

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
 Data File : BF117994.D
 Acq On : 26 Nov 2019 4:33
 Operator : JU
 Sample : K5999-03 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 IDLEWILD-BH-03A

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-BF111319.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	2.163	8	13	25	rVB	404696	504474	32.71%	2.706%
2	5.093	507	511	519	rVB	265378	268299	17.40%	1.439%
3	5.498	576	580	584	rBV	1405559	1333658	86.49%	7.155%
4	6.516	748	753	764	rBV	1581547	1477330	95.80%	7.926%
5	6.657	773	777	781	rBV	1828018	1542055	100.00%	8.273%
6	6.893	813	817	820	rBV	1197948	957297	62.08%	5.136%
7	7.045	840	843	847	rBV	1390660	1214155	78.74%	6.514%
8	7.451	908	912	915	rBV	1114568	884641	57.37%	4.746%
9	8.181	1032	1036	1039	rBV	1523309	1239181	80.36%	6.648%
10	9.257	1215	1219	1222	rBV	1788368	1381184	89.57%	7.410%
11	9.492	1256	1259	1262	rVB	29625	25936	1.68%	0.139%
12	9.598	1273	1277	1280	rBV	295979	224482	14.56%	1.204%
13	9.651	1282	1286	1290	rVB	202225	163133	10.58%	0.875%
