

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
 Data File : BF114068.D
 Acq On : 1 May 2019 14:47
 Operator : JU/SJ
 Sample : K2191-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P-66-TP

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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	2.140	4	9	14	rVB	35418	47403	2.17%	0.228%
2	5.522	579	584	598	rVB	1711954	1677557	76.79%	8.058%
3	6.445	737	741	747	rBV	35722	35664	1.63%	0.171%
4	6.528	750	755	771	rVB	2211135	1961040	89.77%	9.420%
5	6.669	775	779	782	rBV	2267568	1883458	86.22%	9.048%
6	6.898	814	818	821	rBV	819385	652991	29.89%	3.137%
7	7.057	841	845	848	rBV	1572200	1401907	64.17%	6.734%
8	7.457	908	913	923	rBV	1043415	1059581	48.50%	5.090%
9	8.181	1032	1036	1043	rBV	746256	677414	31.01%	3.254%
10	9.075	1182	1188	1192	rBV7	11313	27066	1.24%	0.130%
11	9.133	1193	1198	1203	rVV	39243	70463	3.23%	0.338%
12	9.251	1215	1218	1225	rBV	2374522	2184558	100.00%	10.494%
13	9.333	1230	1232	1239	rBV7	29962	47801	2.19%	0.230%
14	9.392	1239	1242	1246	rBV	66934	65152	2.98%	0.313%
