

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
 Data File : BF096986.D
 Acq On : 24 Jul 2017 12:52
 Operator : SJ/JU
 Sample : I4370-02 5X
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-N6-BASE

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-BF071317.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	2.757	128	131	134	rBV	14021	21440	1.88%	0.161%
2	4.057	348	352	357	rBV3	10483	15187	1.34%	0.114%
3	4.681	455	458	465	rVB	46459	57528	5.06%	0.433%
4	5.081	522	526	534	rBV	21002	32006	2.81%	0.241%
5	5.146	534	537	547	rBV	593044	615646	54.13%	4.630%
6	6.098	695	699	703	rVB4	10721	13565	1.19%	0.102%
7	6.204	714	717	726	rBV	684760	664526	58.42%	4.997%
8	6.275	726	729	732	rVV	488454	391436	34.41%	2.944%
9	6.316	732	736	742	rVB	661049	613991	53.98%	4.617%
10	6.475	760	763	770	rVB	72534	68662	6.04%	0.516%
11	6.540	770	774	780	rVV	984923	977403	85.93%	7.350%
12	6.587	780	782	790	rVB	122547	111844	9.83%	0.841%
13	6.693	797	800	802	rBV	546897	633334	55.68%	4.763%
14	6.828	819	823	826	rBV2	49498	58968	5.18%	0.443%
15	6.869	828	830	834	rVB	26561	20995	1.85%	0.158%
16	6.993	847	851	857	rBV2	52595	74711	6.57%	0.562%
17	7.104	863	870	873	rBV	401487	401805	35.33%	3.022%
18	7.157	877	879	883	rVB	17100	15968	1.40%	0.120%
19	7.263	894	897	900	rVB	31611	26933	2.37%	0.203%
