

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102519\
 Data File : BF117546.D
 Acq On : 25 Oct 2019 19:47
 Operator : JU
 Sample : K5499-19
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 702-27-(0-1)

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-BF101819.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	5.357	553	556	577	rBV	533188	667857	86.51%	9.132%
2	6.386	728	731	748	rBV	677649	754074	97.68%	10.311%
3	6.510	748	752	767	rVB	754231	772001	100.00%	10.556%
4	6.728	786	789	803	rVB	221201	204820	26.53%	2.801%
5	6.886	812	816	830	rBV	654775	550669	71.33%	7.530%
6	7.292	882	885	900	rBV	356497	419071	54.28%	5.730%
7	8.010	1004	1007	1019	rBV	249906	245261	31.77%	3.354%
8	9.086	1186	1190	1198	rBV	869838	718256	93.04%	9.821%
9	9.151	1198	1201	1203	rVB2	31430	27062	3.51%	0.370%
10	9.416	1243	1246	1249	rBV	14388	10579	1.37%	0.145%
11	9.480	1254	1257	1263	rBV	100572	80584	10.44%	1.102%
12	9.763	1302	1305	1315	rVB	314664	259730	33.64%	3.552%
13	10.557	1437	1440	1451	rBV	375403	343109	44.44%	4.692%
14	11.251	1554	1558	1560	rBV	237076	210497	27.27%	2.878%
15	11.274	1560	1562	1566	rVV	89340	76036	9.85%	1.040%