15	9.639	1282	1284	1289	rVB	238432	218343	9.99%	1.049%
16	9.798	1309	1311	1315	rBV4	17615	24351	1.11%	0.117%
17	9.851	1317	1320	1325	rVB2	52623	58527	2.68%	0.281%
18	9.933	1331	1334	1339	rVB	1105631	992185	45.42%	4.766%
19	10.622	1449	1451	1457	rVB6	20367	37069	1.70%	0.178%
20	10.722	1464	1468	1472	rBV	1416453	1421030	65.05%	6.826%
21	10.839	1486	1488	1492	rVB3	30960	37473	1.72%	0.180%
22	10.951	1504	1507	1510	rBV3	23591	34514	1.58%	0.166%
23	11.016	1514	1518	1521	rBV	46102	54816	2.51%	0.263%
24	11.133	1537	1538	1541	rBV3	21710	27288	1.25%	0.131%
25	11.422	1583	1587	1593	rBV	1075326	978887	44.81%	4.702%
26	11.710	1633	1636	1640	rVB4	45201	54120	2.48%	0.260%
27	11.945	1673	1676	1680	rBV	350638	302941	13.87%	1.455%
28	11.975	1680	1681	1683	rVB2	46013	26092	1.19%	0.125%
29	12.727	1807	1809	1814	rBV5	65257	79466	3.64%	0.382%
30	13.004	1852	1856	1860	rBV	2006077	1796230	82.22%	8.629%
31	13.692	1971	1973	1976	rBV2	85960	75595	3.46%	0.363%
32	13.927	2008	2013	2022	rBV3	163153	436953	20.00%	2.099%
