

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
 Data File : BF108240.D
 Acq On : 17 Aug 2018 13:52
 Operator : JU/SJ
 Sample : J4511-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RA-081518-FL-031

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-BF080818.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	5.249	491	495	502	rVB	144857	168927	4.47%	0.495%
2	5.637	556	561	564	rBV	3167104	3002537	79.52%	8.799%
3	6.631	725	730	738	rBV	3066551	3280119	86.87%	9.613%
4	6.784	751	756	759	rBV	3624615	3152000	83.47%	9.237%
5	7.013	791	795	799	rBV	1153366	924593	24.49%	2.710%
6	7.172	818	822	825	rBV	2886183	2449356	64.87%	7.178%
7	7.578	886	891	894	rBV	2132114	2096489	55.52%	6.144%
8	8.295	1009	1013	1018	rBV	1376176	1178896	31.22%	3.455%
9	9.372	1191	1196	1199	rBV	4376113	3775993	100.00%	11.066%
10	9.437	1204	1207	1210	rVV2	47838	44125	1.17%	0.129%
11	9.760	1259	1262	1265	rBV	471225	351195	9.30%	1.029%
12	10.060	1309	1313	1317	rBV	1491157	1293047	34.24%	3.789%
13	10.236	1340	1343	1345	rBV4	33236	44563	1.18%	0.131%
14	10.372	1363	1366	1369	rBV	69037	98790	2.62%	0.290%
15	10.466	1380	1382	1386	rVB	88385	80750	2.14%	0.237%
16	10.854	1443	1448	1460	rBV	2287231	2394834	63.42%	7.018%
17	10.954	1461	1465	1473	rVB2	99437	192118	5.09%	0.563%
18	11.395	1537	1540	1542	rBV	83609	72363	1.92%	0.212%
19	11.554	1564	1567	1570	rBV	1490292	1294563	34.28%	3.794%
20	11.578	1570	1571	1575	rVB	185817	117266	3.11%	0.344%
21	12.060	1650	1653	1656	rBV2	232936	259731	6.88%	0.761%
22	12.783	1773	1776	1778	rVB	207877	179857	4.76%	0.527%
23	13.007	1812	1814	1820	rVB	202797	204035	5.40%	0.598%
24	13.142	1833	1837	1840	rBV	3520233	3065194	81.18%	8.983%
25	14.048	1988	1991	2000	rVB3	253076	421490	11.16%	1.235%
26	14.207	2014	2018	2021	rBV	1188524	1204049	31.89%	3.529%
27	14.648	2091	2093	2098	rVB	213283	203233	5.38%	0.596%
28	14.977	2146	2149	2152	rVB	272586	273721	7.25%	0.802%
