

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102919\
 Data File : BF117589.D
 Acq On : 29 Oct 2019 14:31
 Operator : JU
 Sample : K5503-17
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 171-64-(0-1.8)

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	4.945	483	486	497	rBV	13794	21885	2.10%	0.282%
2	5.357	553	556	580	rBV	754108	960969	92.06%	12.402%
3	6.386	727	731	747	rBV	910287	1026435	98.34%	13.247%
4	6.504	747	751	760	rVV	1089985	1043806	100.00%	13.471%
5	6.728	786	789	800	rVB	255873	229562	21.99%	2.963%
6	6.881	812	815	832	rBV	797164	729634	69.90%	9.417%
7	7.292	882	885	897	rBV	499468	562297	53.87%	7.257%
8	8.010	1004	1007	1028	rBV	222864	268009	25.68%	3.459%
9	9.080	1185	1189	1206	rBV	853343	827790	79.30%	10.684%
10	9.480	1254	1257	1267	rBV	52814	58107	5.57%	0.750%
11	9.763	1301	1305	1319	rBB	235561	246183	23.59%	3.177%
12	10.557	1436	1440	1456	rBV	307954	353064	33.82%	4.557%
13	11.251	1554	1558	1567	rBV	179563	190339	18.24%	2.457%
14	11.774	1645	1647	1656	rBV	20643	25522	2.45%	0.329%
15	12.827	1822	1826	1830	rBV	636637	540675	51.80%	6.978%
16	13.733	1976	1980	1990	rBV2	46607	87034	8.34%	1.123%