33	14.074	2034	2038	2044	rBV	756887	767147	35.12%	3.685%
34	15.580	2290	2294	2302	rVB	438183	659106	30.17%	3.166%

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-66-TP

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.915	2517	2521	2524	rBV5	111712	203988	9.34%	0.980%
36	17.304	2584	2587	2594	rBV7	126206	220058	10.07%	1.057%
37	17.604	2636	2638	2641	rBV3	91143	65668	3.01%	0.315%
38	17.927	2692	2693	2696	rBV3	88858	51141	2.34%	0.246%
39	18.174	2733	2735	2740	rBV5	101546	172081	7.88%	0.827%
40	18.386	2769	2771	2774	rVB2	108081	64158	2.94%	0.308%
41	18.568	2800	2802	2809	rVB6	109797	166113	7.60%	0.798%

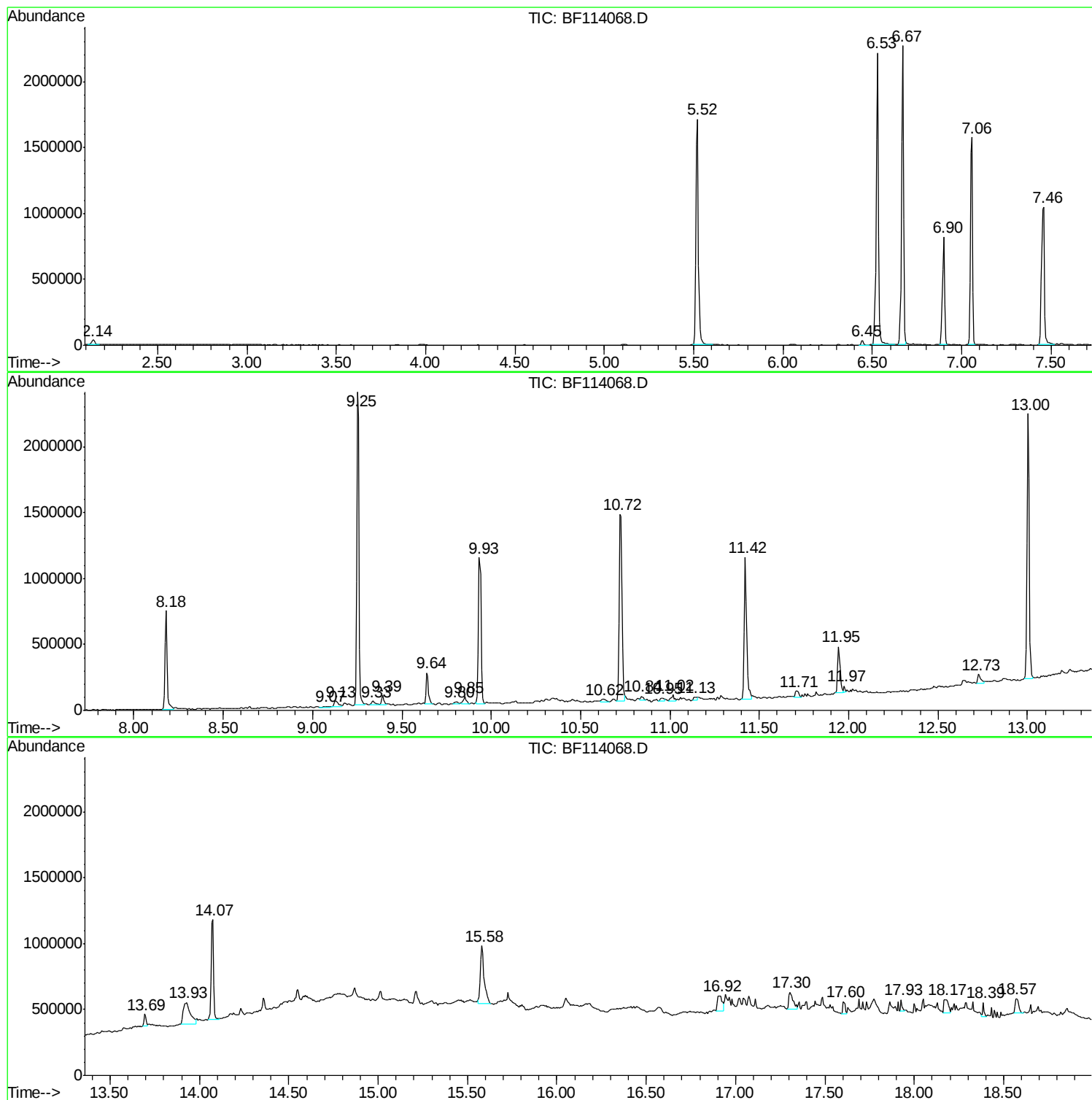
Sum of corrected areas: 20817395

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
P-66-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-66-TP

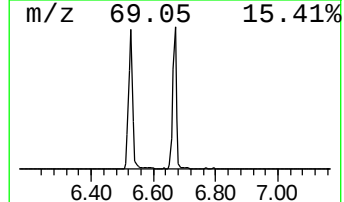
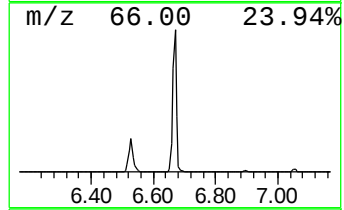
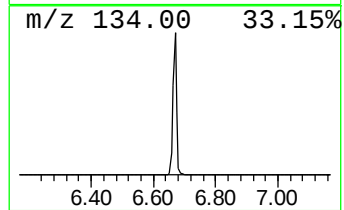
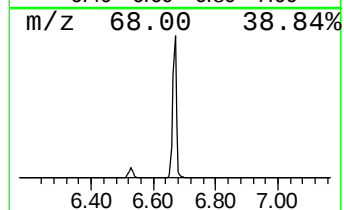
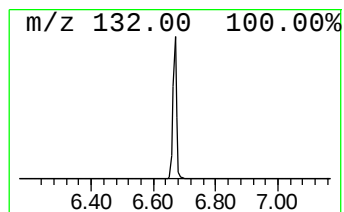
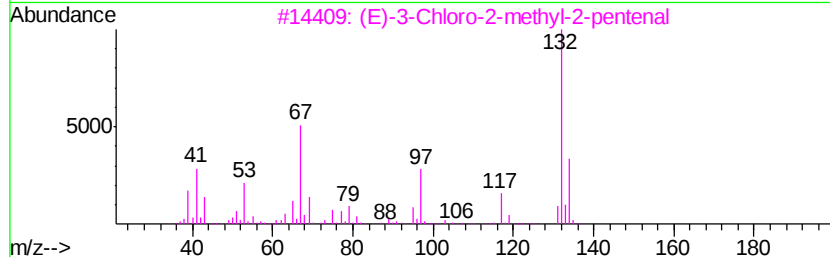