14	9.775	1305	1307	1309	rBV	26282	21386	1.39%	0.115%
15	9.798	1309	1311	1314	rVB	28402	27913	1.81%	0.150%
16	9.945	1331	1336	1338	rBV	1201219	1181910	76.65%	6.341%
17	10.563	1438	1441	1445	rBV	36334	29139	1.89%	0.156%
18	10.692	1457	1463	1464	rBV3	22517	19408	1.26%	0.104%
19	10.733	1464	1470	1473	rVV2	815852	969588	62.88%	5.202%
20	11.198	1546	1549	1552	rVB	36334	29638	1.92%	0.159%
21	11.375	1576	1579	1584	rBV6	13729	20897	1.36%	0.112%
22	11.433	1585	1589	1592	rVV	1085307	929219	60.26%	4.985%
23	11.457	1592	1593	1597	rVV	94573	65238	4.23%	0.350%
24	11.510	1599	1602	1605	rVB	33021	25470	1.65%	0.137%
25	11.663	1625	1628	1633	rBV5	16145	29382	1.91%	0.158%
26	11.957	1675	1678	1683	rVB2	167374	159998	10.38%	0.858%
27	12.051	1692	1694	1698	rBV	31908	34323	2.23%	0.184%
28	12.651	1793	1796	1799	rBV	201264	186046	12.06%	0.998%
29	12.745	1809	1812	1817	rVB2	89243	125666	8.15%	0.674%
30	12.880	1833	1835	1838	rVB	196444	159587	10.35%	0.856%
31	13.022	1856	1859	1863	rBV	1272413	1153069	74.77%	6.186%