17	13.892	2003	2007	2017	rBV	198367	213491	20.45%	2.755%
18	14.345	2079	2084	2087	rBV4	15785	19938	1.91%	0.257%
19	14.645	2132	2135	2140	rVB	22331	20643	1.98%	0.266%
20	14.715	2143	2147	2150	rVV	45292	44805	4.29%	0.578%
21	14.957	2185	2188	2191	rVB	28238	29676	2.84%	0.383%
22	15.333	2245	2252	2259	rVB	123718	186286	17.85%	2.404%
23	15.427	2265	2268	2273	rVB6	11354	14855	1.42%	0.192%
24	15.721	2314	2318	2324	rVB	18719	26991	2.59%	0.348%
25	16.351	2422	2425	2433	rVB6	11705	20265	1.94%	0.262%

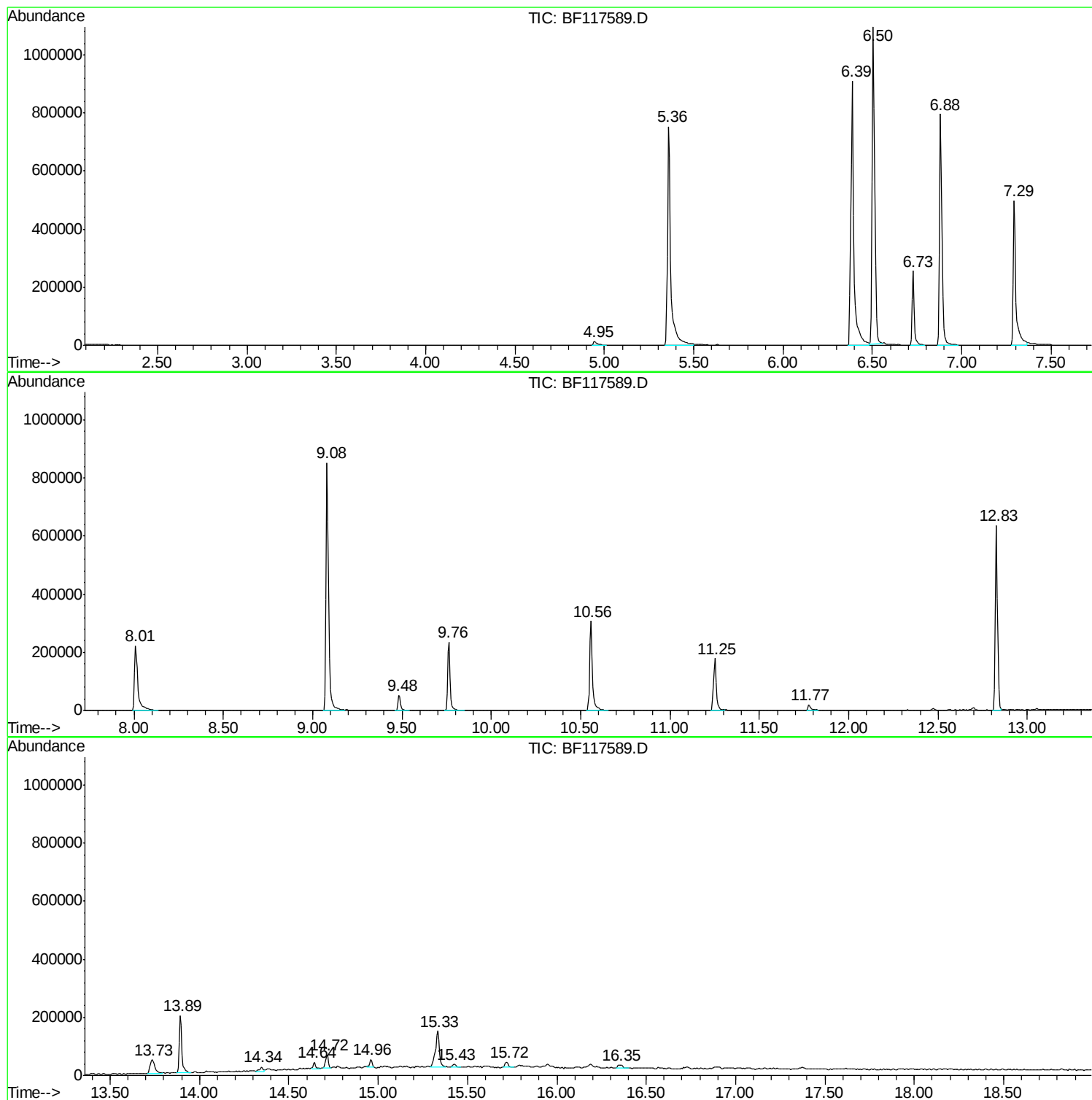
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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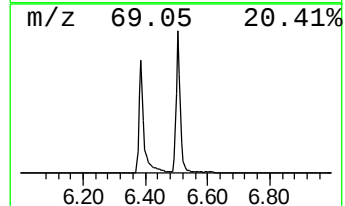
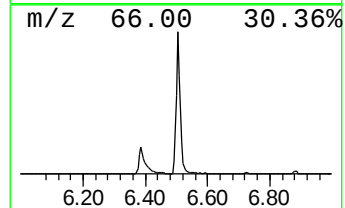
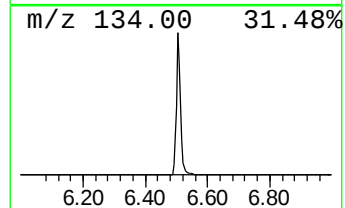
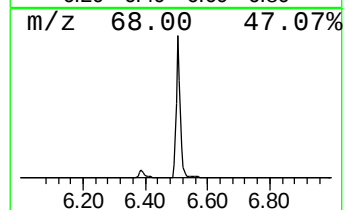
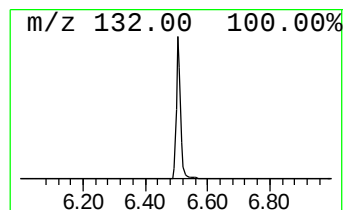
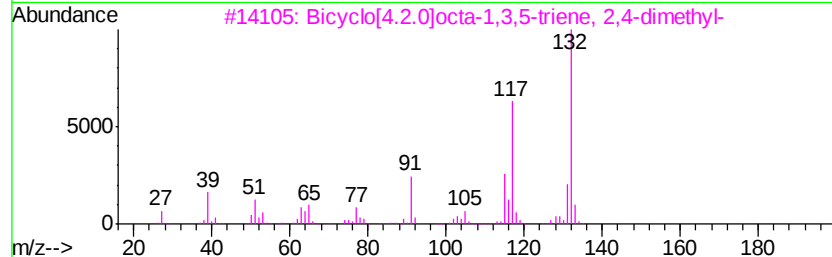
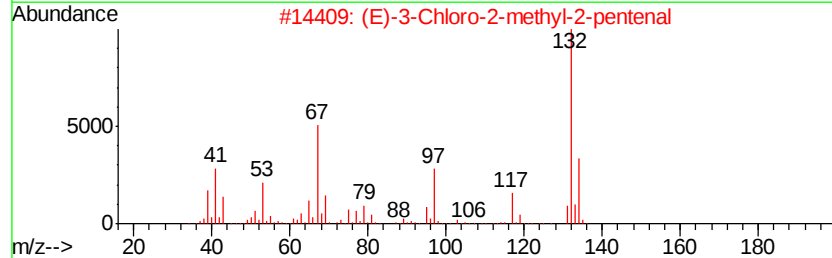
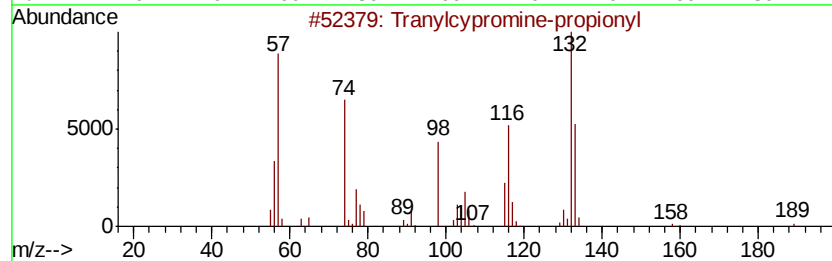
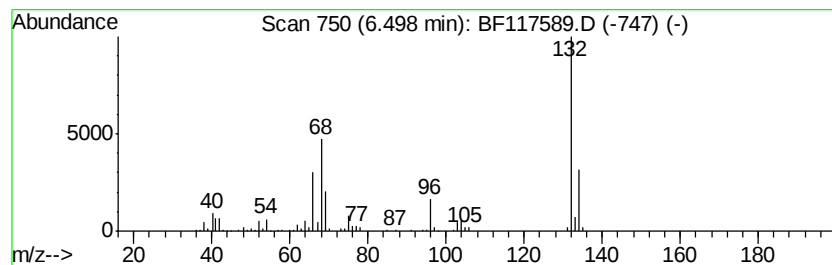