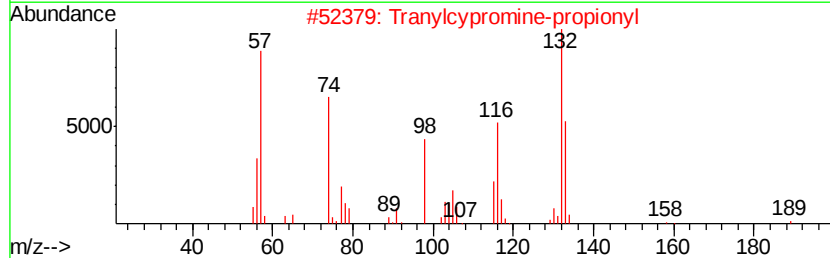
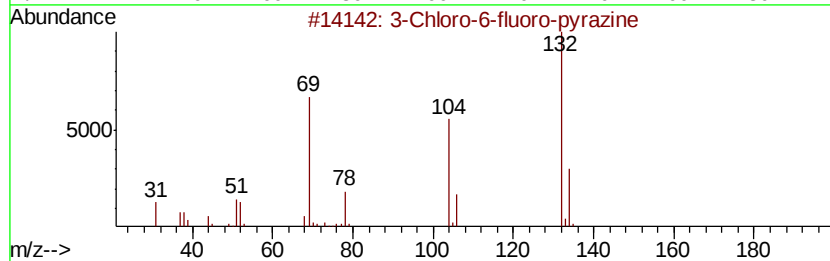
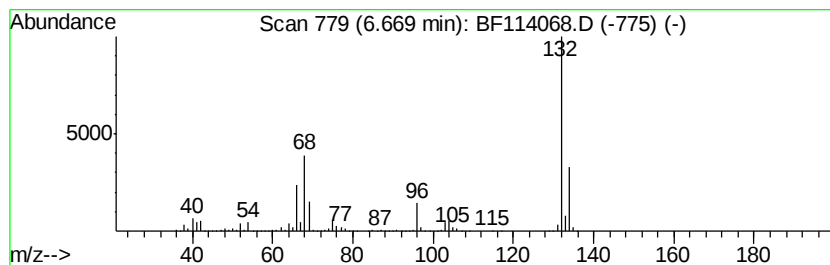
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	57.69 ng	1883460	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

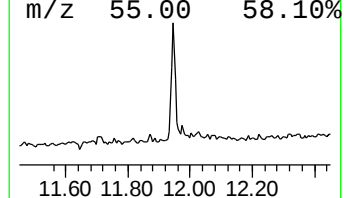
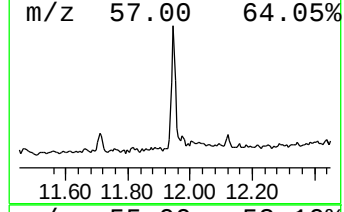
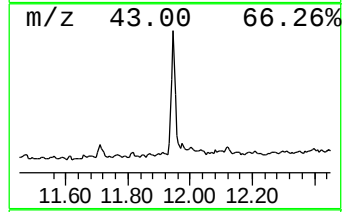
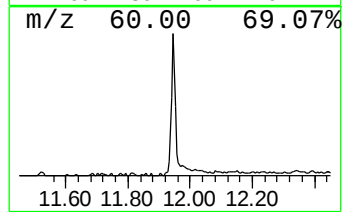
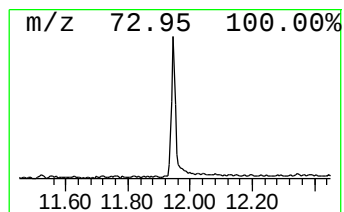
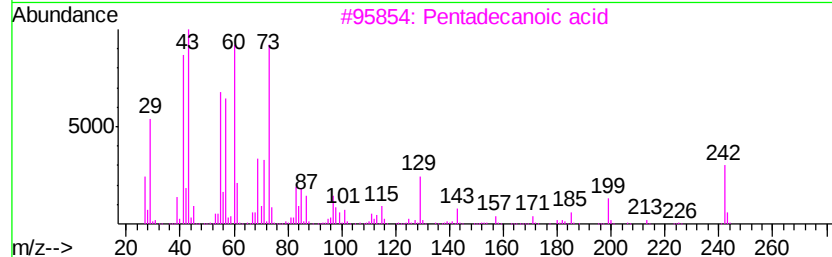
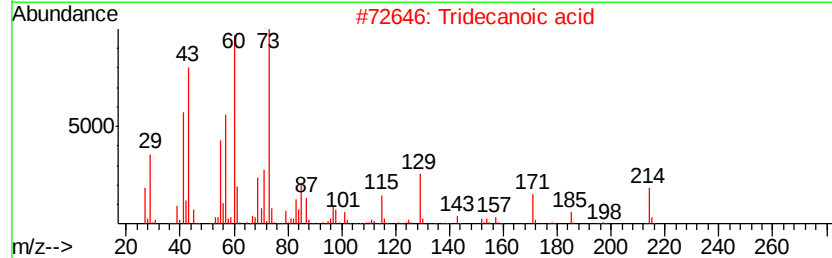
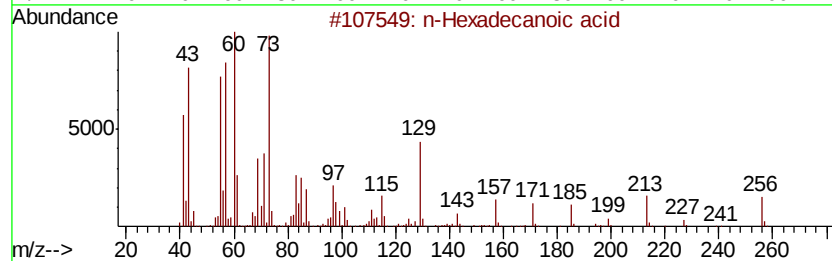
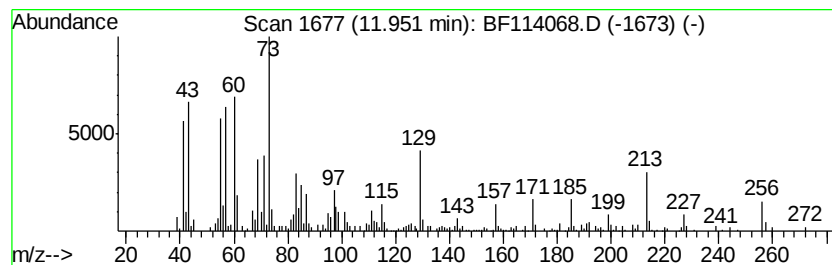
Instrument :
BNA_F
ClientSampleId :
P-66-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.95	6.19 ng	302941	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Hexadecane	226	C16H34	000544-76-3	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-66-TP

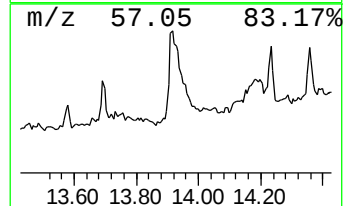
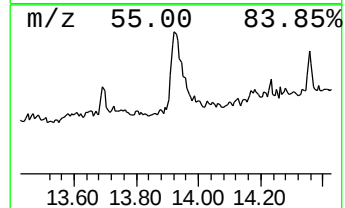
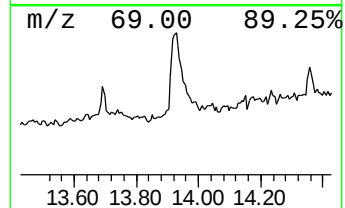
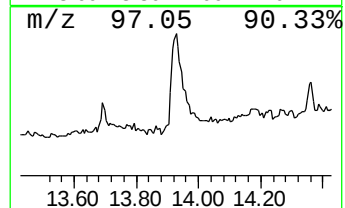