32	14.063	2033	2036	2037	rBV	187131	194376	12.60%	1.043%
33	14.086	2037	2040	2043	rVB	1101633	975782	63.28%	5.235%
34	15.592	2292	2296	2313	rVB	697108	1086265	70.44%	5.828%

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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
IDLEWILD-BH-03A

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-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

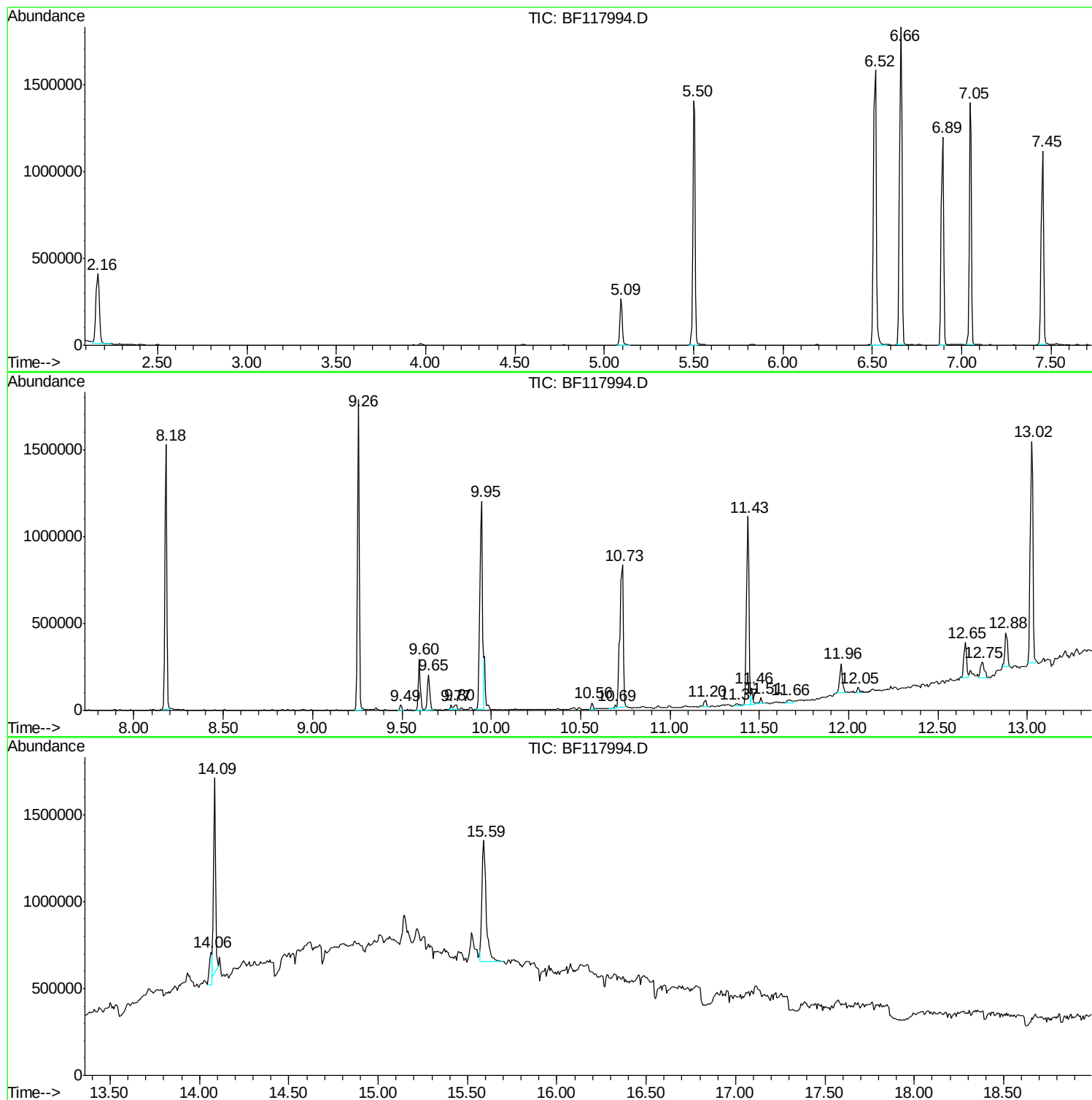
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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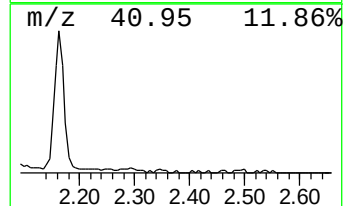
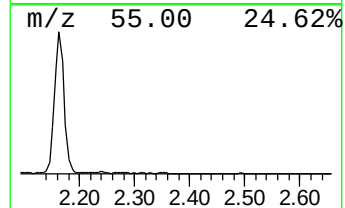
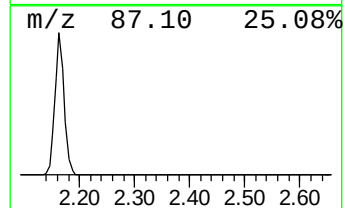
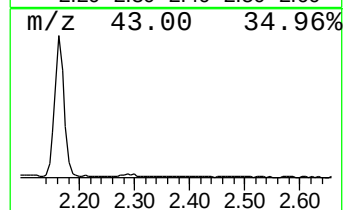
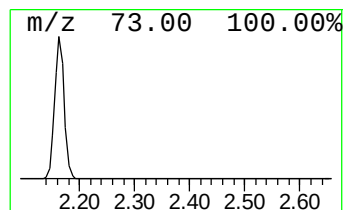
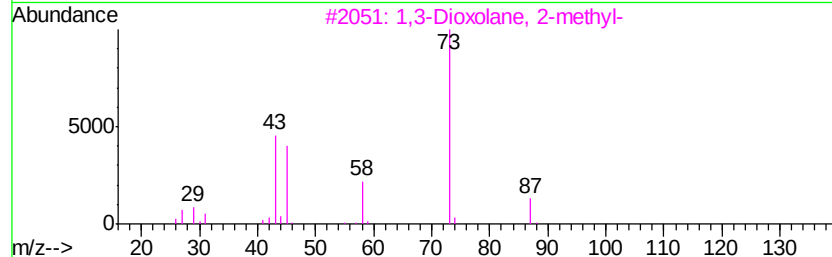
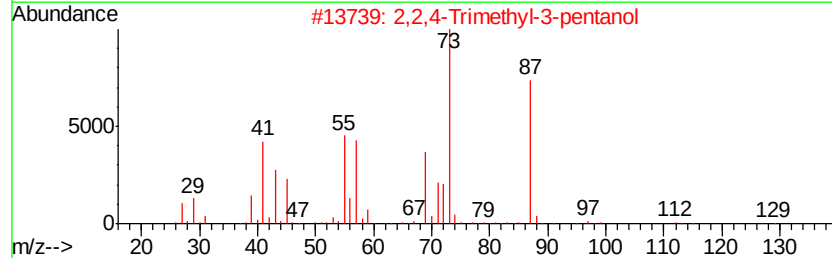
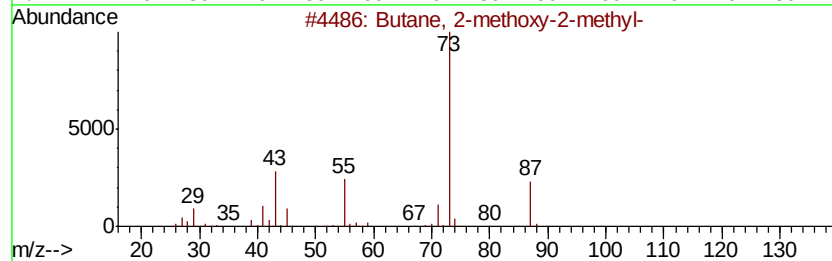
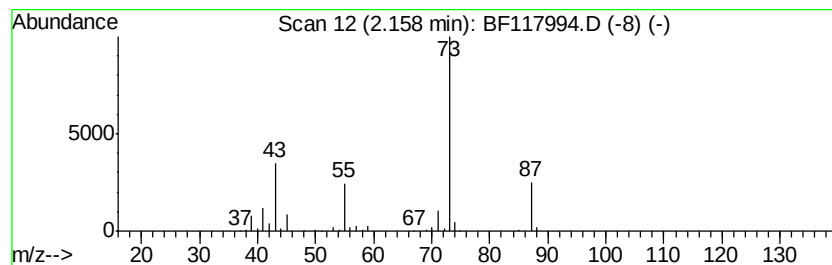