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	90.94 ng	1043810	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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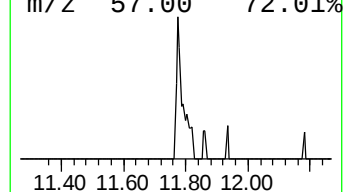
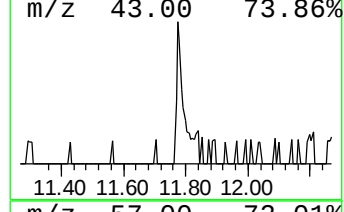
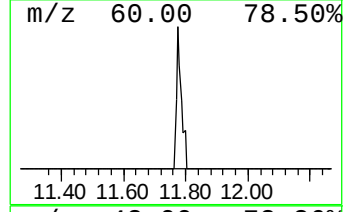
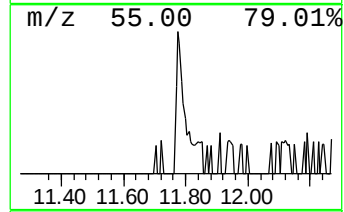
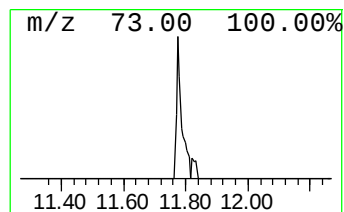
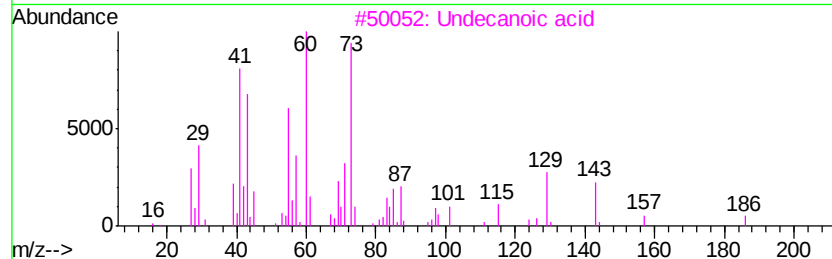
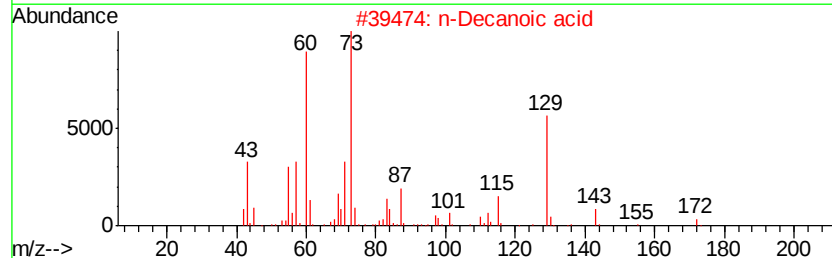
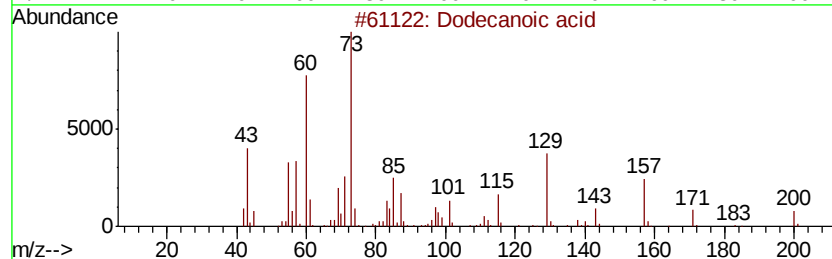
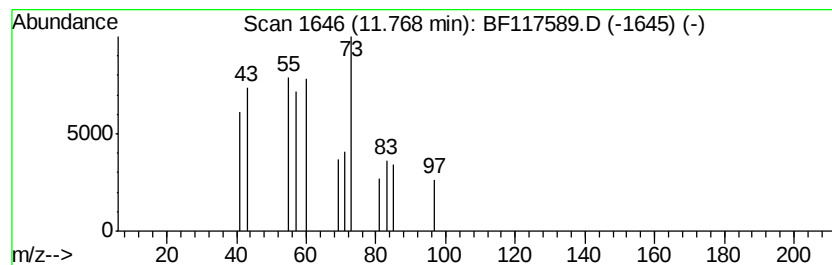
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Peak Number 3 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.77	2.68 ng	25522	Phenanthrene-d10		11.25	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid		200	C12H24O2	000143-07-7	59
2	n-Decanoic acid		172	C10H20O2	000334-48-5	59
3	Undecanoic acid		186	C11H22O2	000112-37-8	50
4	Butyraldehyde, semicarbazone		129	C5H11N3O	013183-21-6	43
5	1-Decanol, 2-hexyl-		242	C16H34O	002425-77-6	27



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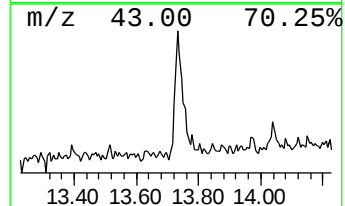
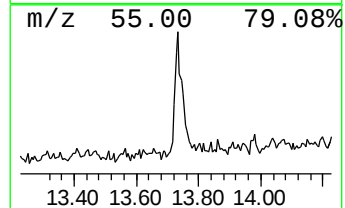
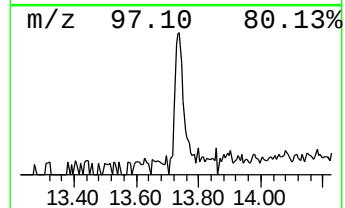