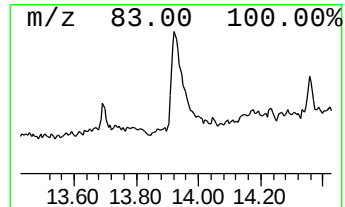
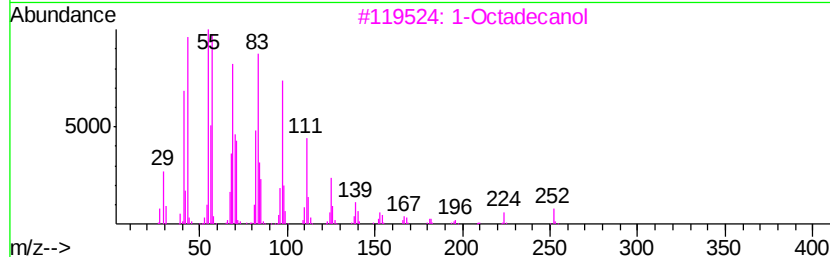
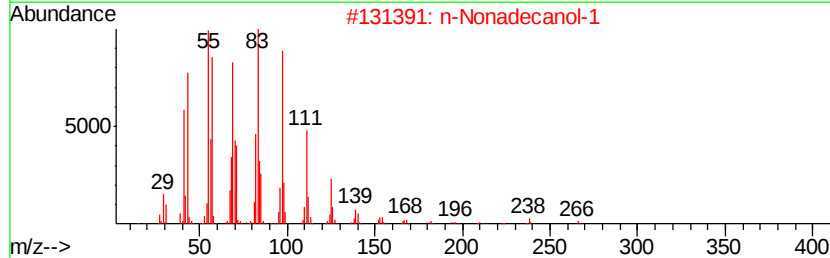
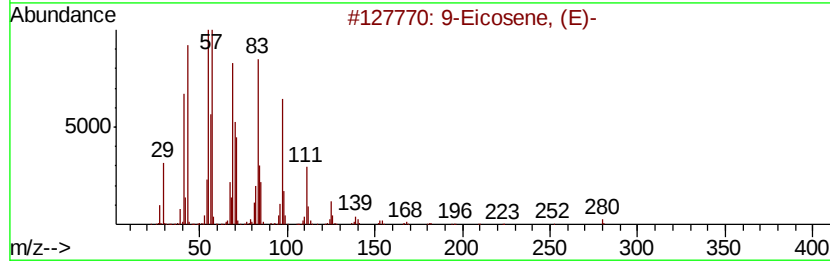
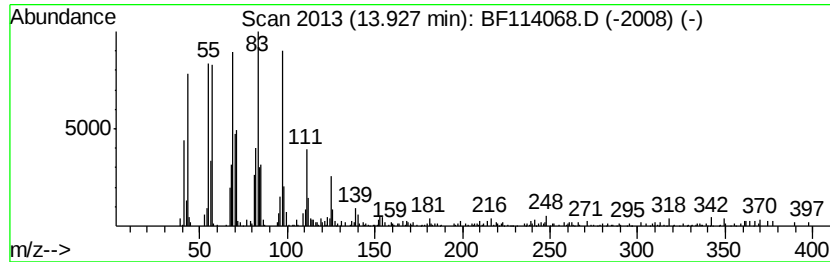
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 9-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	11.39 ng	436953	Chrysene-d12	14.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Eicosene, (E)-	280	C20H40	074685-29-3	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3		1-Octadecanol	270	C18H38O	000112-92-5	94
4		Behenic alcohol	326	C22H46O	000661-19-8	93
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-66-TP

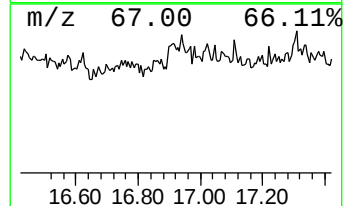
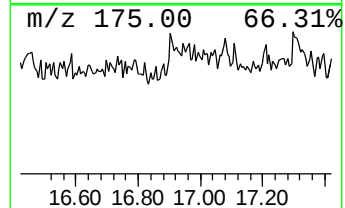
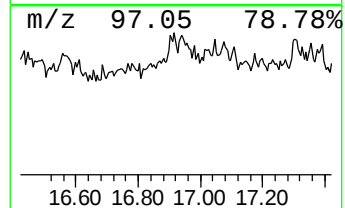
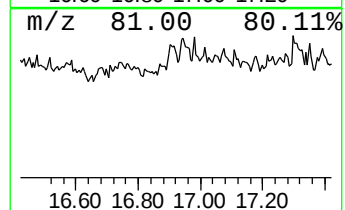
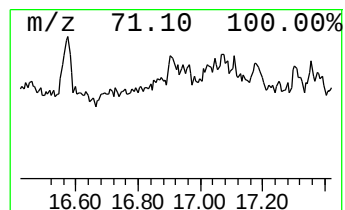
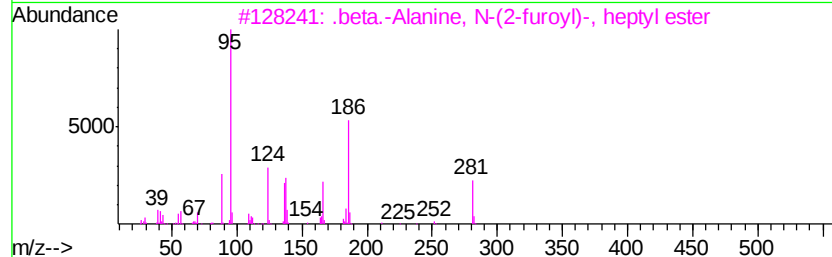
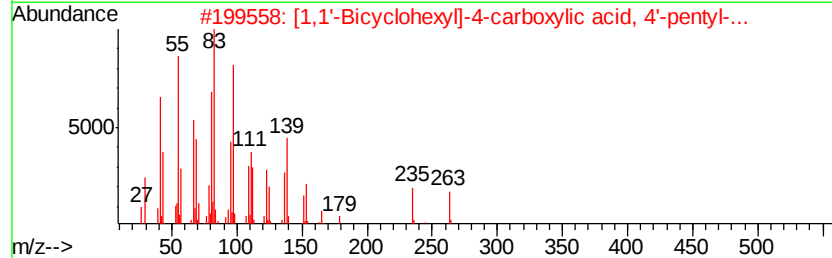
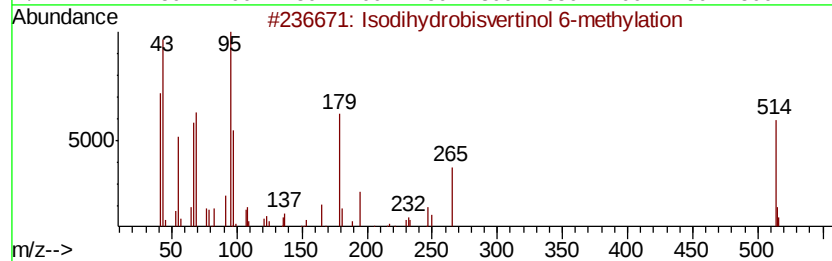
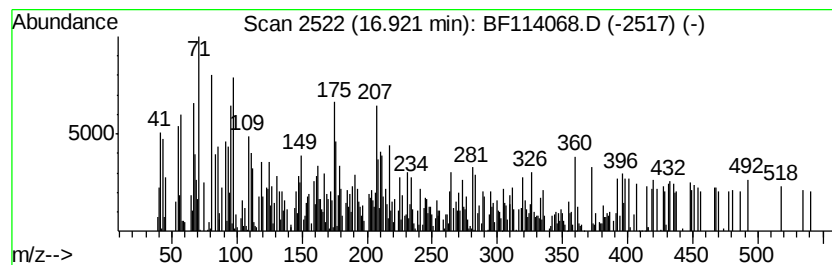