20	7.345	909	911	916	rVB3	12161	13950	1.23%	0.105%
21	7.510	932	939	944	rBV4	22819	48367	4.25%	0.364%
22	7.563	944	948	951	rBV4	11662	14491	1.27%	0.109%
23	7.598	951	954	956	rBV2	24631	22522	1.98%	0.169%
24	7.640	956	961	967	rVB	72388	118223	10.39%	0.889%
25	7.704	970	972	975	rVB	21702	15345	1.35%	0.115%
26	7.734	975	977	980	rBV3	23866	25697	2.26%	0.193%
27	7.769	980	983	986	rVB	147744	117825	10.36%	0.886%
28	7.822	987	992	995	rBV	1293672	1137407	100.00%	8.553%
29	7.987	1015	1020	1023	rBV	97206	97937	8.61%	0.736%
30	8.110	1039	1041	1048	rVB7	11594	15813	1.39%	0.119%
31	8.204	1051	1057	1062	rBV	51689	56258	4.95%	0.423%
32	8.298	1070	1073	1076	rVB	30729	28395	2.50%	0.214%
33	8.328	1076	1078	1083	rBV	50576	52740	4.64%	0.397%
34	8.475	1098	1103	1105	rBV3	15966	25665	2.26%	0.193%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
 Data File : BF096986.D
 Acq On : 24 Jul 2017 12:52
 Operator : SJ/JU
 Sample : I4370-02 5X
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-N6-BASE

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-BF071317.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	8.534	1109	1113	1117	rBV	97594	89531	7.87%	0.673%
36	8.598	1121	1124	1127	rBV5	16523	16997	1.49%	0.128%
37	8.634	1127	1130	1132	rBV	104830	81709	7.18%	0.614%