16	11.327	1568	1571	1576	rVB	12968	14213	1.84%	0.194%
17	11.492	1594	1599	1605	rBV4	7373	11589	1.50%	0.158%
18	11.751	1640	1643	1645	rBV	15024	13699	1.77%	0.187%
19	11.780	1645	1648	1655	rVB3	61820	65402	8.47%	0.894%
20	11.863	1659	1662	1665	rBV2	16561	16463	2.13%	0.225%
21	12.092	1698	1701	1704	rBV4	11635	10622	1.38%	0.145%
22	12.198	1713	1719	1721	rBV6	5271	8447	1.09%	0.116%
23	12.304	1733	1737	1740	rBV2	13411	16639	2.16%	0.228%
24	12.398	1750	1753	1757	rBV3	11040	12575	1.63%	0.172%
25	12.468	1761	1765	1768	rBV	182590	182392	23.63%	2.494%
26	12.563	1779	1781	1786	rBV4	19804	22714	2.94%	0.311%
27	12.615	1788	1790	1792	rVV3	15238	11685	1.51%	0.160%
28	12.692	1798	1803	1809	rVB	171150	187289	24.26%	2.561%
29	12.833	1823	1827	1830	rBV	653164	556437	72.08%	7.609%
30	12.857	1830	1831	1837	rVB6	11487	11263	1.46%	0.154%
31	12.915	1837	1841	1846	rBV5	16161	31705	4.11%	0.434%
32	13.004	1852	1856	1857	rBV4	17744	21425	2.78%	0.293%
33	13.092	1869	1871	1873	rBV2	12217	9769	1.27%	0.134%
34	13.133	1875	1878	1879	rBV2	17730	15488	2.01%	0.212%

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702-27-(0-1)