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown16.92 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.92	6.19 ng	203988	Perylene-d12	15.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isodihydrobisvertinol 6-methylation	514	C29H38O8	1000145-05-7	38
2		[1,1'-Bicyclohexyl]-4-carboxylic...	374	C24H35FO2	088878-50-6	35
3		.beta.-Alanine, N-(2-furoyl)-, h...	281	C15H23NO4	1000321-97-7	20
4		Propanamide, 3-(5-methylfuryl)-N...	263	C14H14ClNO2	307540-63-2	20
5		1-Bromo-11-iodoundecane	360	C11H22BrI	139123-69-6	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-66-TP

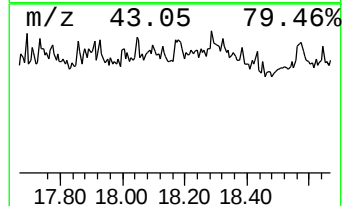
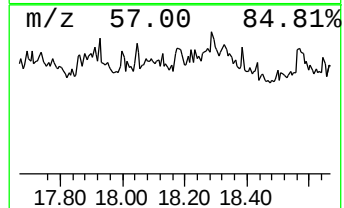
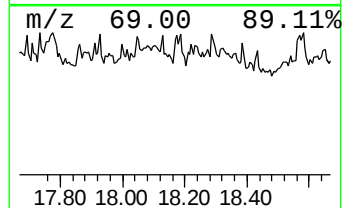
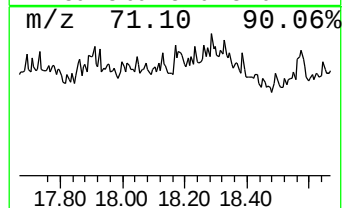
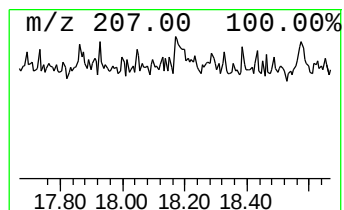
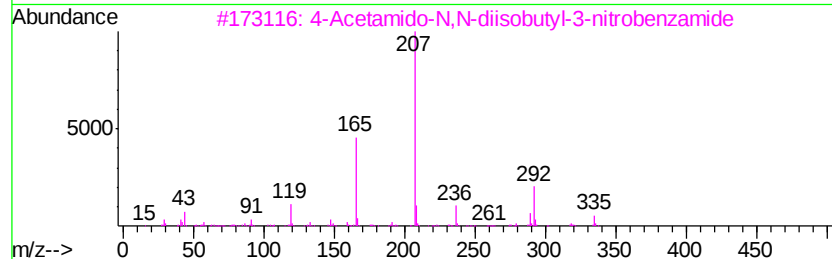
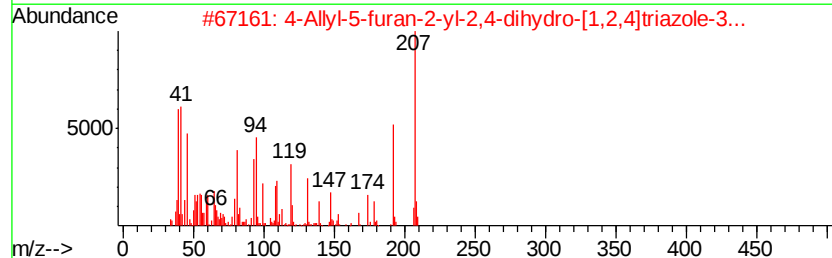
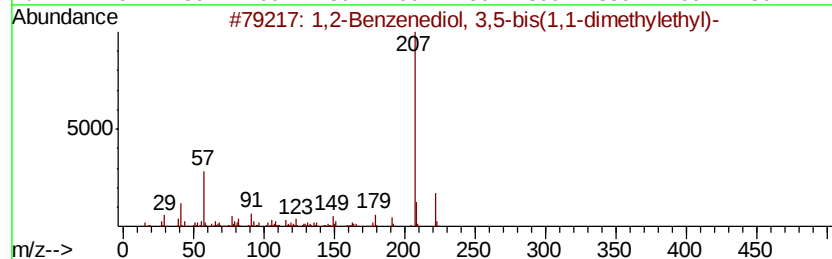
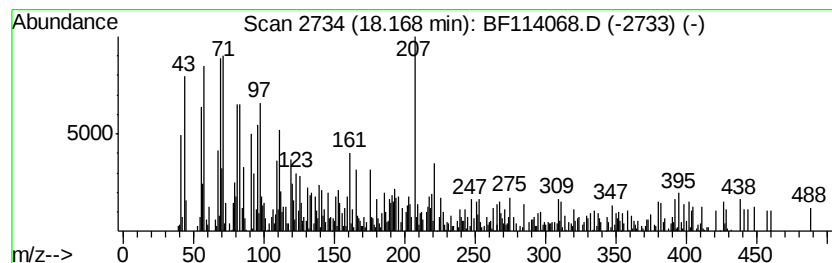