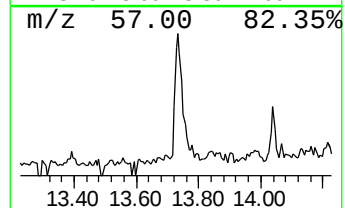
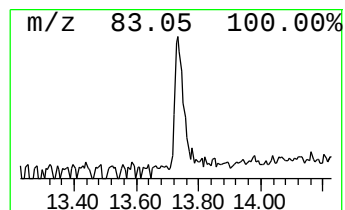
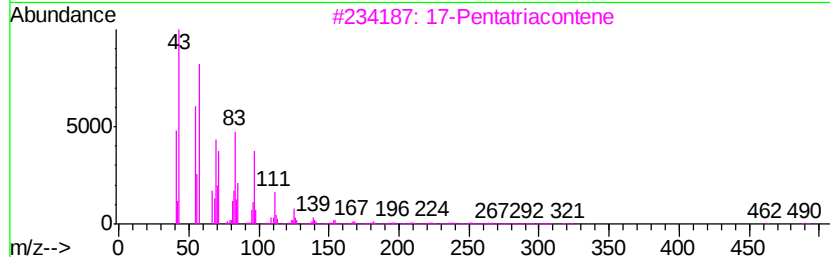
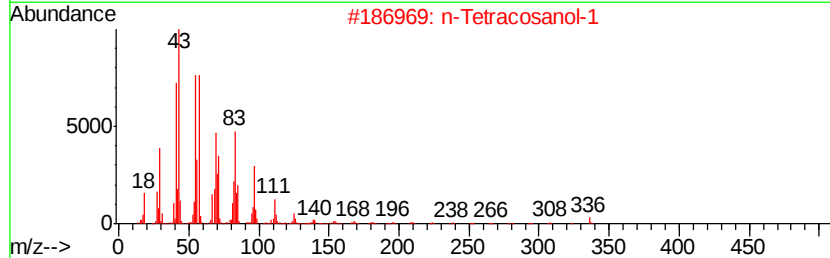
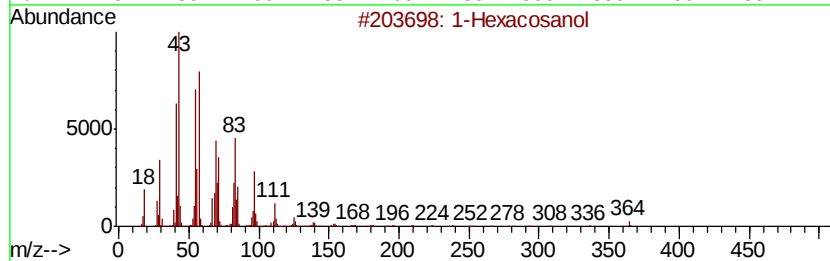
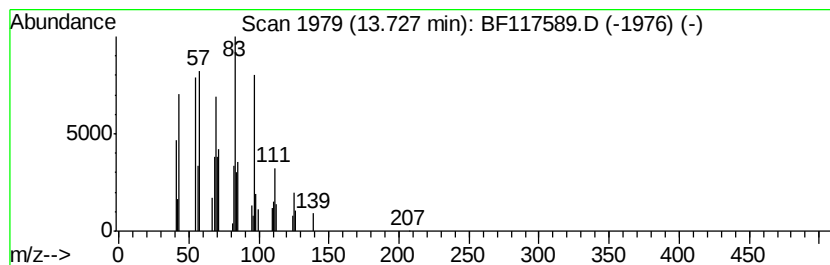
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	8.15 ng	87034	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexacosanol	382	C26H54O	000506-52-5	87
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3		17-Pentatriacontene	491	C35H70	006971-40-0	78
4		1-Eicosanol	298	C20H42O	000629-96-9	68
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	58



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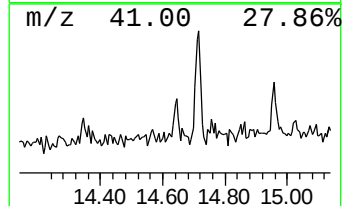
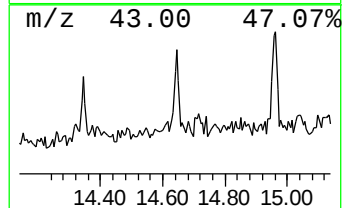
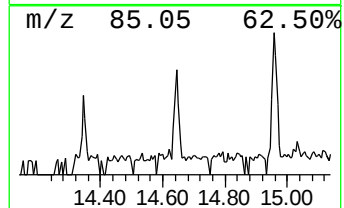
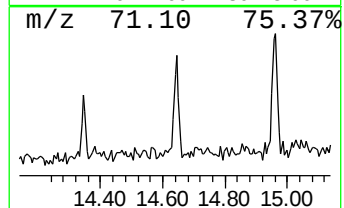
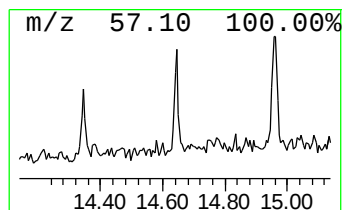
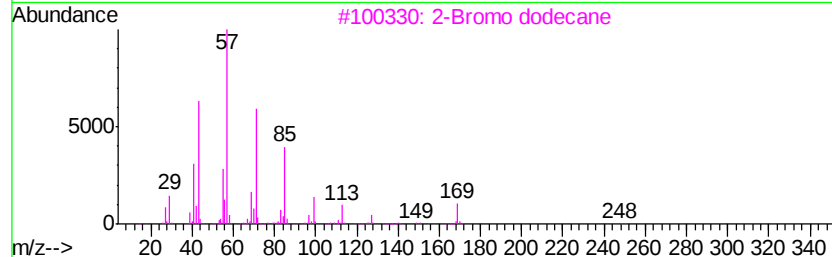
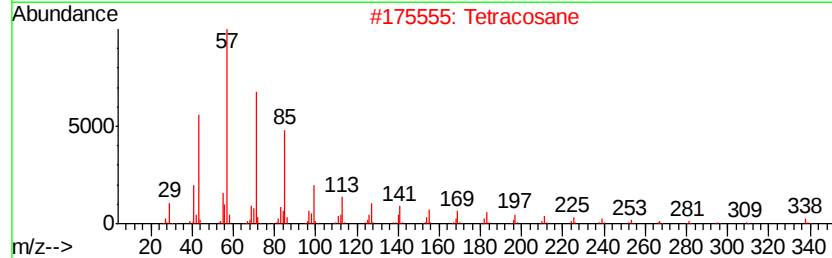
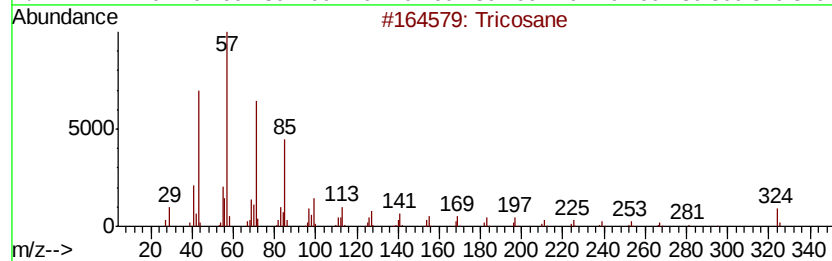
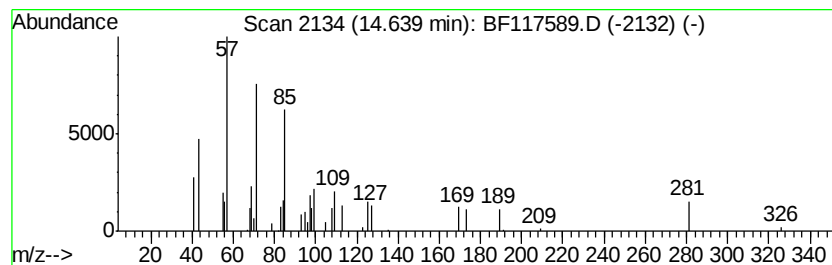
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.22 ng	20643	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	64