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-BF101819.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.221	1890	1893	1896	rBV3	23875	30967	4.01%	0.423%
36	13.257	1897	1899	1900	rBV2	17111	12252	1.59%	0.168%
37	13.739	1977	1981	1990	rVB4	73050	145891	18.90%	1.995%
38	13.862	1999	2002	2004	rBV	49002	54052	7.00%	0.739%
39	13.898	2004	2008	2010	rVV2	243694	316065	40.94%	4.322%
40	13.921	2010	2012	2017	rVB	89015	93598	12.12%	1.280%
41	15.727	2317	2319	2324	rVB	83698	100964	13.08%	1.381%

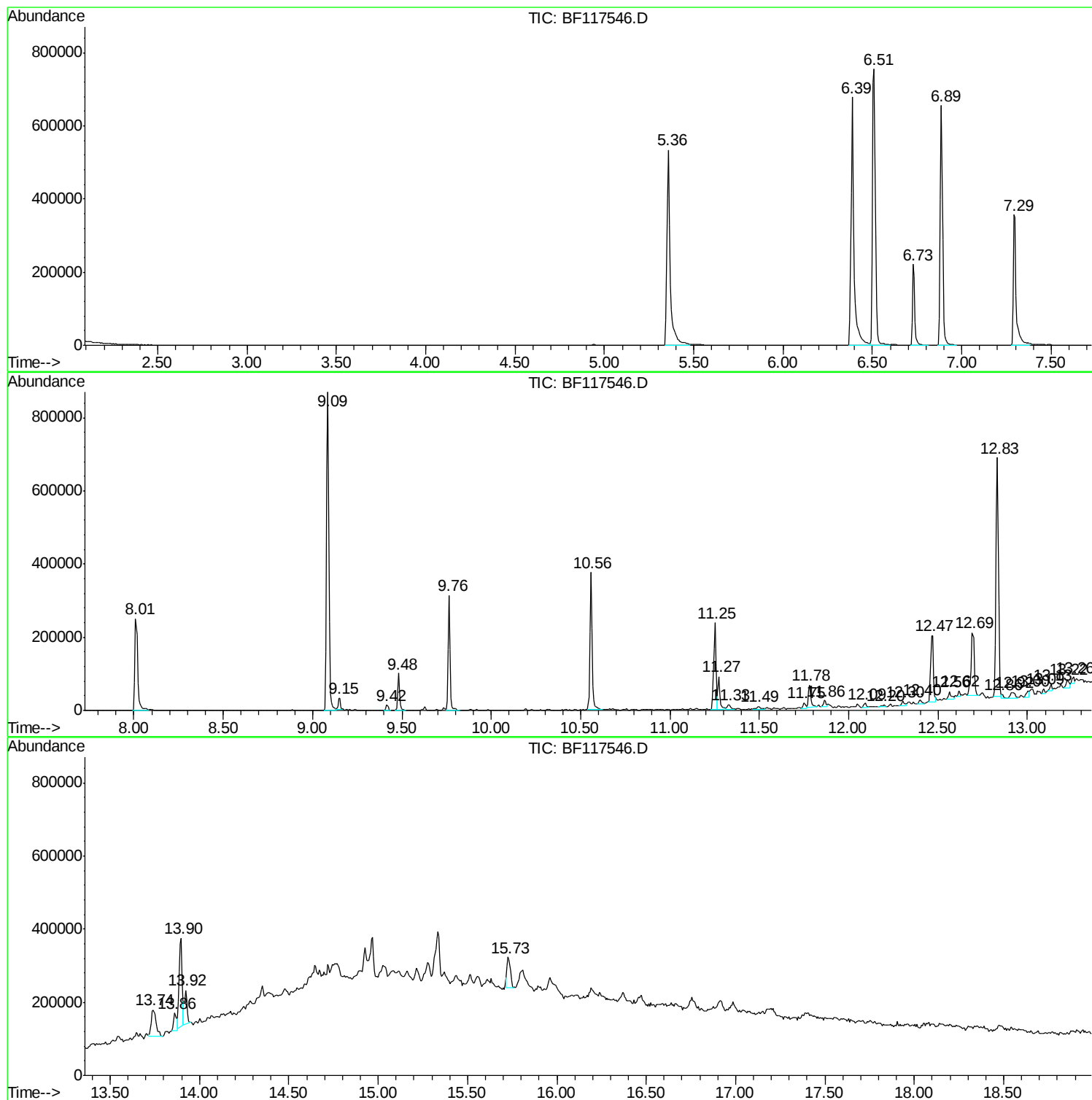
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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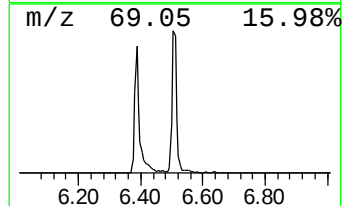
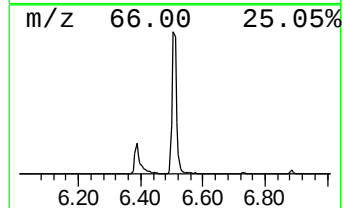
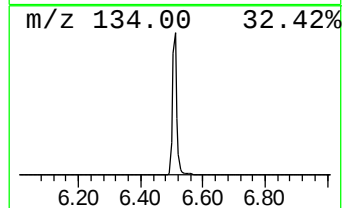
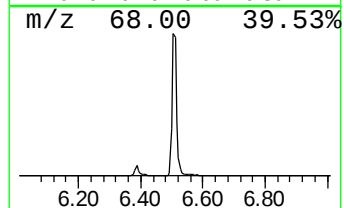
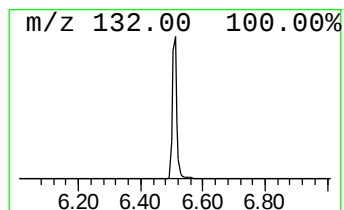
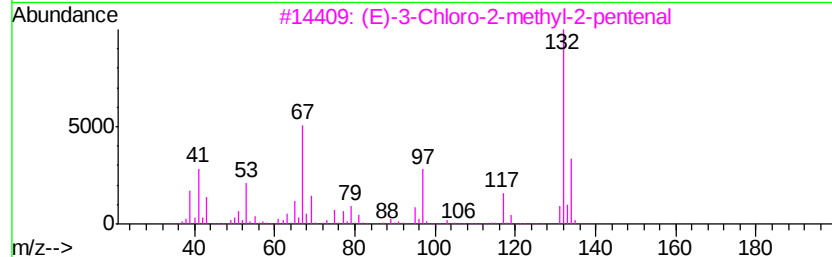
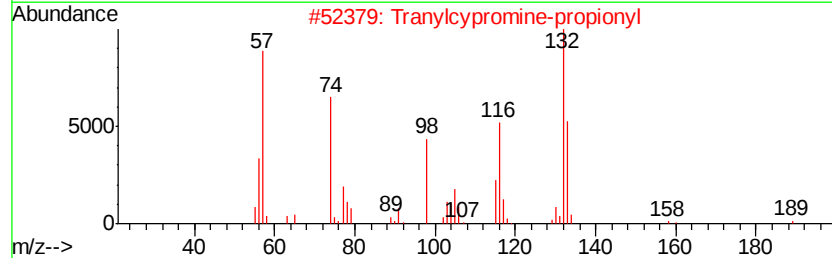
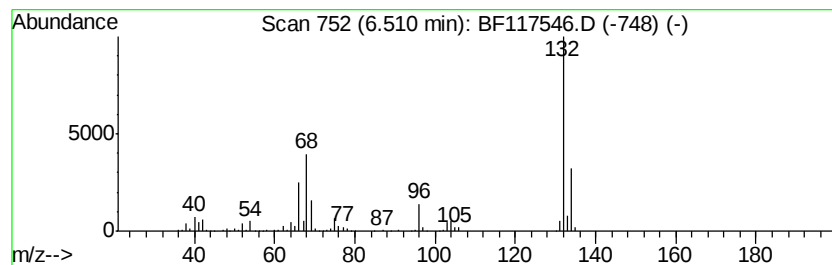
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	75.38 ng	772001	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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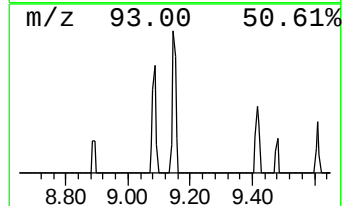