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown18.17 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.17	5.22 ng	172081	Perylene-d12	15.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenediol, 3,5-bis(1,1-dim...	222	C14H22O2	001020-31-1	46
2		4-Allyl-5-furan-2-yl-2,4-dihydro...	207	C9H9N3OS	1000300-01-3	46
3		4-Acetamido-N,N-diisobutyl-3-nit...	335	C17H25N3O4	093993-07-8	41
4		Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	41
5		N-Methyl-1-adamantaneacetamide	207	C13H21NO	031897-93-5	41



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

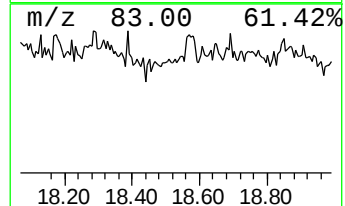
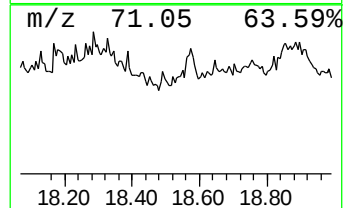
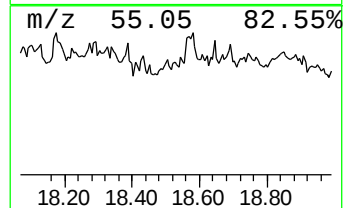
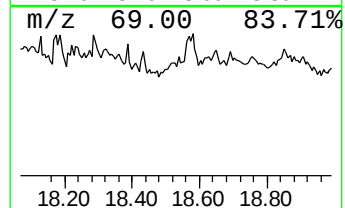
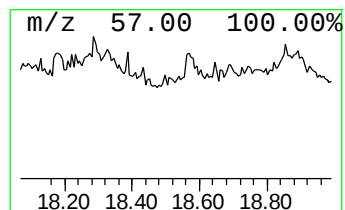
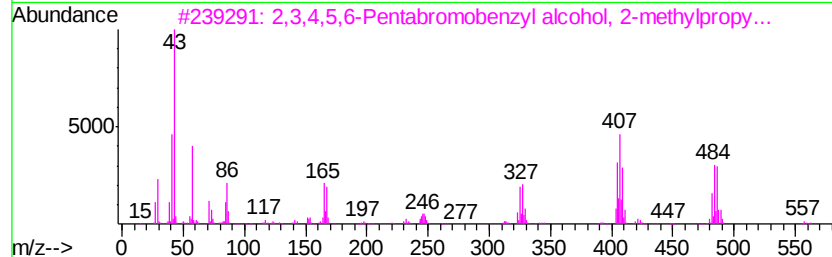
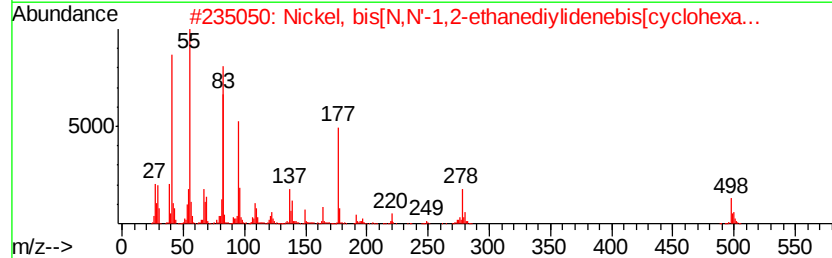
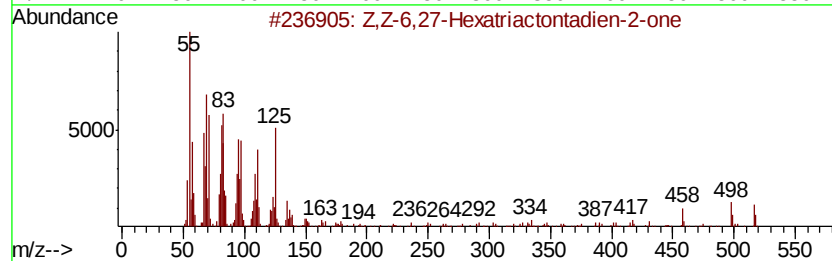
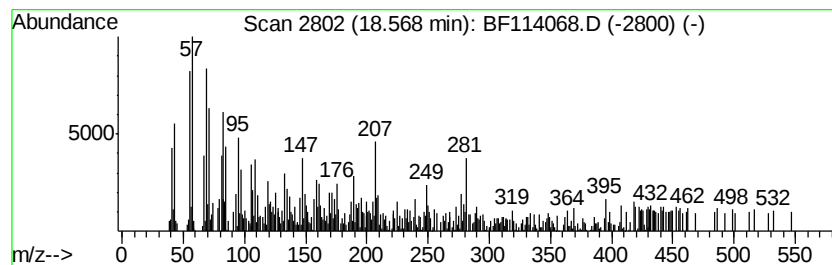
Instrument :
BNA_F
ClientSampleId :
P-66-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.57 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	5.04 ng	166113	Perylene-d12	15.58