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	10.54 ng	504474	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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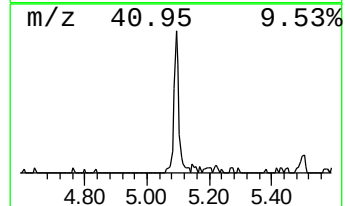
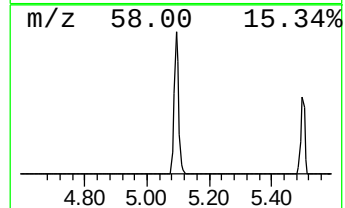
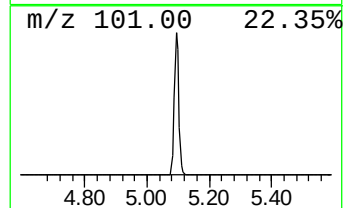
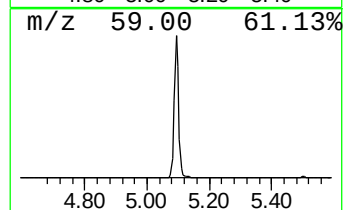
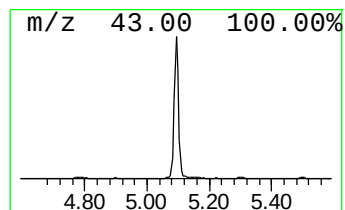
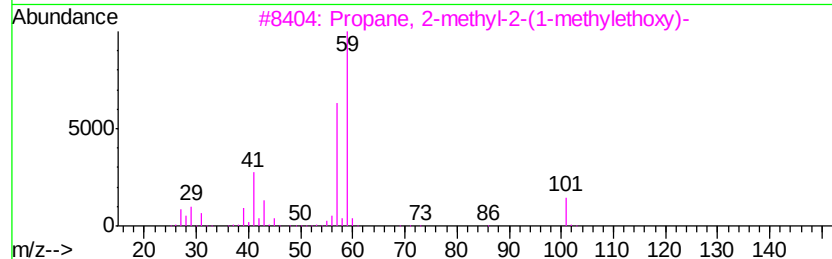
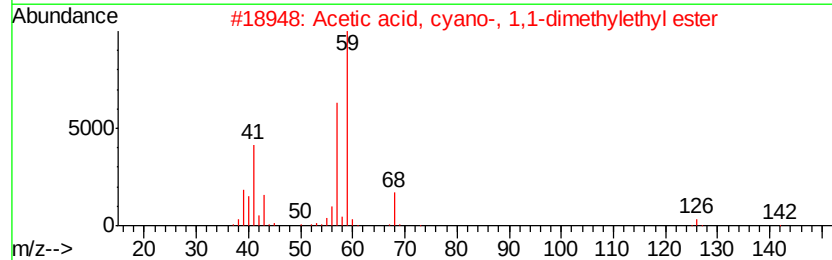
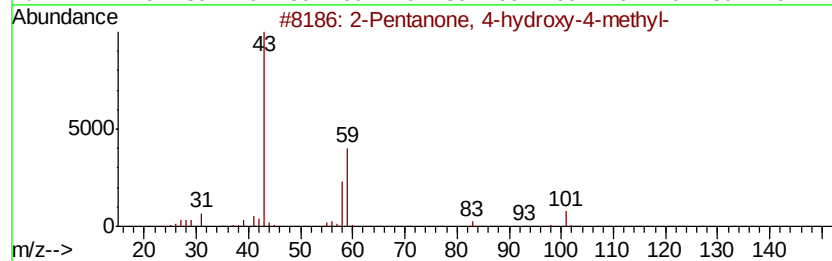
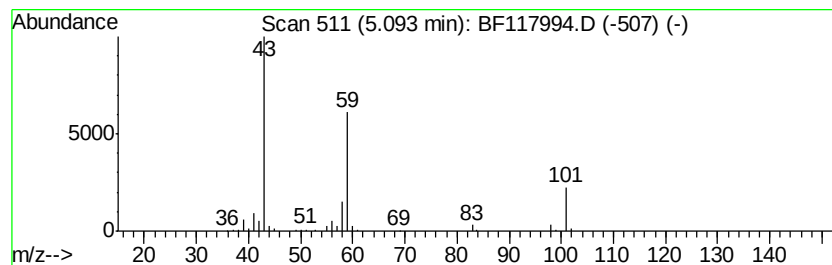
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.09	5.61 ng	268299	1,4-Dichlorobenzene-d4	6.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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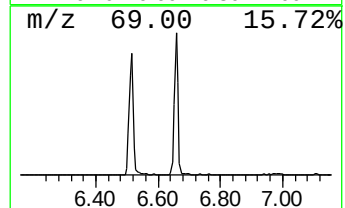
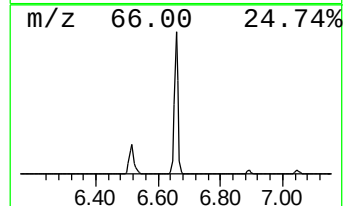
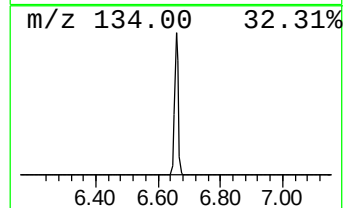
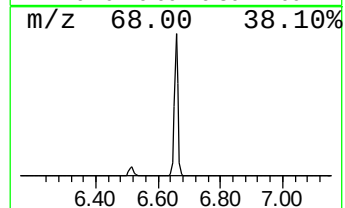
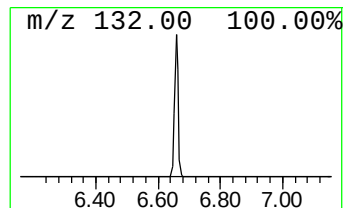
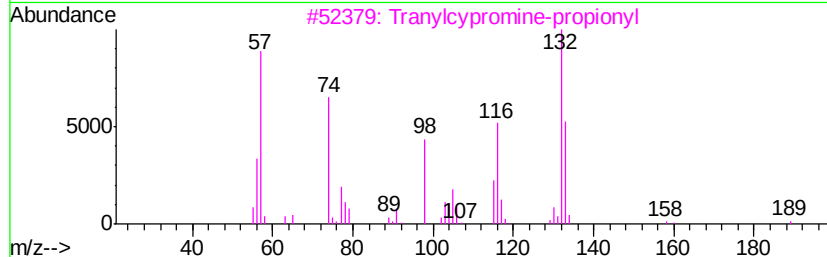
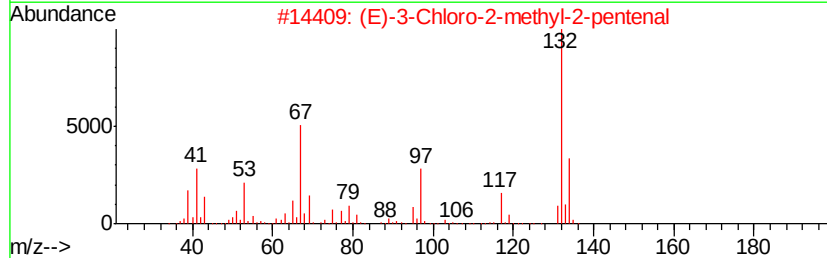
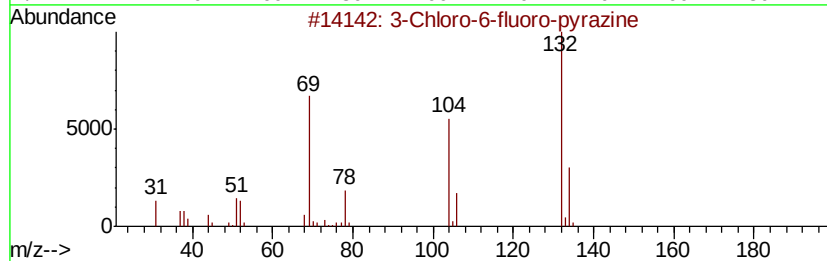
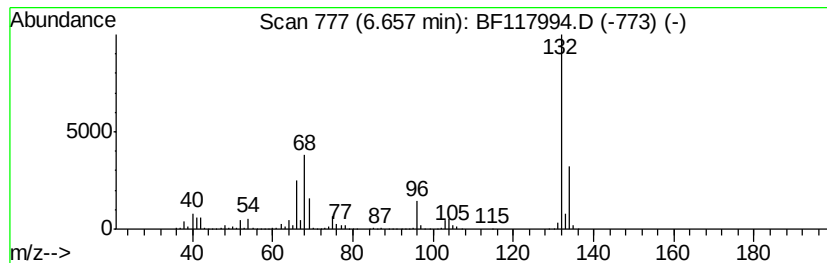