38	8.698	1137	1141	1144	rBV5	21965	35888	3.16%	0.270%
39	8.751	1148	1150	1152	rBV3	14514	13391	1.18%	0.101%
40	8.816	1156	1161	1164	rBV6	21846	46477	4.09%	0.349%
41	8.898	1171	1175	1178	rBV	799104	641341	56.39%	4.823%
42	8.957	1183	1185	1186	rBV	32719	24962	2.19%	0.188%
43	9.092	1206	1208	1213	rVB5	22915	35196	3.09%	0.265%
44	9.163	1217	1220	1222	rVB2	26009	27105	2.38%	0.204%
45	9.234	1229	1232	1235	rBV	45338	53402	4.70%	0.402%
46	9.257	1235	1236	1239	rVV2	32115	24767	2.18%	0.186%
47	9.298	1240	1243	1248	rVB	123922	115217	10.13%	0.866%
48	9.428	1263	1265	1268	rBV	32560	34240	3.01%	0.257%
49	9.569	1284	1289	1293	rBV2	1213693	1105306	97.18%	8.312%
50	9.998	1359	1362	1364	rVB	91086	79186	6.96%	0.595%
51	10.022	1364	1366	1369	rBV3	30151	25290	2.22%	0.190%
52	10.357	1419	1423	1431	rVB	325469	330323	29.04%	2.484%
53	11.045	1536	1540	1543	rBV	1095977	928421	81.63%	6.982%
54	11.598	1631	1634	1637	rBV2	106072	94430	8.30%	0.710%
55	12.298	1751	1753	1757	rVB5	36232	43701	3.84%	0.329%
56	12.380	1764	1767	1775	rVB	151803	146328	12.87%	1.100%
57	12.475	1781	1783	1786	rBV	40660	33320	2.93%	0.251%
58	12.627	1805	1809	1814	rVB	400250	386971	34.02%	2.910%
59	12.716	1822	1824	1827	rVB	32459	26467	2.33%	0.199%
60	13.174	1899	1902	1904	rBV	36678	34853	3.06%	0.262%