2	Tetracosane		338	C24H50	000646-31-1	59
3	2-Bromo dodecane		248	C12H25Br	013187-99-0	53
4	Sulfurous acid, butyl tetradecyl...		334	C18H38O3S	1000309-18-1	53
5	Heneicosane		296	C21H44	000629-94-7	53



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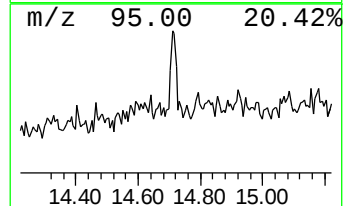
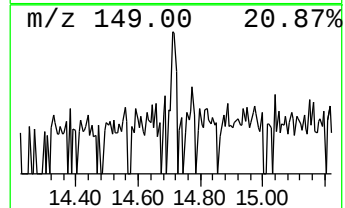
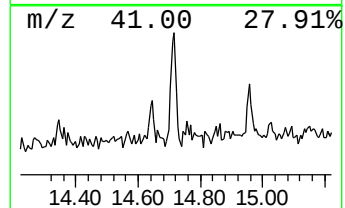
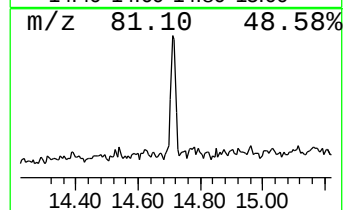
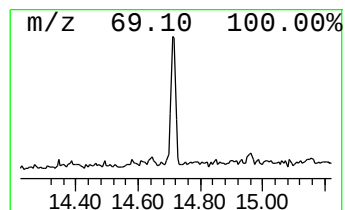
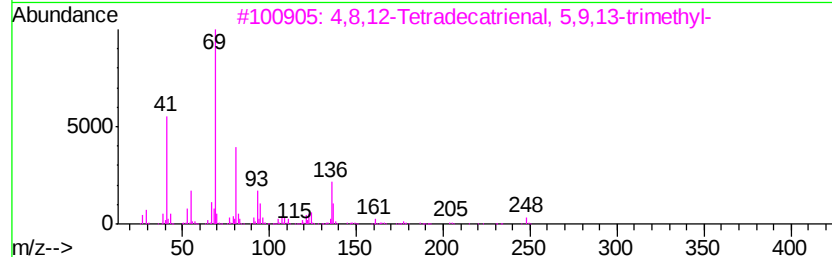
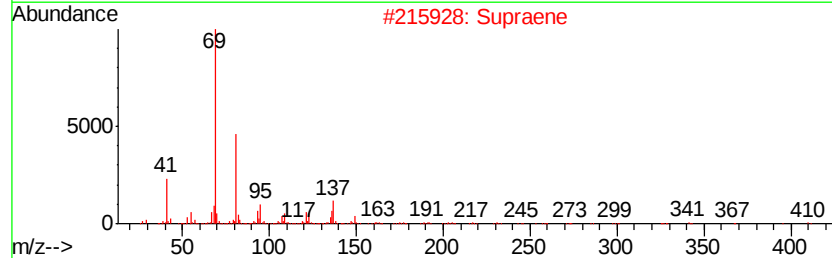
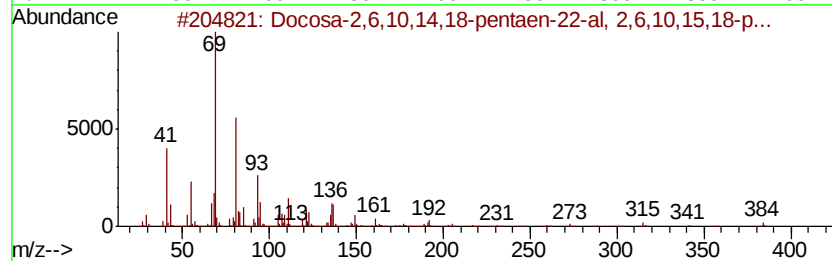
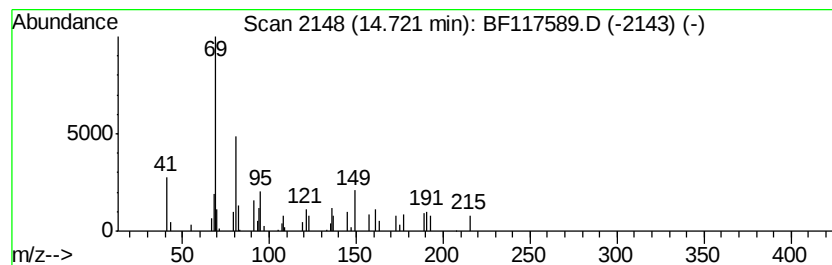
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Docosa-2,6,10,14,18-pentaen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	4.81 ng	44805	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
2		Supraene	410	C30H50	007683-64-9	74
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4		Squalene	410	C30H50	000111-02-4	64
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	53



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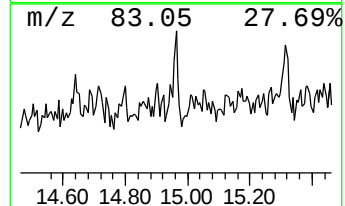