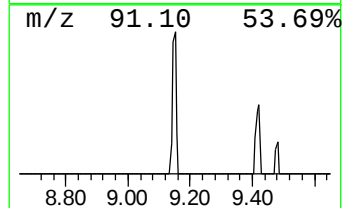
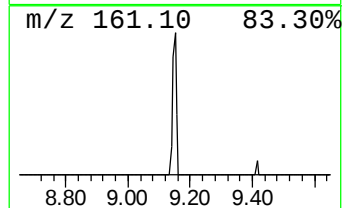
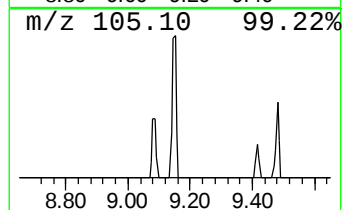
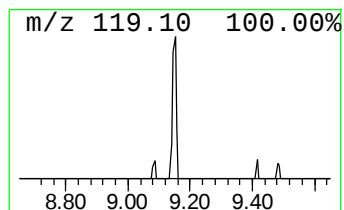
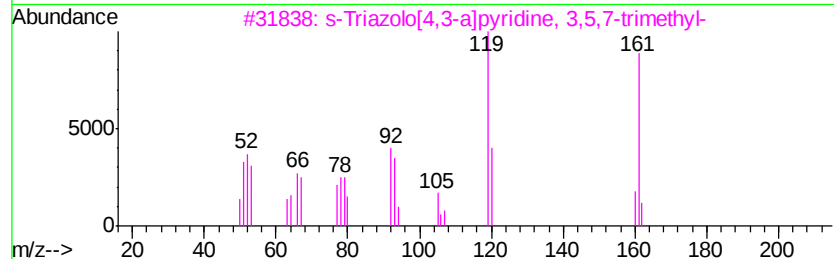
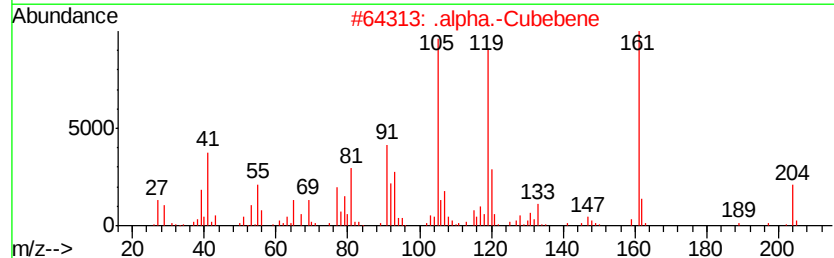
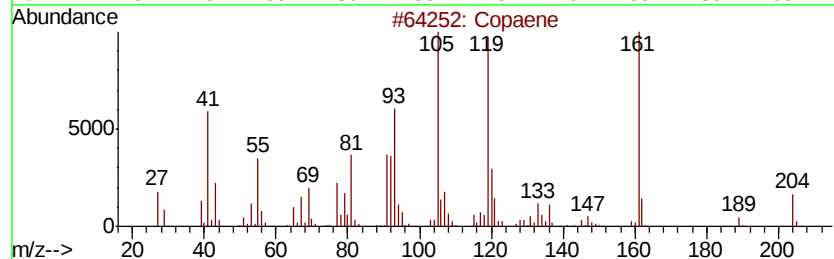
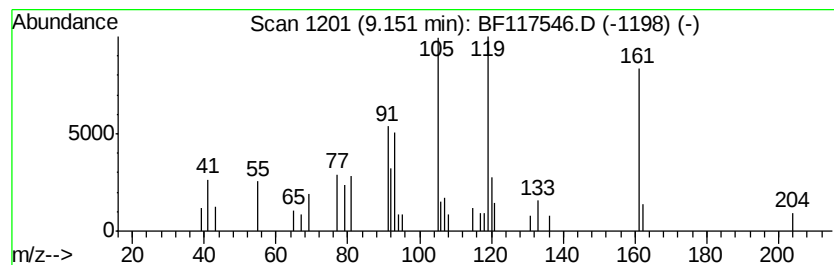
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Copaene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.15	2.08 ng	27062	Acenaphthene-d10	9.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Copaene	204	C15H24	003856-25-5	96
2		.alpha.-Cubebene	204	C15H24	017699-14-8	95
3		s-Triazolo[4,3-a]pyridine, 3,5,7...	161	C9H11N3	004919-15-7	74
4		cis-muurolo-3,5-diene	204	C15H24	1000365-95-4	70
5		.beta.-copaene	204	C15H24	1000374-18-9	55



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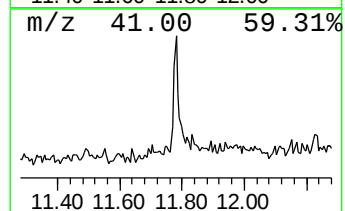
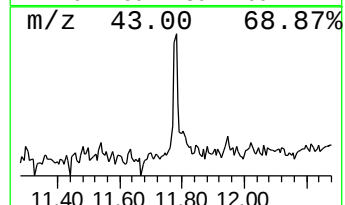
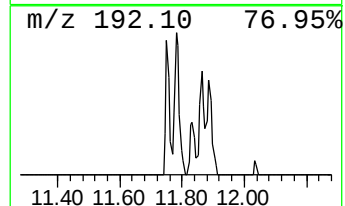
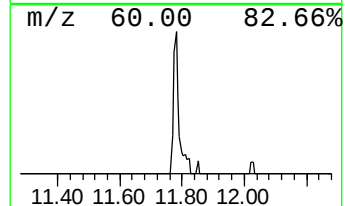
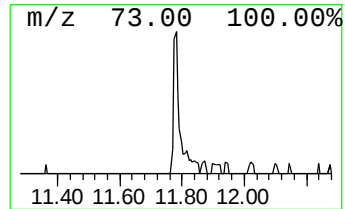