61	13.280	1918	1920	1923	rBV4	19099	25452	2.24%	0.191%
62	13.539	1962	1964	1970	rVB6	45207	52744	4.64%	0.397%
63	13.669	1982	1986	1993	rVB	659116	646764	56.86%	4.864%
64	14.463	2119	2121	2125	rVB4	36350	32908	2.89%	0.247%
65	14.663	2152	2155	2163	rVB	101120	155338	13.66%	1.168%
66	14.921	2196	2199	2204	rVB	104456	114643	10.08%	0.862%
67	14.974	2206	2208	2212	rVV	38206	53547	4.71%	0.403%
68	15.027	2214	2217	2224	rVB	475411	583775	51.33%	4.390%
69	15.568	2306	2309	2313	rVB5	54761	70750	6.22%	0.532%
70	15.627	2317	2319	2329	rVB5	34105	85306	7.50%	0.641%
71	16.280	2426	2430	2440	rVB2	76085	128236	11.27%	0.964%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

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-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.657	2489	2494	2503	rVB	63855	123436	10.85%	0.928%
73	16.768	2509	2513	2524	rVB	58326	143871	12.65%	1.082%

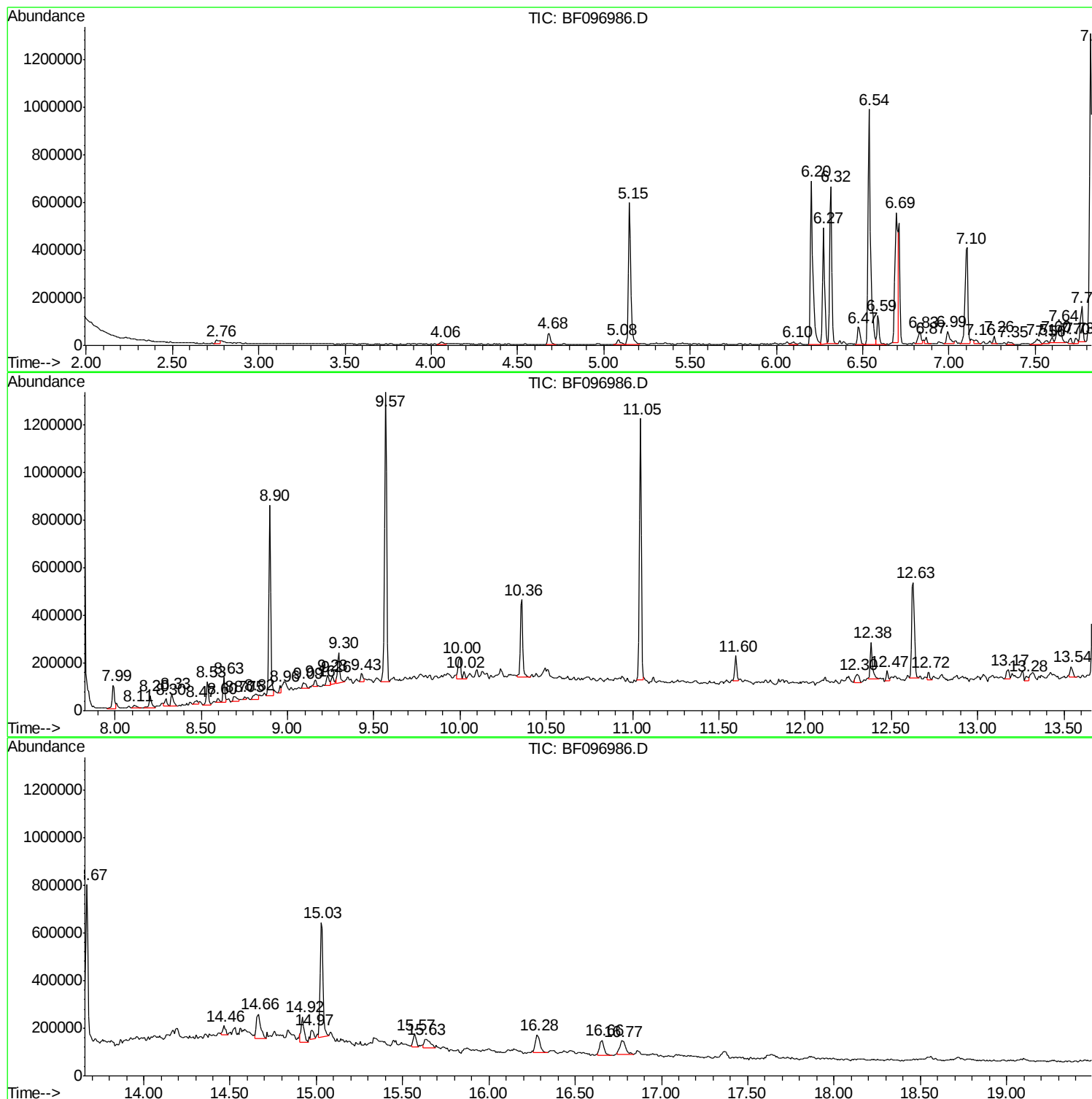
Sum of corrected areas: 13298172

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

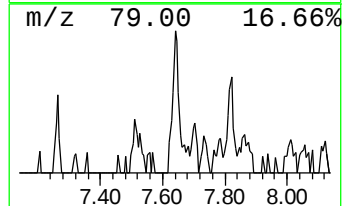
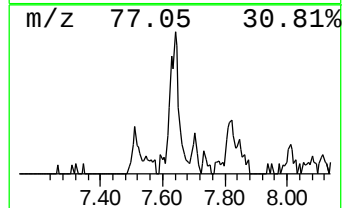
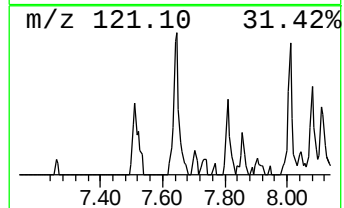
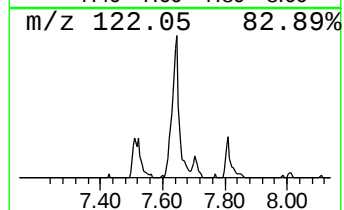
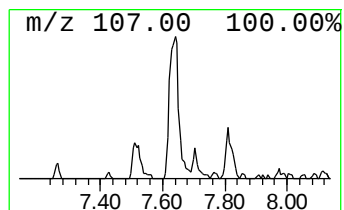
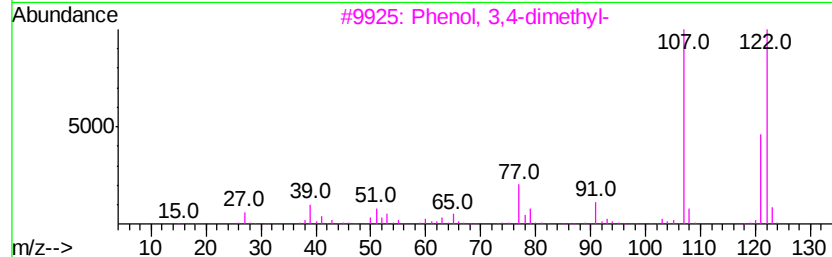