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	32.22 ng	1542060	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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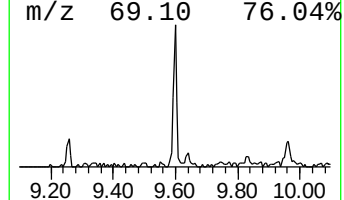
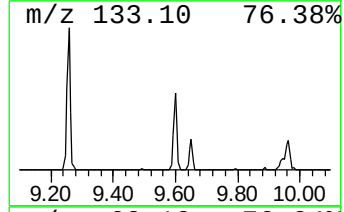
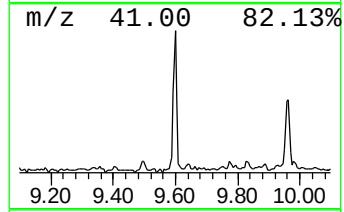
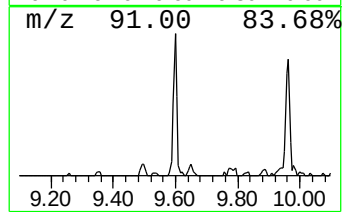
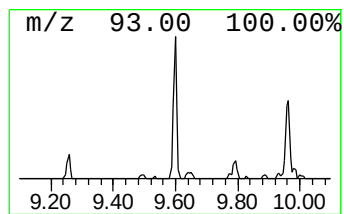
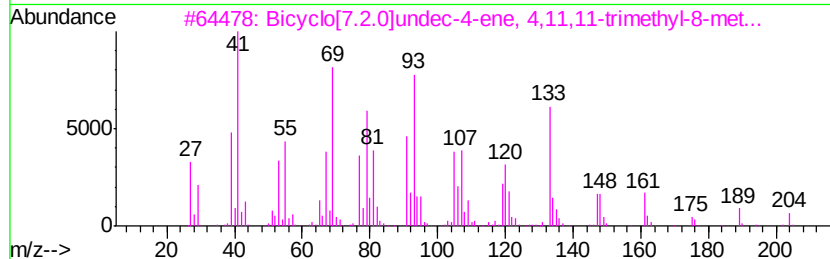
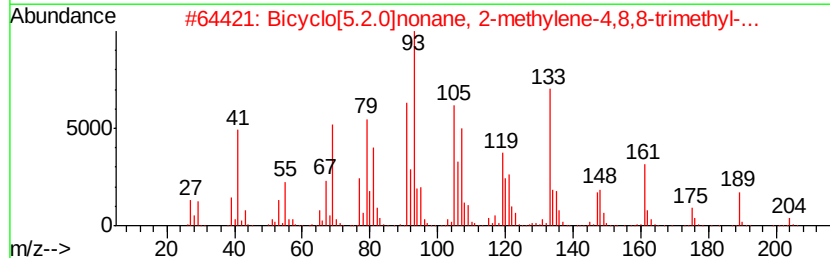
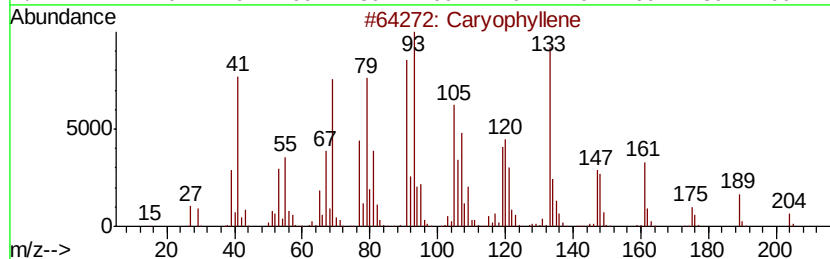
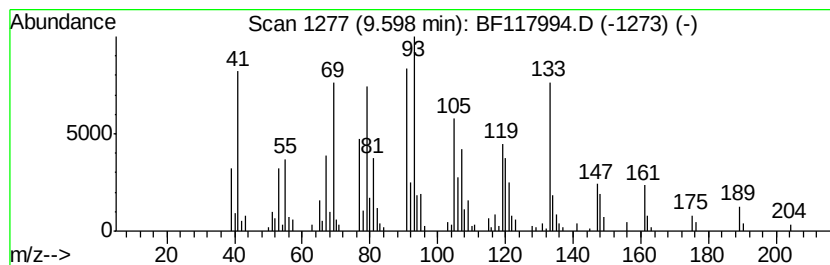
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Caryophyllene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.60	3.80 ng	224482	Acenaphthene-d10	9.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carvophyllene	204	C15H24	000087-44-5	99
2	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	92
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
4	(Z,Z)-.alpha.-Farnesene	204	C15H24	1000293-03-1	41
5	(-)-delta.-Panasinsine	204	C15H24	1000156-11-8	30