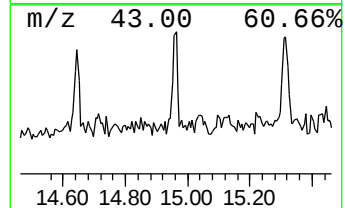
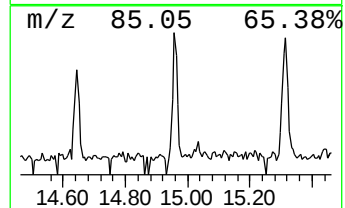
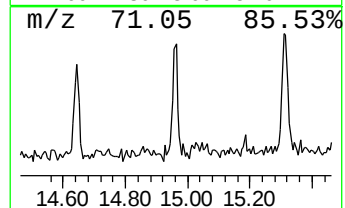
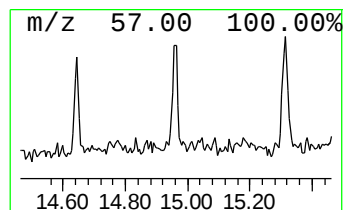
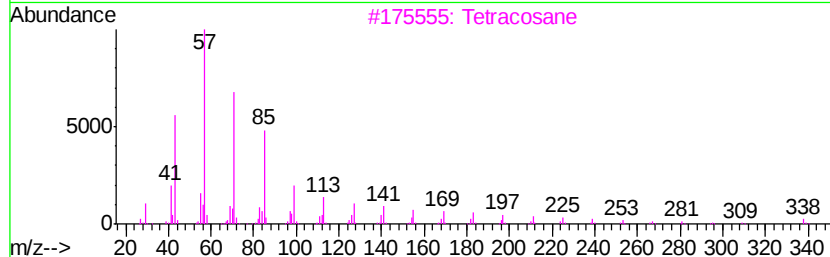
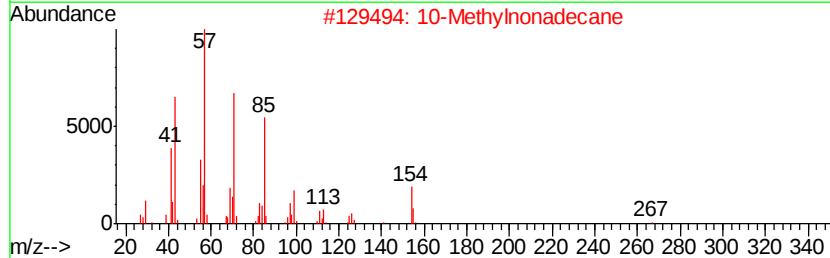
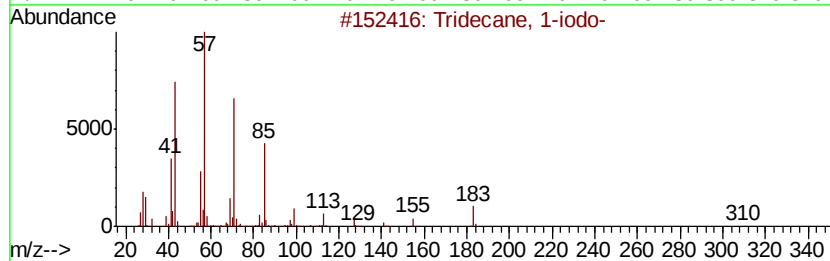
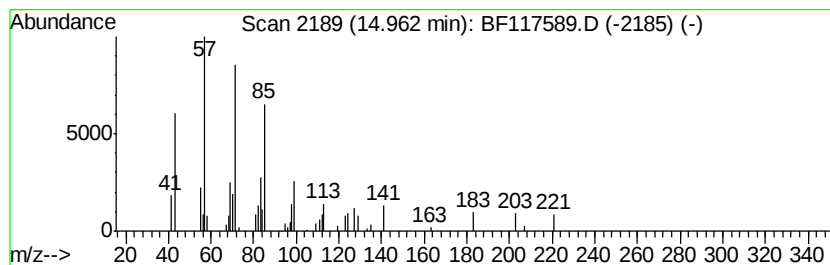
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tridecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.19 ng	29676	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	59
2		10-Methylnonadecane	282	C20H42	056862-62-5	59
3		Tetracosane	338	C24H50	000646-31-1	53
4		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53
5		Hentriacontane	437	C31H64	000630-04-6	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117589.D
Acq On : 29 Oct 2019 14:31
Operator : JU
Sample : K5503-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
171-64-(0-1.8)

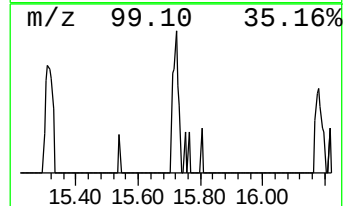
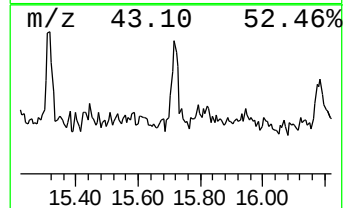
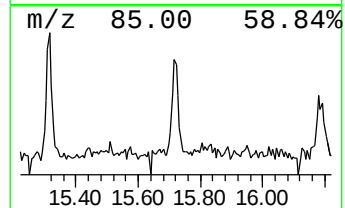
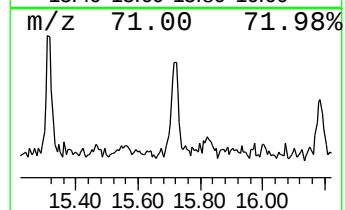
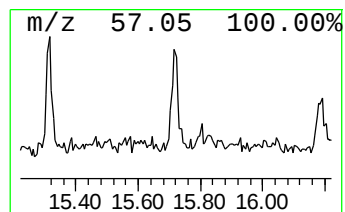