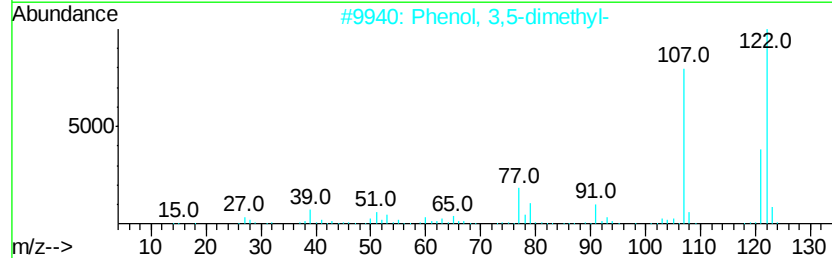
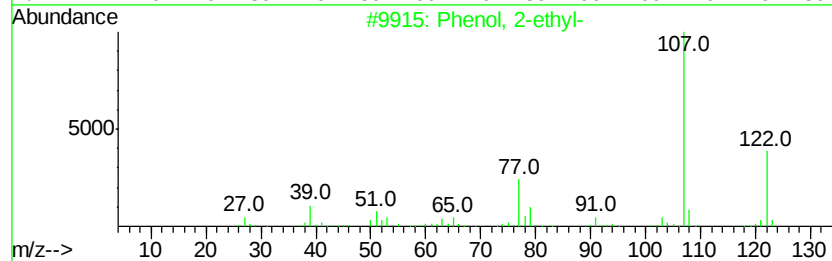
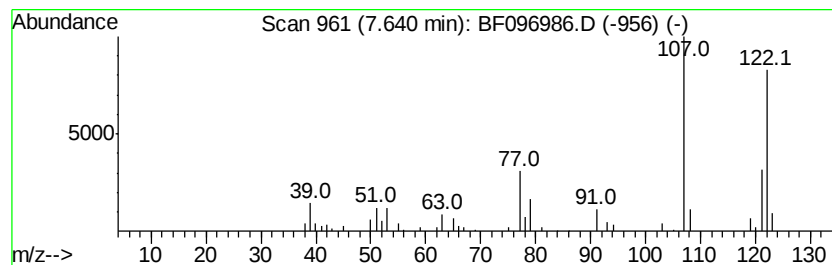
Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Phenol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	2.08 ng	118223	Napthalene-d8	7.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phenol, 2-ethyl-	122	C8H10O	000090-00-6 91
2	Phenol, 3,5-dimethyl-	122	C8H10O	000108-68-9 91
3	Phenol, 3,4-dimethyl-	122	C8H10O	000095-65-8 91
4	Phenol, 2,4-dimethyl-	122	C8H10O	000105-67-9 90
5	Phenol, 2,3-dimethyl-	122	C8H10O	000526-75-0 90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

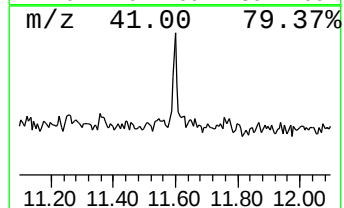
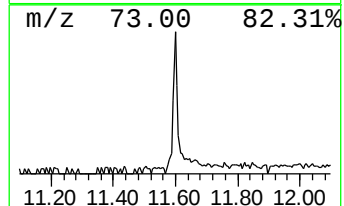
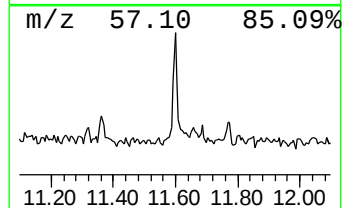
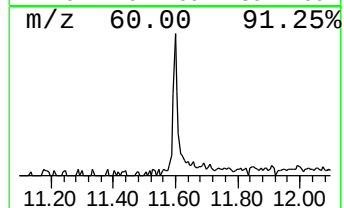
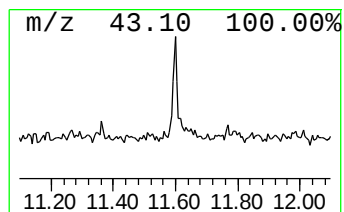
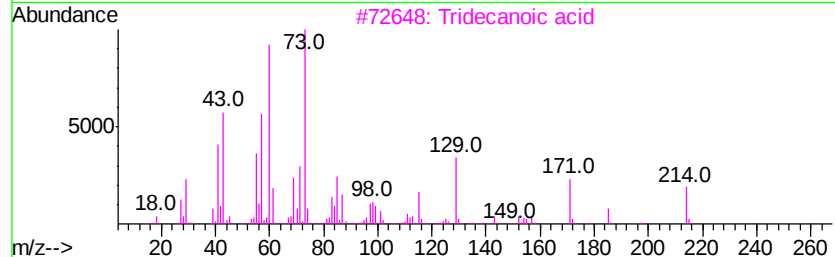
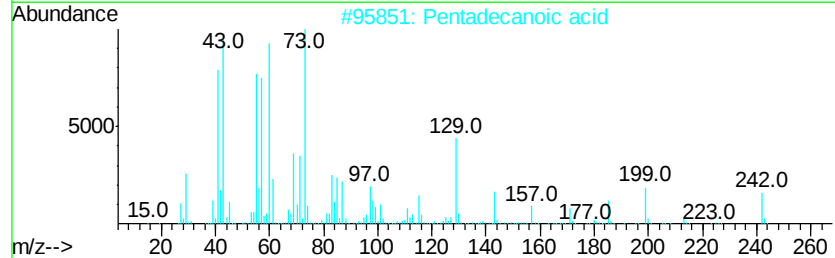
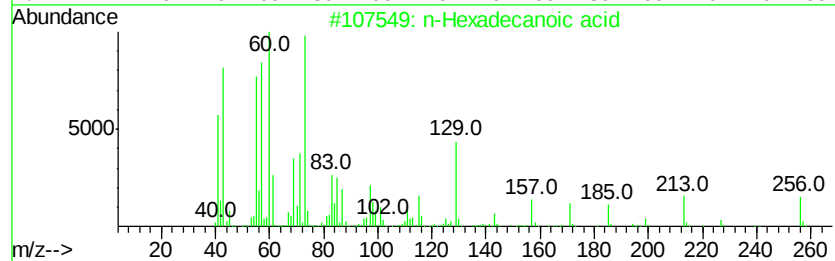
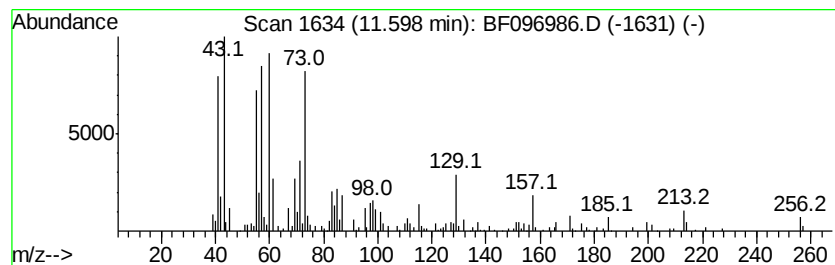
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	2.03 ng	94430	Phenanthrene-d10	11.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		Dodecanoic acid	200	C12H24O2	000143-07-7	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

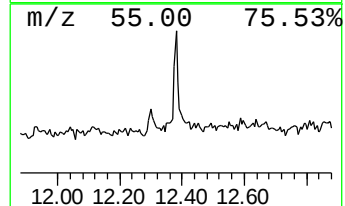