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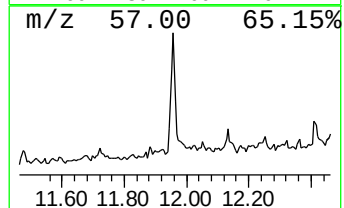
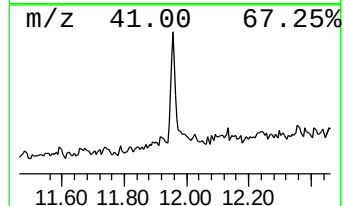
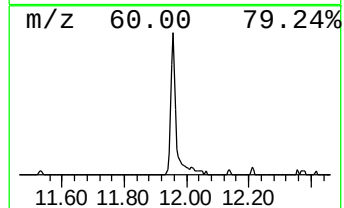
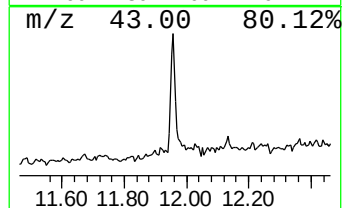
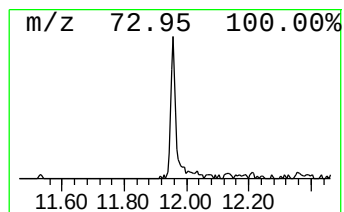
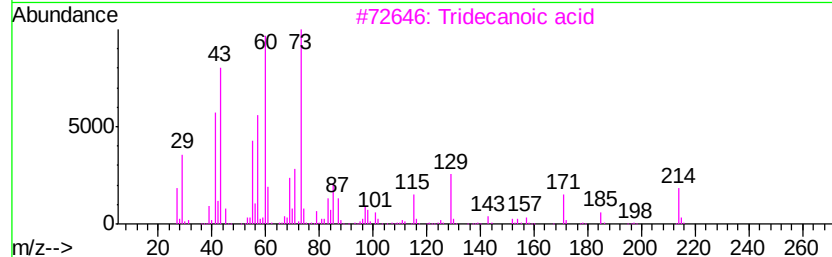
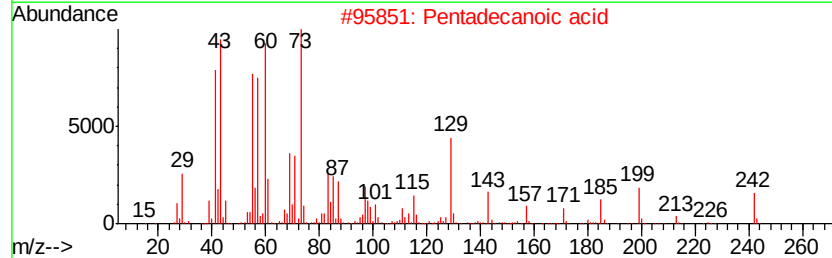
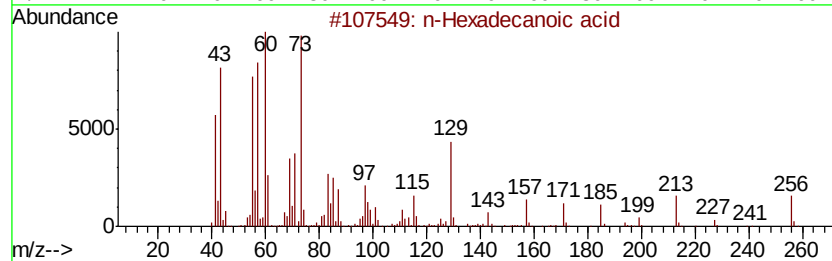
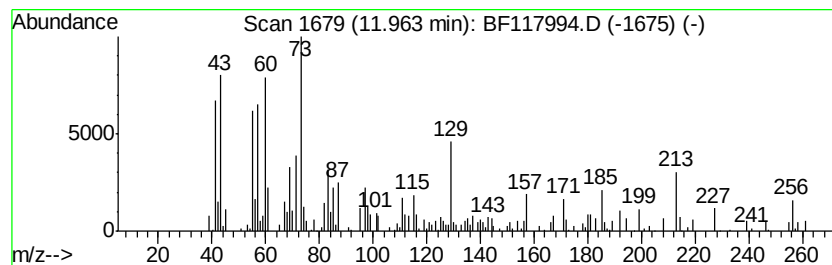
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TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.96	3.44 ng	159998	Phenanthrene-d10		11.43
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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Misc :
ALS Vial : 21 Sample Multiplier: 1

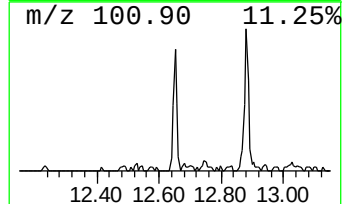
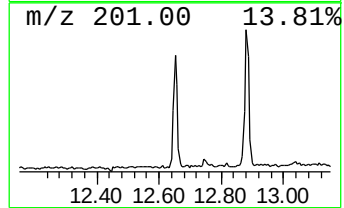
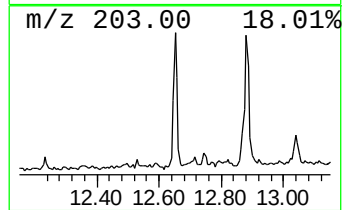
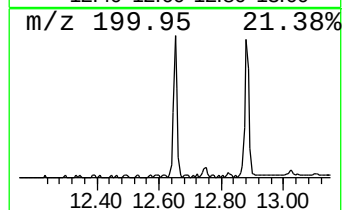
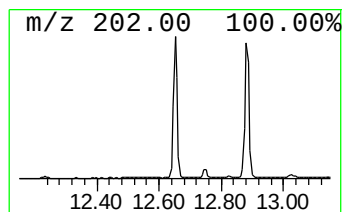
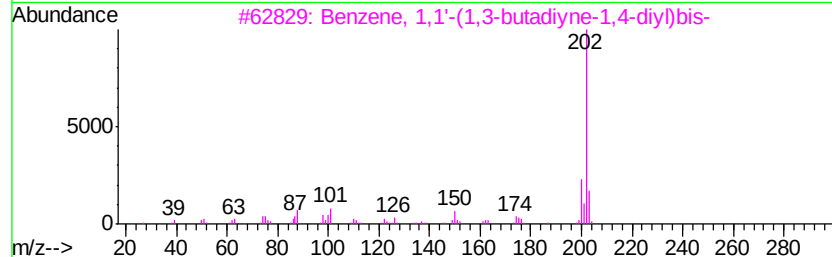
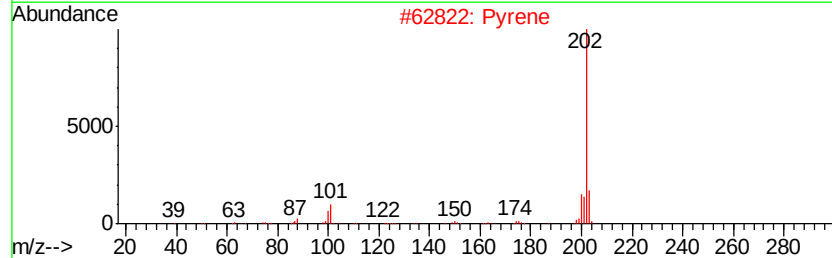
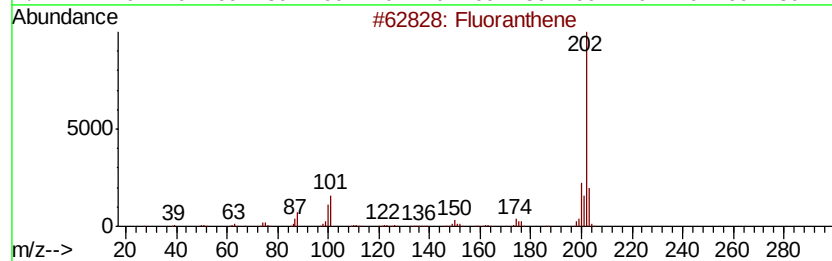