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Z,Z-6,27-Hexatriactontadien-2-one	517 C36H68O	133530-19-5 10
2		Nickel, bis[N,N'-1,2-ethanedivli...	498 C28H48N4Ni	063576-86-3 10
3		2,3,4,5,6-Pentabromobenzvl alcoh...	554 C11H11Br5O	1000375-31-7 10
4		2,3,4,5,6-Pentabromobenzvl alcoh...	540 C10H9Br5O	1000375-31-6 9
5		2,3,4,5,6-Pentabromobenzyl alcoh...	568 C12H13Br5O	1000375-31-3 7



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF050119\
Data File : BF114068.D
Acq On : 1 May 2019 14:47
Operator : JU/SJ
Sample : K2191-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-66-TP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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
unknown6.67	6.67	57.7	ng	1883460	1	6.90	652991	20.0
n-Hexadecanoic acid	11.95	6.2	ng	302941	4	11.42	978887	20.0
9-Eicosene, (E)-	13.93	11.4	ng	436953	5	14.07	767147	20.0
unknown16.92	16.92	6.2	ng	203988	6	15.58	659106	20.0
unknown18.17	18.17	5.2	ng	172081	6	15.58	659106	20.0
unknown18.57	18.57	5.0	ng	166113	6	15.58	659106	20.0