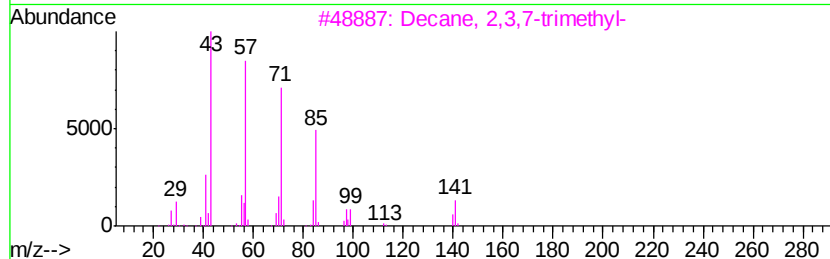
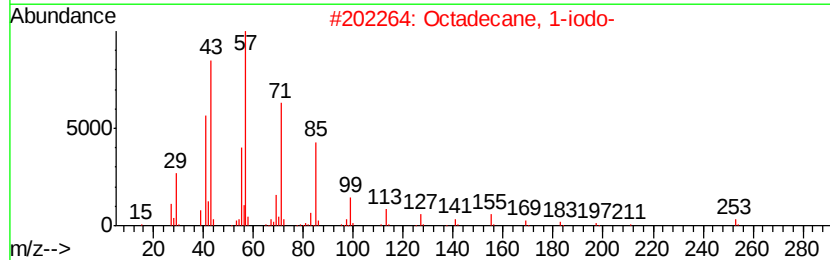
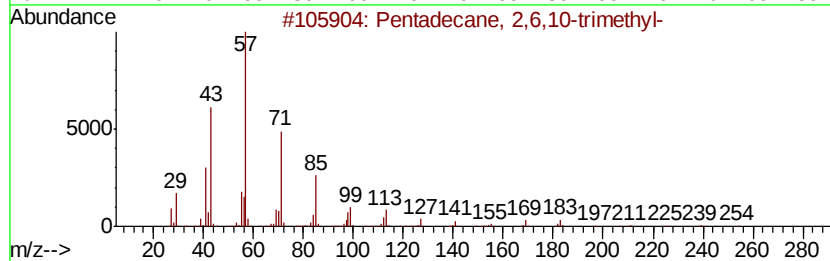
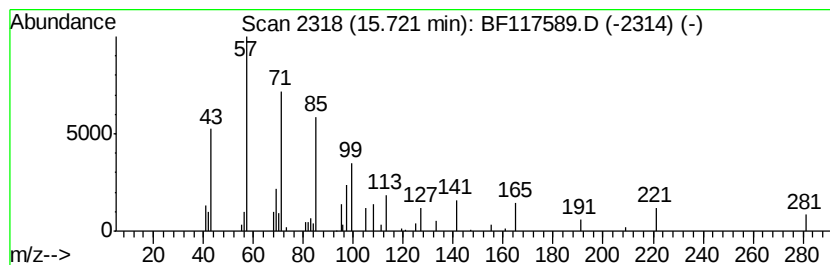
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.90 ng	26991	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	59
2		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	50
3		Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	47
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	47
5		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117589.D
Acq On : 29 Oct 2019 14:31
Operator : JU
Sample : K5503-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

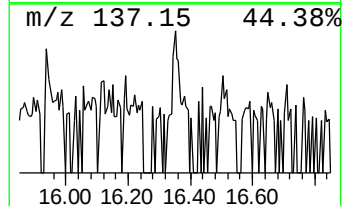
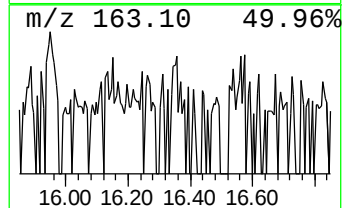
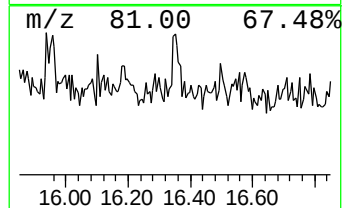
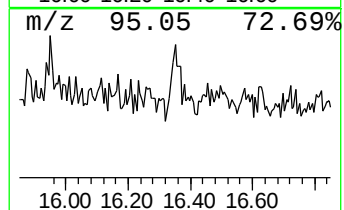
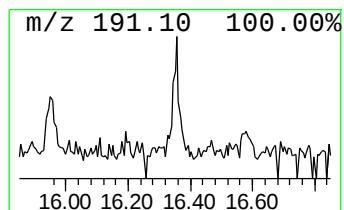
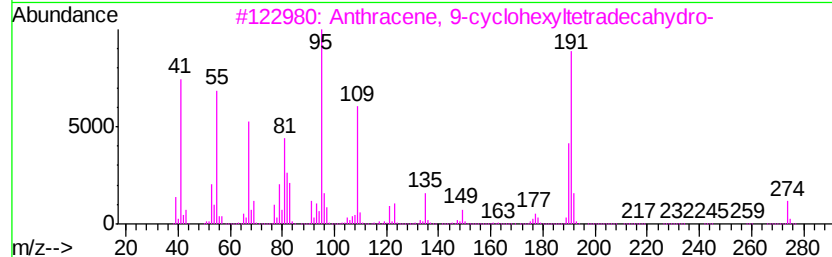
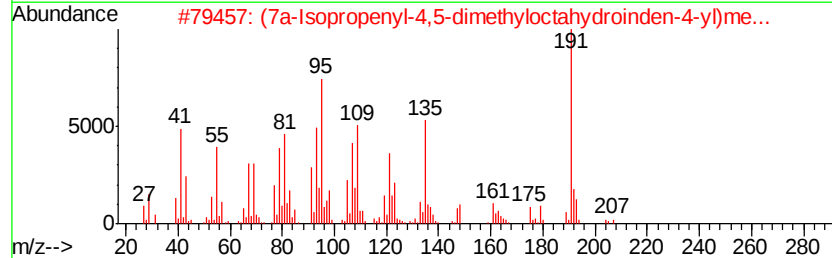
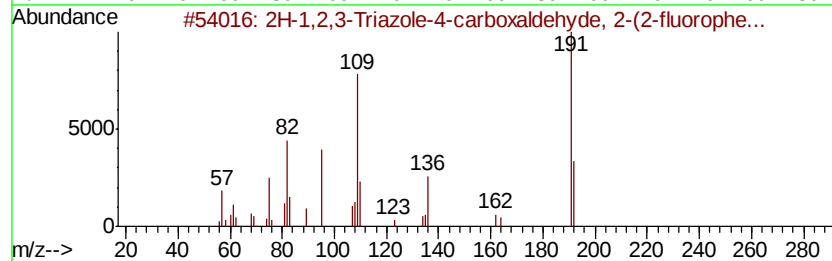
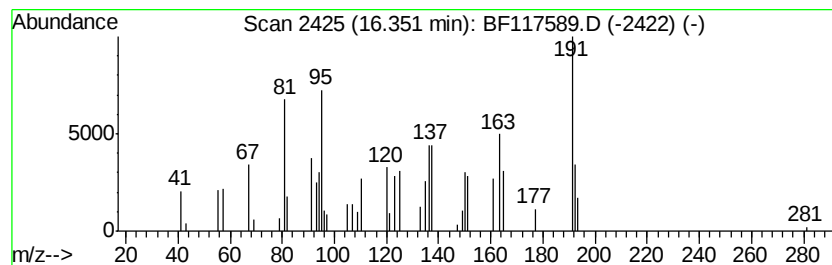