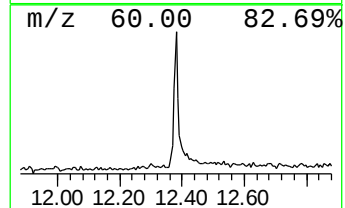
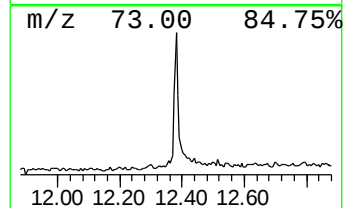
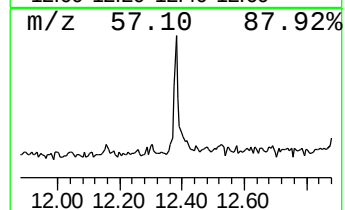
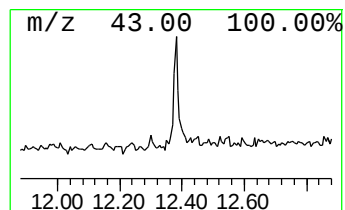
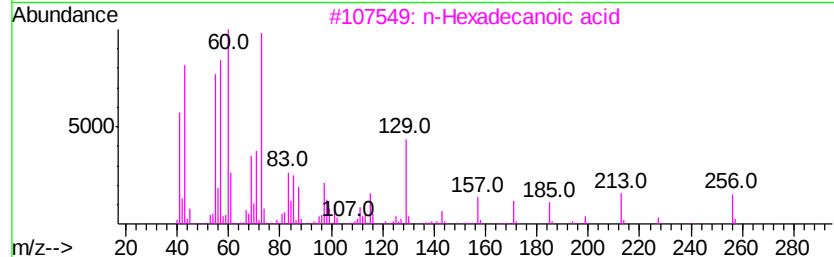
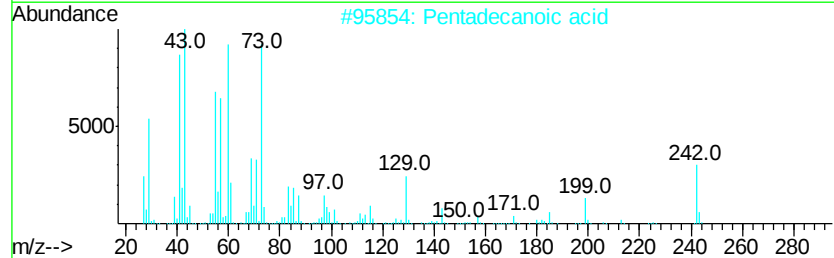
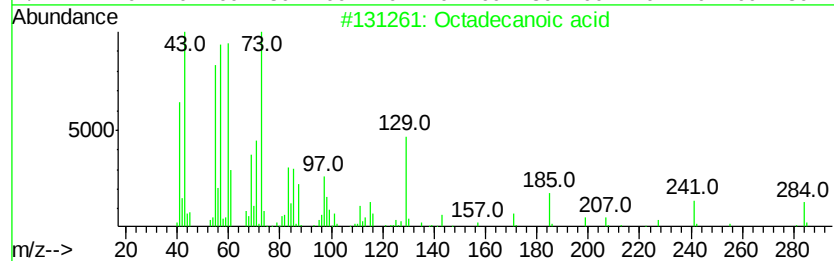
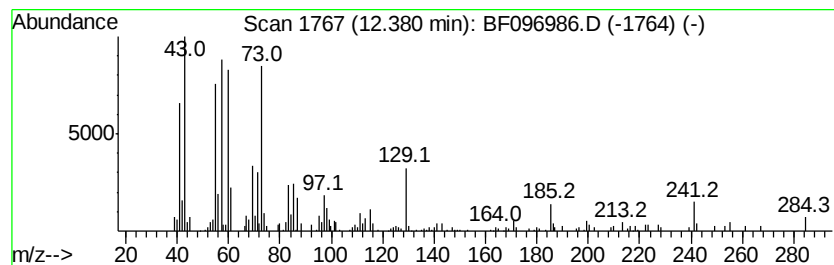
Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.38	4.52 ng	146328	Chrysene-d12		13.67	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

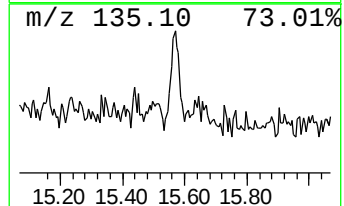
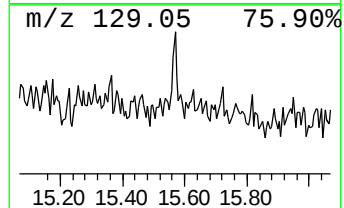
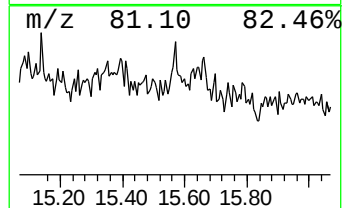
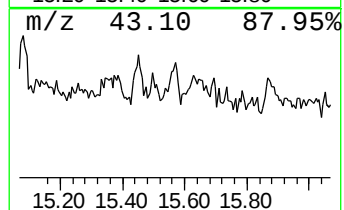
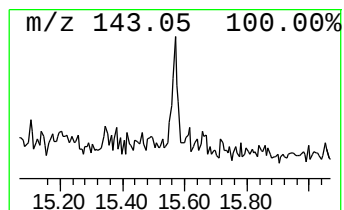
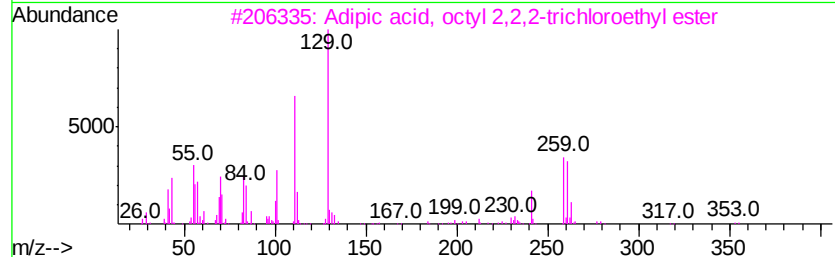
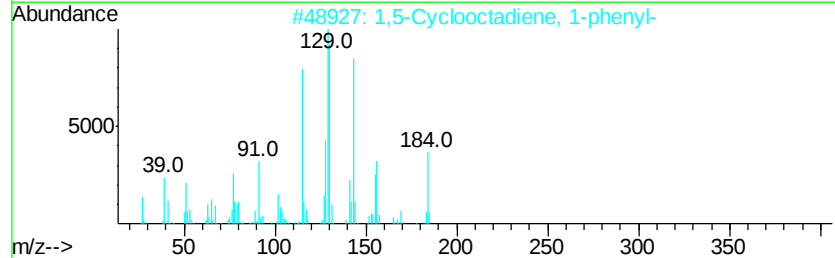
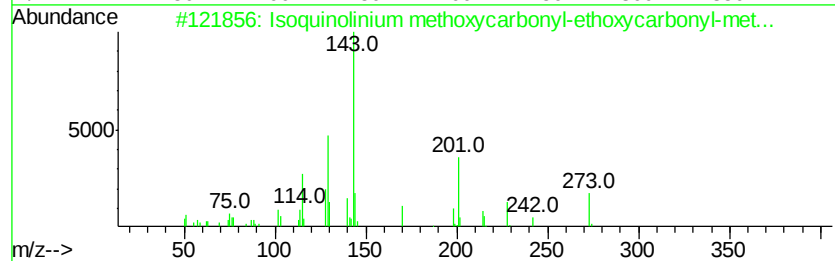
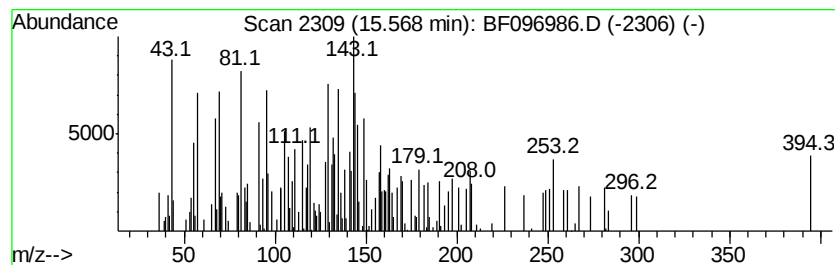
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown15.57 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.42 ng	70750	Perylene-d12	15.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isoquinolinium methoxycarbonyl-e...	273	C15H15N04	1000146-40-5	35
2		1,5-Cyclooctadiene, 1-phenyl-	184	C14H16	016538-84-4	27
3		Adipic acid, octyl 2,2,2-trichlo...	388	C16H27Cl3O4	1000353-48-0	14
4		Thiophene, 2-nitro-	129	C4H3NO2S	000609-40-5	10
