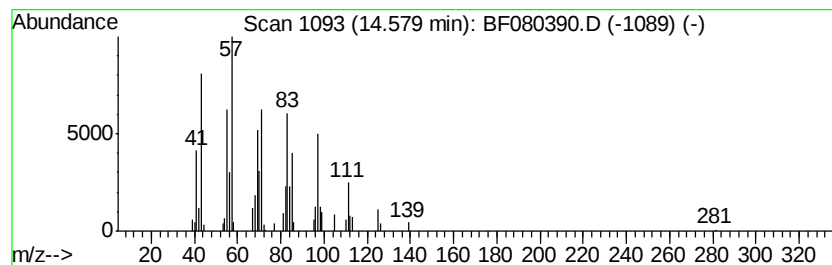
Instrument :
BNA_F
ClientSampleId :
RB3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexadecanesulfonyl chloride Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.58	7.50 ng	207272	Chrysene-d12	14.77		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	91
4		Pentafluoropropionic acid, octadecyl-	416	C21H37F5O2	1000280-07-7	87
5		Pentafluoropropionic acid, heptadecyl-	402	C20H35F5O2	1000283-04-2	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070815\
Data File : BF080390.D
Acq On : 8 Jul 2015 16:23
Operator : TP/UM
Sample : G2905-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB3

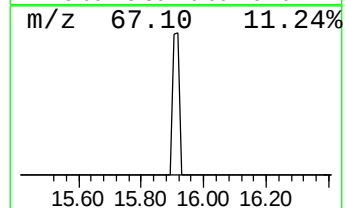
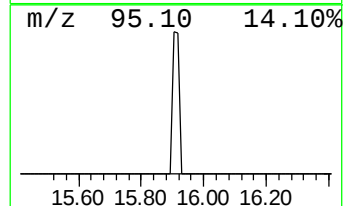
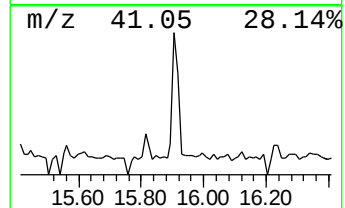
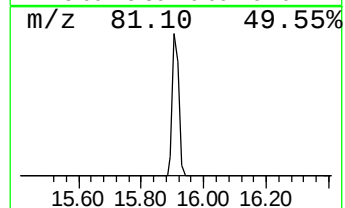
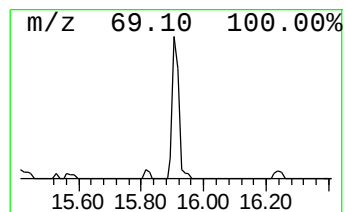
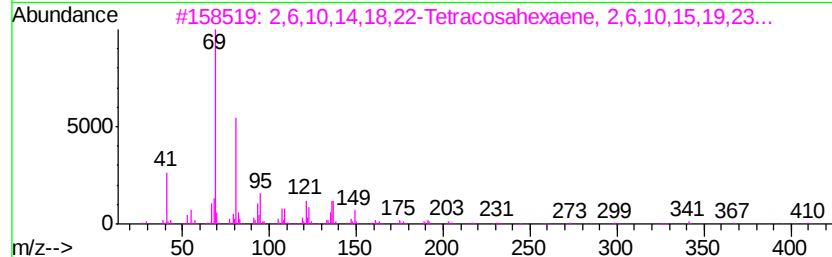
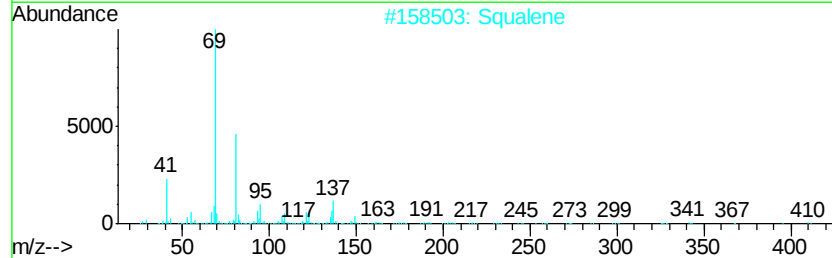
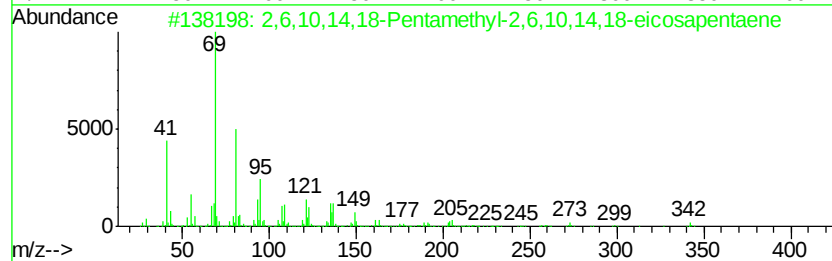
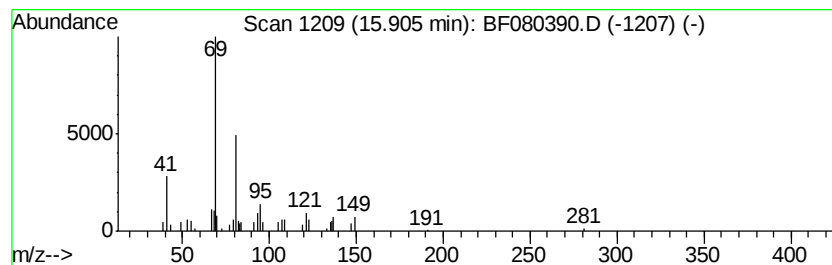
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,6,10,14,18-Pentamethyl-2,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.41 ng	48584	Perylene-d12	16.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	72		
2	Squalene	410	C30H50	007683-64-9	72		
3	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	64		
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	64		
5	1-Hexadecyn-3-ol, 3,7,11,15-tetr...	294	C20H38O	029171-23-1	64		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070815\
Data File : BF080390.D
Acq On : 8 Jul 2015 16:23
Operator : TP/UM
Sample : G2905-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.40	66.8	ng	812390	1	7.21	243371	20.0
3-Penten-2-one, 4...	4.81	2.5	ng	30967	1	7.21	243371	20.0
2-Pentanone, 4-hy...	5.40	12.4	ng	150663	1	7.21	243371	20.0
unknown6.21	6.21	3.1	ng	37301	1	7.21	243371	20.0
unknown6.97	6.97	51.5	ng	626615	1	7.21	243371	20.0
1-Hexadecanesulfo...	14.58	7.5	ng	207272	5	14.77	552863	20.0
2,6,10,14,18-Pent...	15.91	2.4	ng	48584	6	16.63	402723	20.0