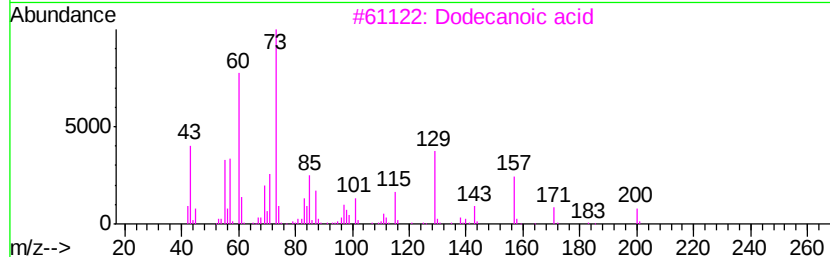
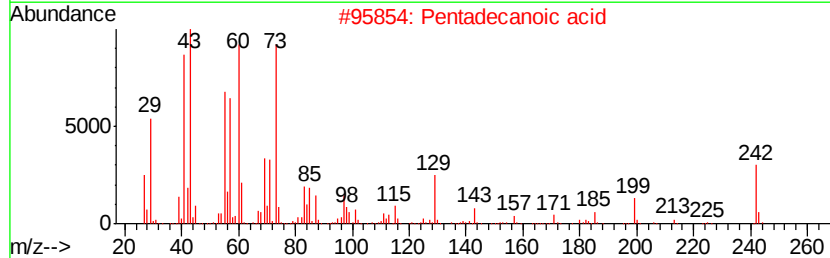
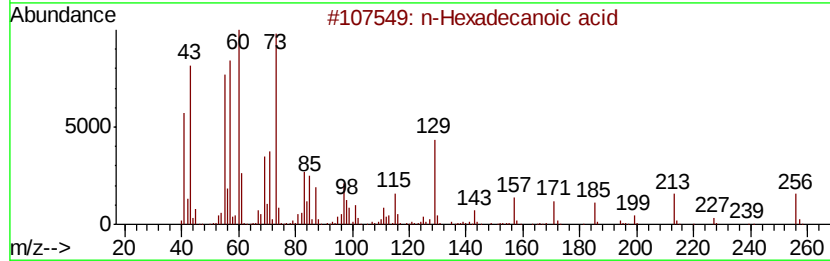
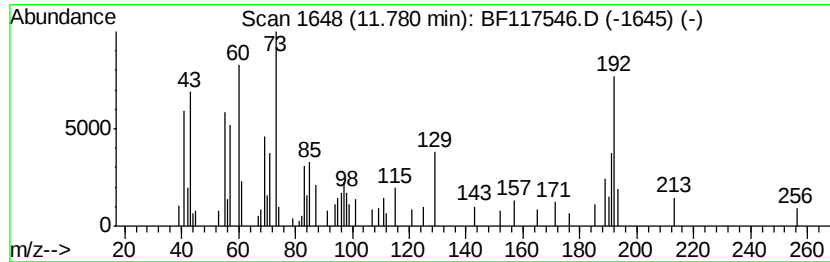
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.78	6.21 ng	65402	Phenanthrene-d10		11.25
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
3	Dodecanoic acid	200	C12H24O2	000143-07-7	43
4	Tridecanoic acid	214	C13H26O2	000638-53-9	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38



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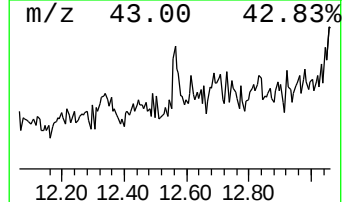
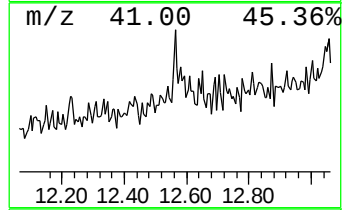
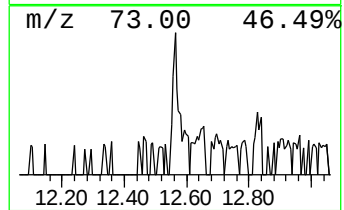
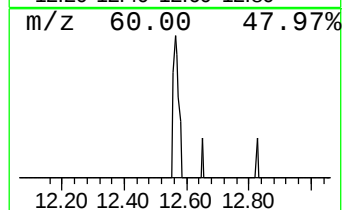
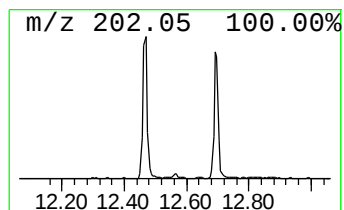
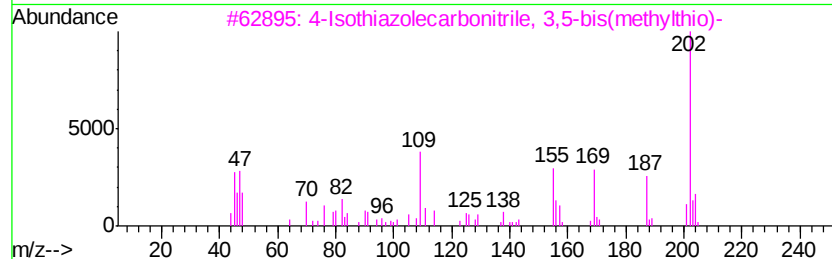
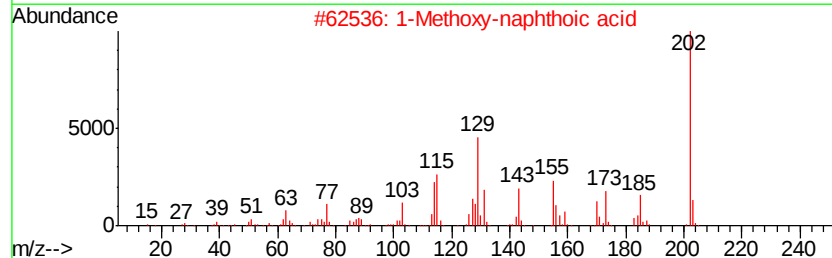
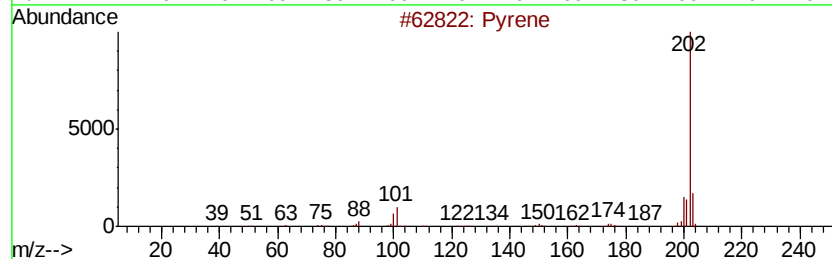
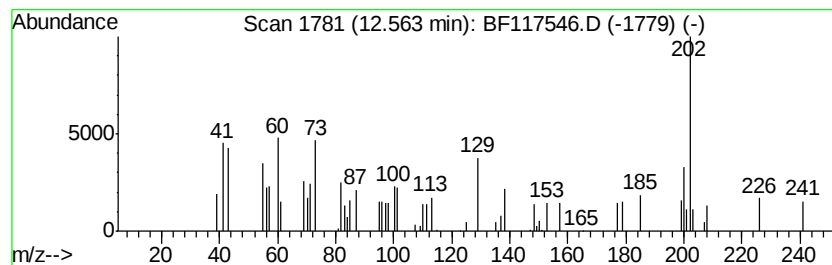
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown12.56 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.56	2.16 ng	22714	Phenanthrene-d10		11.25	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pyrene	202	C16H10	000129-00-0	38