5		Adipic acid, nonyl 2,2,2-trichlo...	402	C17H29Cl3O4	1000353-48-1	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

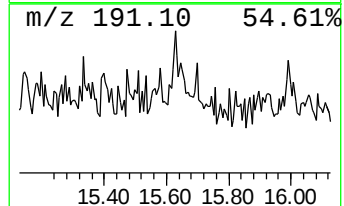
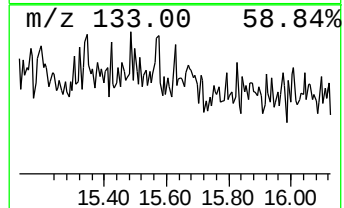
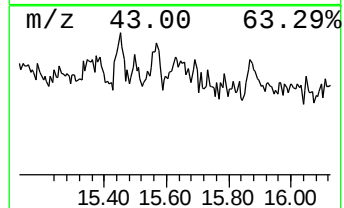
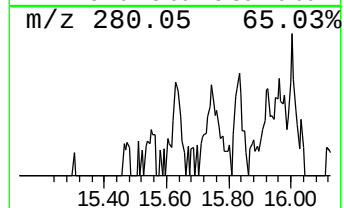
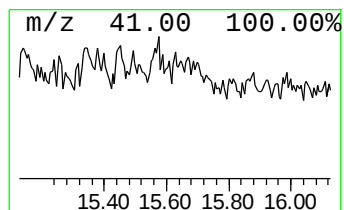
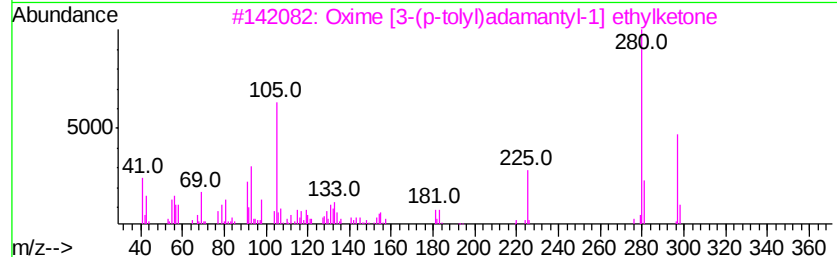
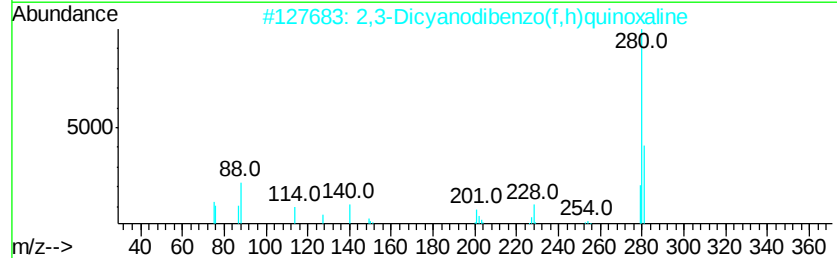
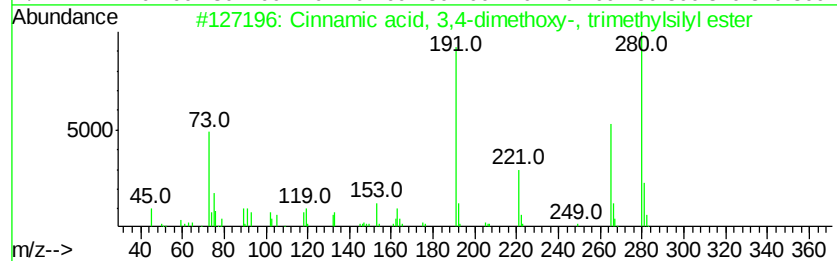
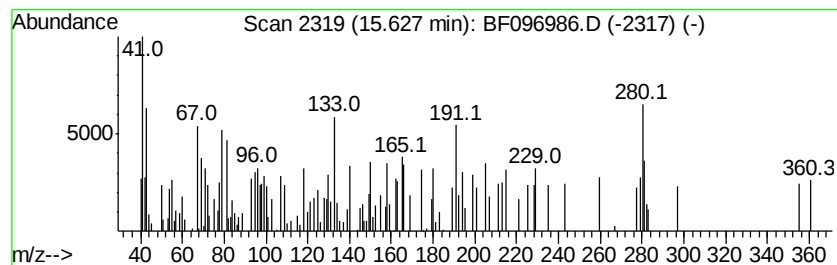
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	2.92 ng	85306	Perylene-d12	15.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cinnamic acid, 3,4-dimethoxy-, t...	280	C14H20O4Si	027750-71-6	22
2		2,3-Dicyanodibenzo(f,h)quinoxaline	280	C18H8N4	055408-49-6	14
3		Oxime [3-(p-tolyl)adamantyl-1] e...	297	C20H27NO	1000140-84-9	14
4		Benzo[al]cyclopropa[cd]pentalene-...	398	C26H22O4	040897-27-6	12
5		Anisole, 2,3,4,5,6-pentachloro-	278	C7H3Cl5O	001825-21-4	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

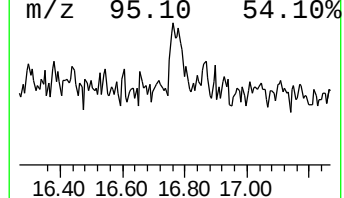
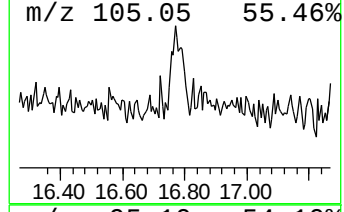
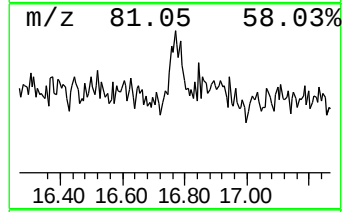
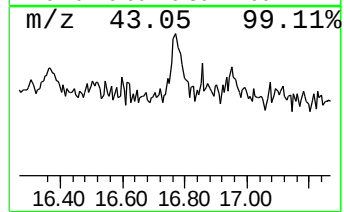
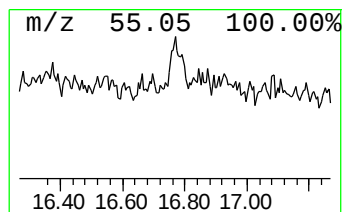
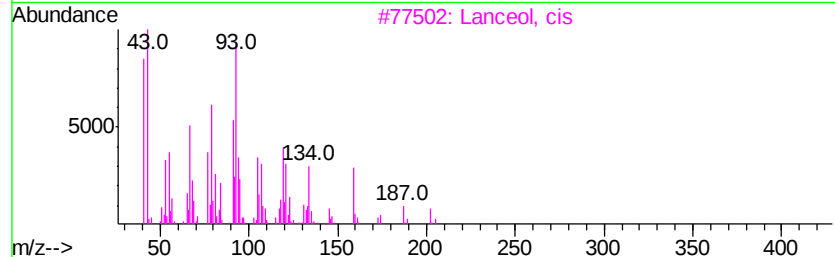