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.35 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.35	2.18 ng	20265	Perylene-d12	15.33		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehv...	191	C9H6FN3O	051306-43-5	35	
2	(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1000187-02-9	25	
3	Anthracene, 9-cvclohexyltetradec...	274	C20H34	055255-70-4	22	
4	4(1H)-Pteridinone, 2-amino-6,7-d...	191	C8H9N5O	000611-55-2	14	
5	Naphthalene, 1-(1,1-dimethylethy...	194	C14H26	056292-64-9	14	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102919\
Data File : BF117589.D
Acq On : 29 Oct 2019 14:31
Operator : JU
Sample : K5503-17
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
171-64-(0-1.8)

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
unknown6.50	6.50	90.9	ng	1043810	1	6.73	229562	20.0
Dodecanoic acid	11.77	2.7	ng	25522	4	11.25	190339	20.0
1-Hexacosanol	13.73	8.2	ng	87034	5	13.89	213491	20.0
Tricosane	14.64	2.2	ng	20643	6	15.33	186286	20.0
Docosa-2,6,10,14,...	14.72	4.8	ng	44805	6	15.33	186286	20.0
Tridecane, 1-iodo-	14.96	3.2	ng	29676	6	15.33	186286	20.0
Pentadecane, 2,6,...	15.72	2.9	ng	26991	6	15.33	186286	20.0
unknown16.35	16.35	2.2	ng	20265	6	15.33	186286	20.0