2		1-Methoxy-naphthoic acid	202	C12H10O3	000883-21-6	22
3		4-Isothiazolecarbonitrile, 3,5-b...	202	C6H6N2S3	004886-13-9	14
4		7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	000486-60-2	14
5		5-Methyl-1-phenylpyrazole-4-carb...	202	C11H10N2O2	091138-00-0	14



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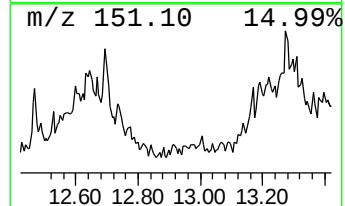
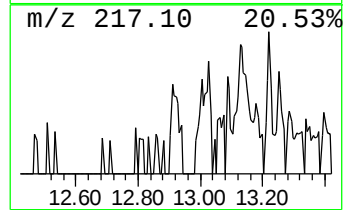
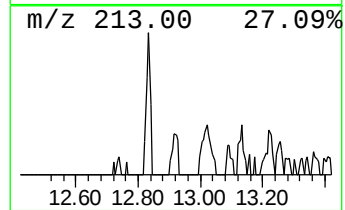
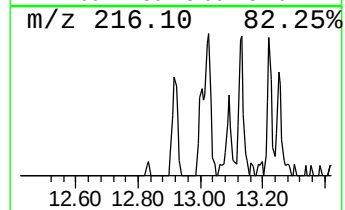
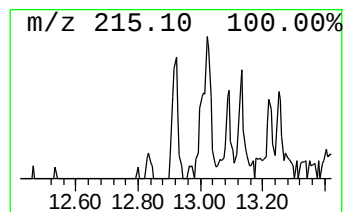
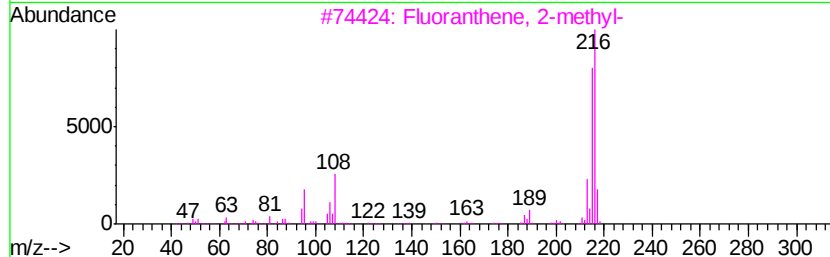
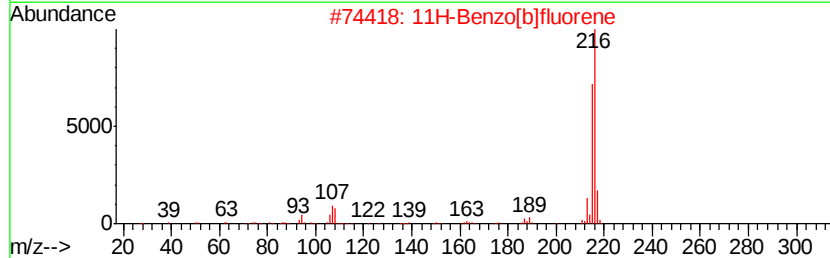
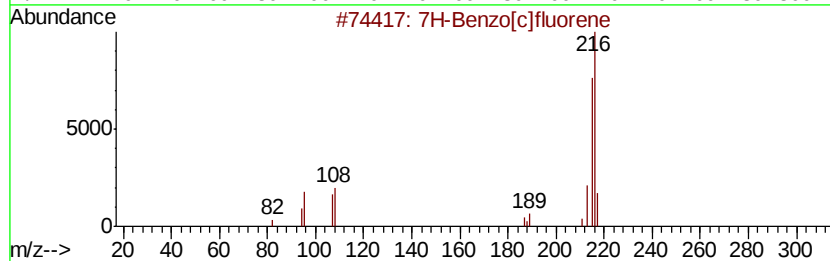
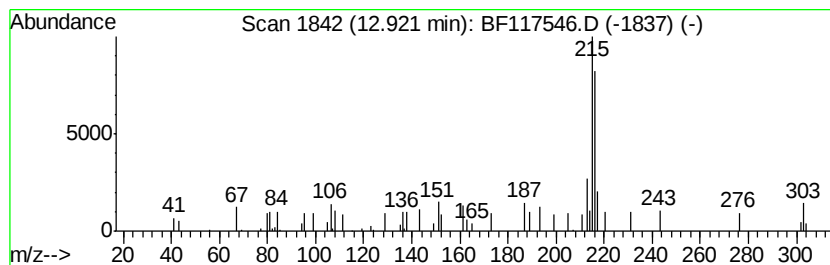
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 7H-Benzo[c]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	2.01 ng	31705	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	58
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	53
3		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	52
4		Pvrene, 1-methyl-	216	C17H12	002381-21-7	50
5		.beta.-Carboline, 1,2,3,4-tetra...	260	C14H16N2O3	1000124-14-2	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102519\