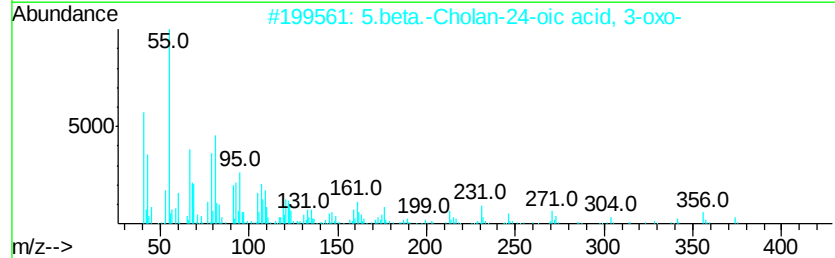
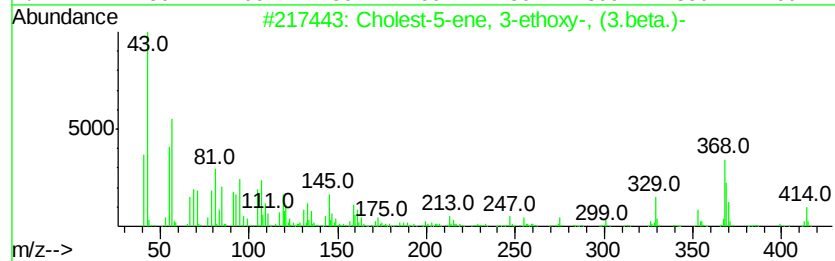
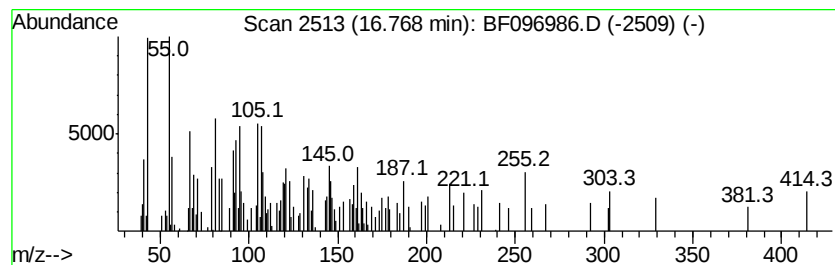
Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cholest-5-ene, 3-ethoxy-, (... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	4.93 ng	143871	Perylene-d12	15.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cholest-5-ene, 3-ethoxy-, (3.beta...	414 C29H500	000986-19-6 50
2		5.beta.-Cholan-24-oic acid, 3-oxo-	374 C24H3803	001553-56-6 38
3		Lanceol, cis	220 C15H240	010067-28-4 12
4		5.alpha.-Pregnane-3.beta.,20.bet...	362 C23H3803	017182-23-9 10
5		5-Methoxy-2,2,6-trimethyl-1-(3-m...	236 C15H2402	1000194-09-1 10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072417\
Data File : BF096986.D
Acq On : 24 Jul 2017 12:52
Operator : SJ/JU
Sample : I4370-02 5X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
E2-N6-BASE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Phenol, 2-ethyl-	7.64	2.1 ng		118223	2	7.82	1137410	20.0
n-Hexadecanoic acid	11.60	2.0 ng		94430	4	11.05	928421	20.0
Octadecanoic acid	12.38	4.5 ng		146328	5	13.67	646764	20.0
unknown15.57	15.57	2.4 ng		70750	6	15.03	583775	20.0
unknown15.63	15.63	2.9 ng		85306	6	15.03	583775	20.0
Cholest-5-ene, 3-...	16.77	4.9 ng		143871	6	15.03	583775	20.0