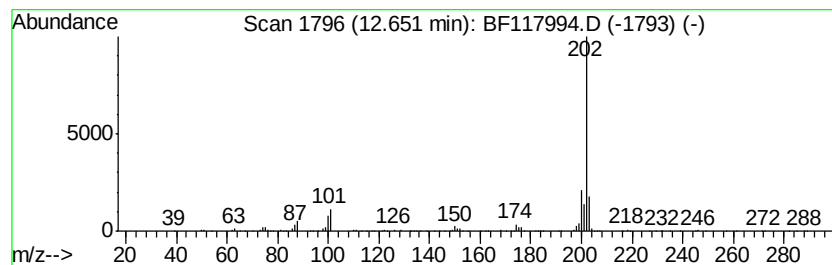
Instrument :
BNA_F
ClientSampleId :
IDLEWILD-BH-03A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.65	4.00 ng	186046	Phenanthrene-d10	11.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	94
2	Pyrene	202	C16H10	000129-00-0	91
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	74
4	Pyrene, 10b,10c-dihydro-10b,10c-...	288	C22H24	028816-94-6	38
5	3H-Benzo[4,5]furo[3,2-d]pyrimidi...	202	C10H6N2OS	062208-70-2	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117994.D
Acq On : 26 Nov 2019 4:33
Operator : JU
Sample : K5999-03 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDLEWILD-BH-03A

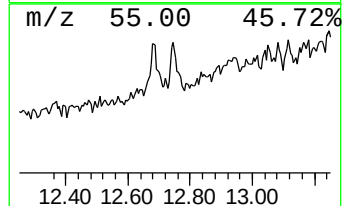
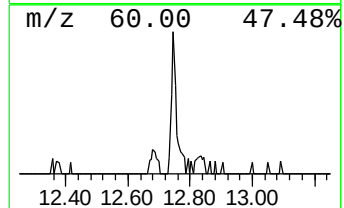
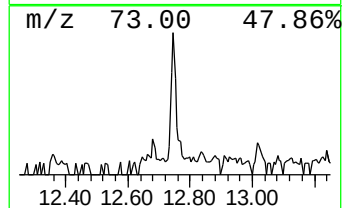
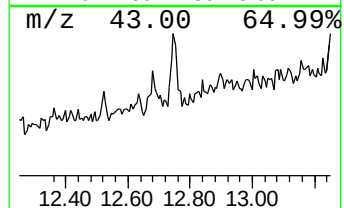
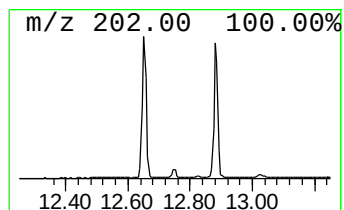
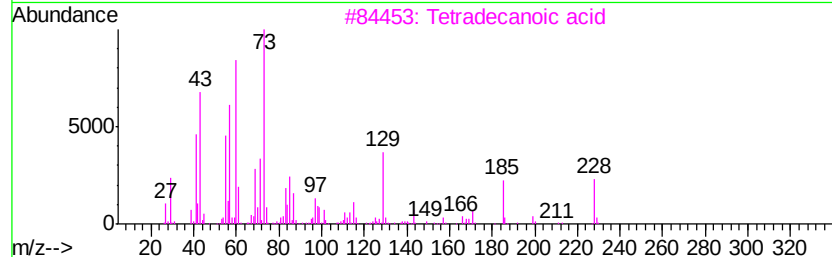
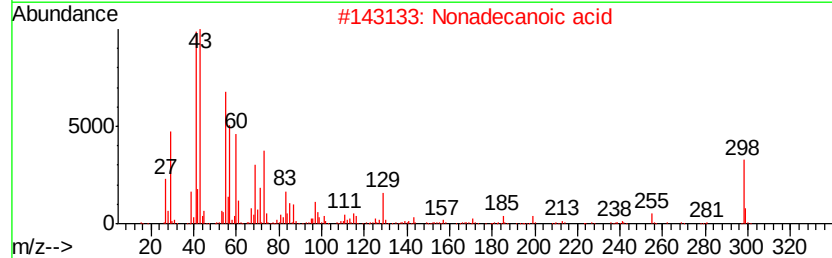
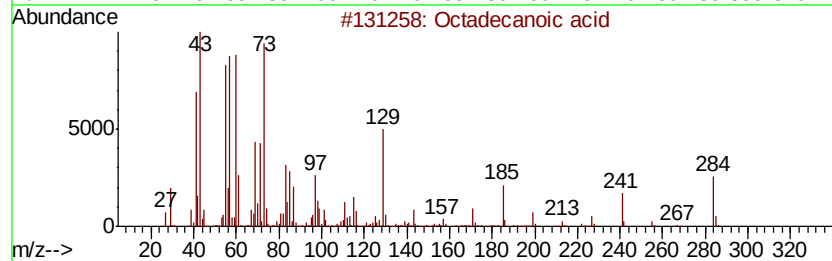
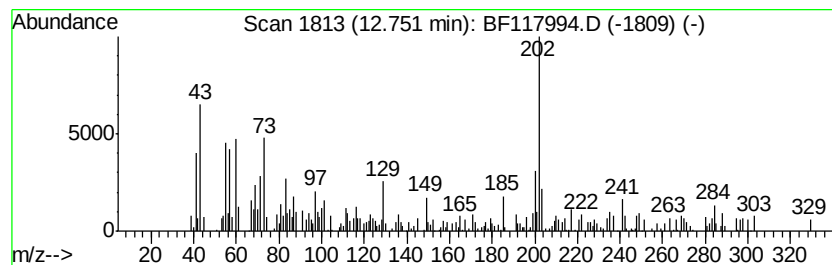
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.75	2.70 ng	125666	Phenanthrene-d10		11.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	78	
2	Nonadecanoic acid	298	C19H38O2	000646-30-0	59	
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43	
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	35	
5	Fluoranthene	202	C16H10	000206-44-0	35	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112519\
Data File : BF117994.D
Acq On : 26 Nov 2019 4:33
Operator : JU
Sample : K5999-03 2X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDLEWILD-BH-03A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.16	10.5	ng	504474	1	6.89	957297	20.0
2-Pentanone, 4-hy...	5.09	5.6	ng	268299	1	6.89	957297	20.0
unknown6.66	6.66	32.2	ng	1542060	1	6.89	957297	20.0
Caryophyllene	9.60	3.8	ng	224482	3	9.95	1181910	20.0
n-Hexadecanoic acid	11.96	3.4	ng	159998	4	11.43	929219	20.0
Benzene, 1,1'-(1,...	12.65	4.0	ng	186046	4	11.43	929219	20.0
Octadecanoic acid	12.75	2.7	ng	125666	4	11.43	929219	20.0