Data File : BF117546.D
Acq On : 25 Oct 2019 19:47
Operator : JU
Sample : K5499-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
702-27-(0-1)

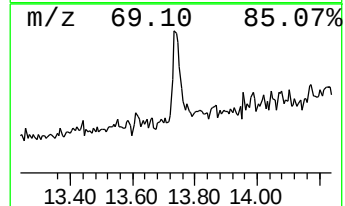
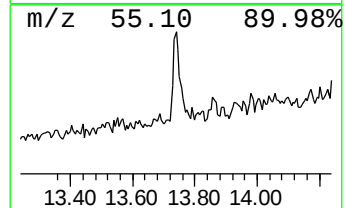
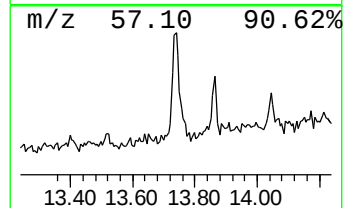
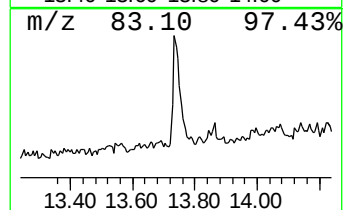
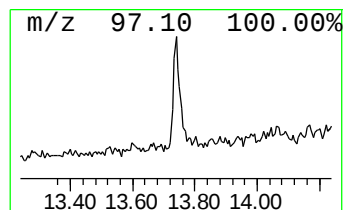
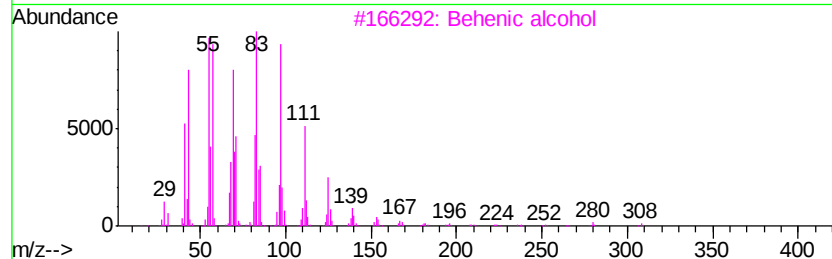
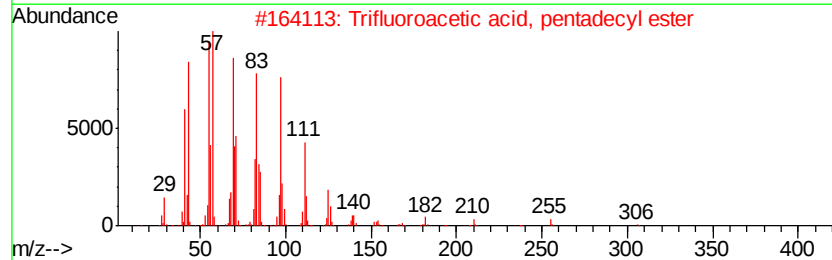
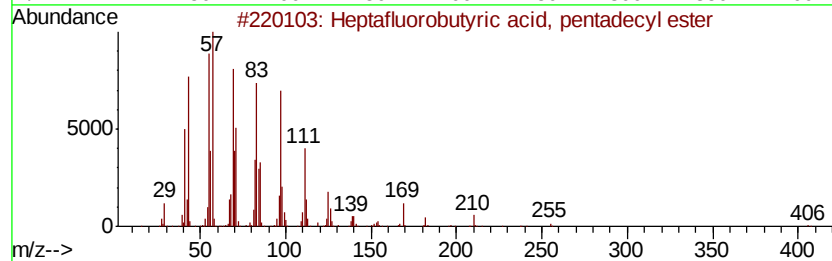
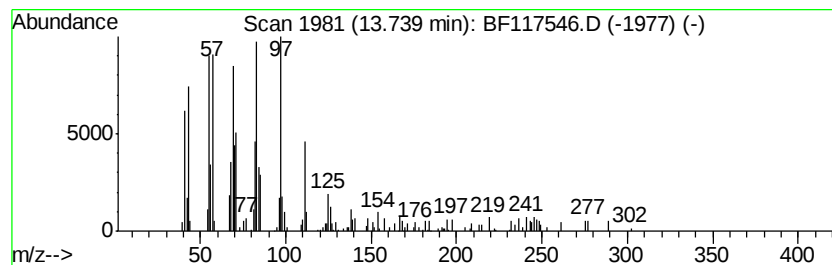
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	9.23 ng	145891	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		Isoheptadecanol	256	C17H36O	057289-07-3	90
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	87



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Data File : BF117546.D
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Operator : JU
Sample : K5499-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
702-27-(0-1)

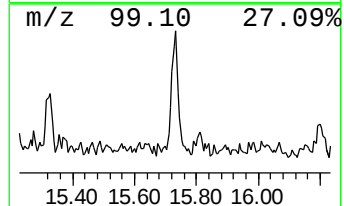
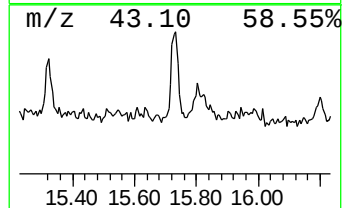
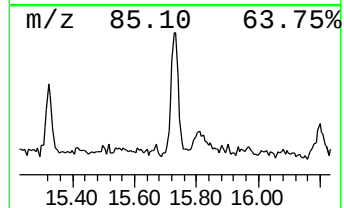
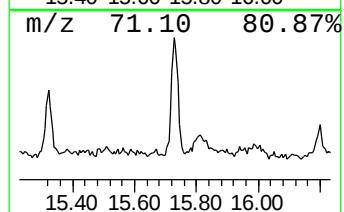
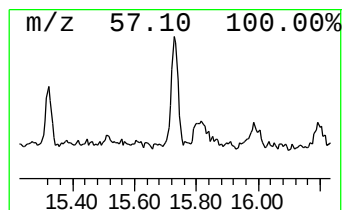
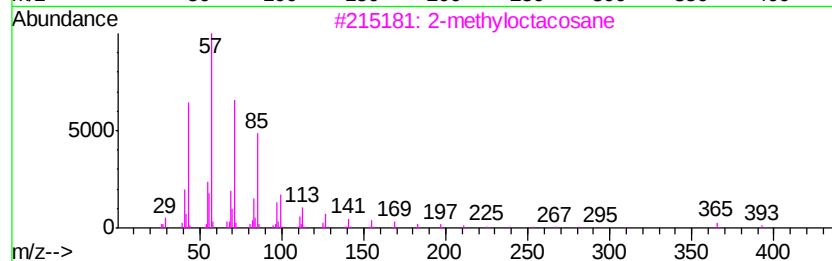
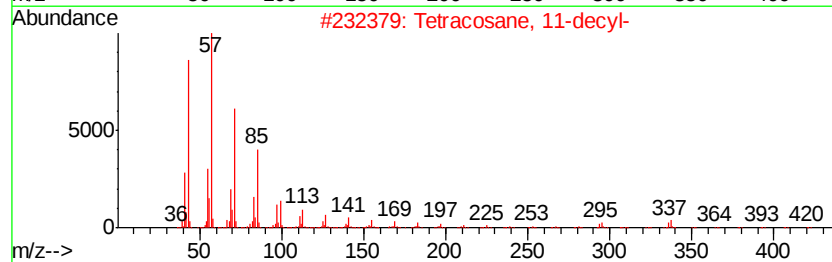
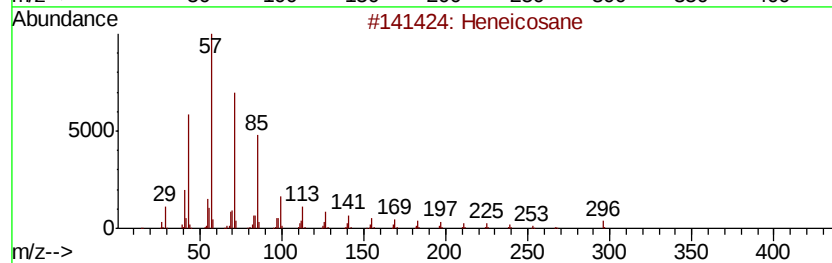
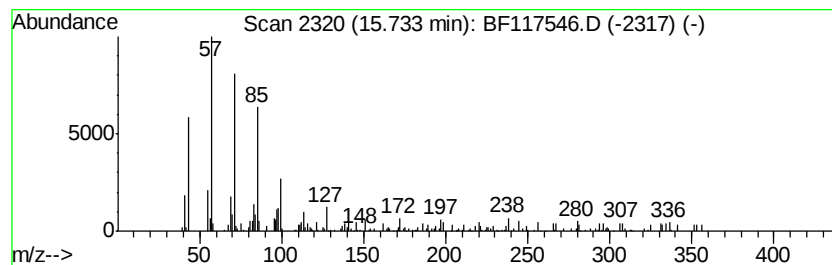
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	20.00 ng	100964	Perylene-d12	15.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Tetracosane, 11-decyl-		479	C34H70	055429-84-0	80
3	2-methyloctacosane		408	C29H60	1000376-72-8	80
4	triacontane		422	C30H62	000638-68-6	74
5	Heptacosane		380	C27H56	000593-49-7	72



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Sample : K5499-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
702-27-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
unknown6.51	6.51	75.4	ng	772001	1	6.73	204820	20.0
Copaene	9.15	2.1	ng	27062	3	9.76	259730	20.0
n-Hexadecanoic acid	11.78	6.2	ng	65402	4	11.25	210497	20.0
unknown12.56	12.56	2.2	ng	22714	4	11.25	210497	20.0
7H-Benzo[c]fluorene	12.92	2.0	ng	31705	5	13.90	316065	20.0
Heptafluorobutyri...	13.74	9.2	ng	145891	5	13.90	316065	20.0
Heneicosane	15.73	20.0	ng	100964	6	15.34	100964	20.0