29	15.342	2208	2211	2218	rVB2	345936	462385	12.25%	1.355%
30	15.771	2278	2284	2289	rBV2	809982	1420583	37.62%	4.163%
31	16.236	2360	2363	2371	rVB	250555	416349	11.03%	1.220%

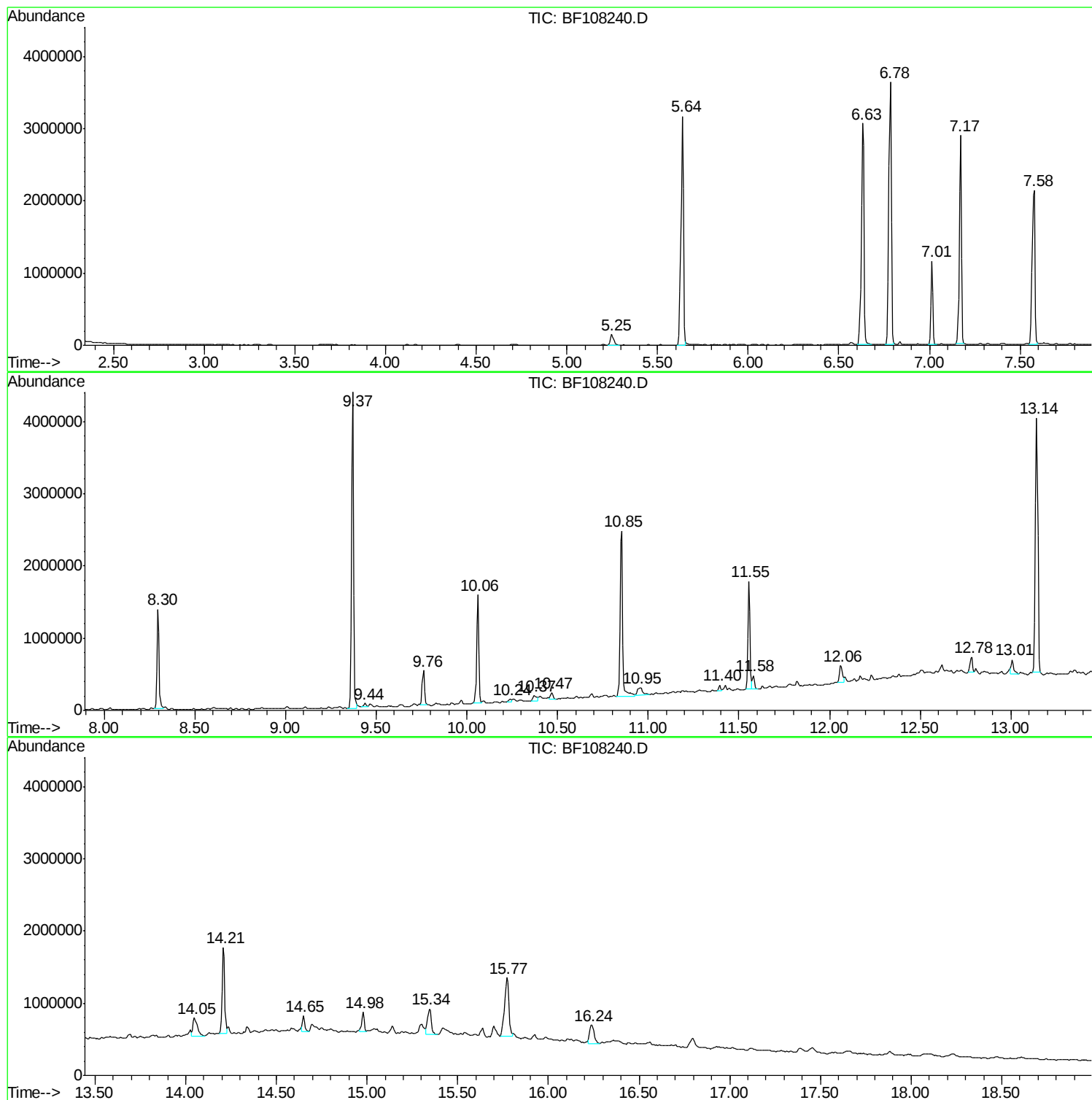
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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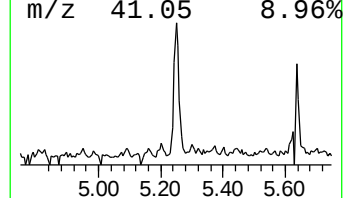
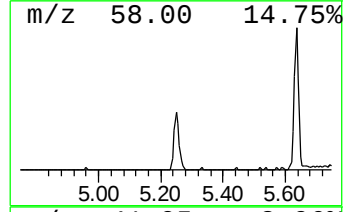
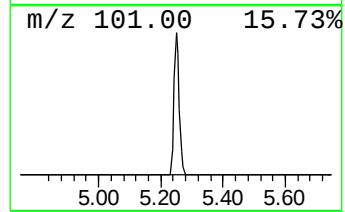
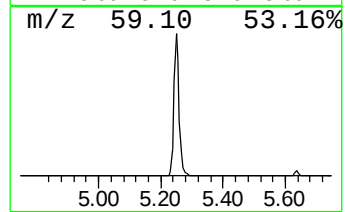
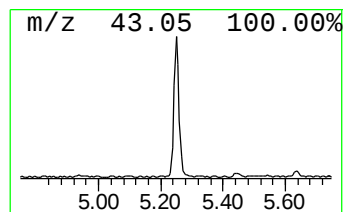
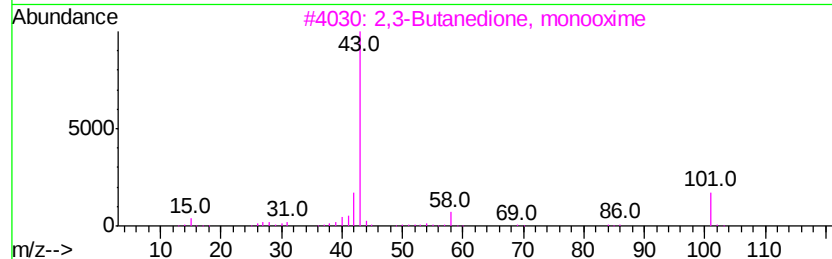
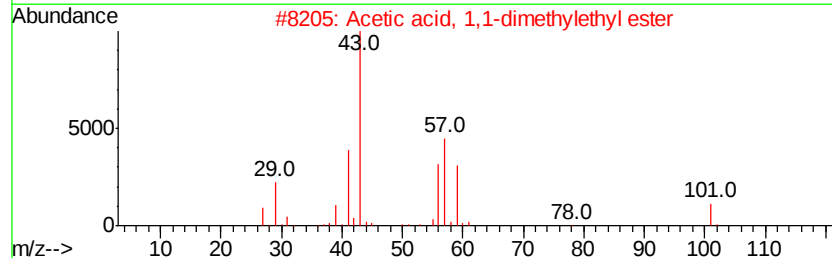
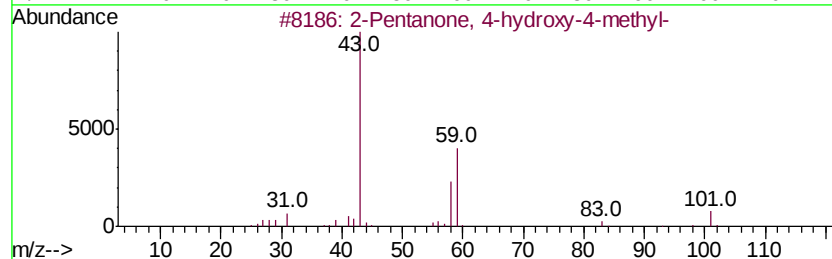
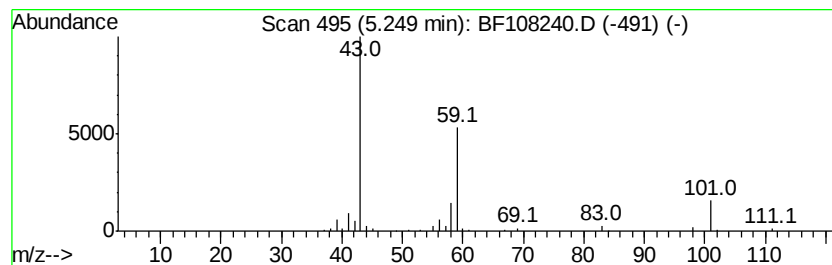
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	3.65 ng	168927	1,4-Dichlorobenzene-d4	7.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23



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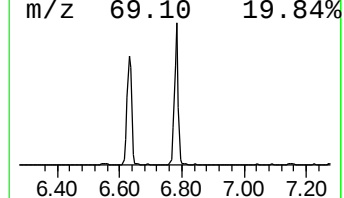
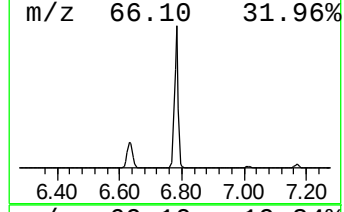
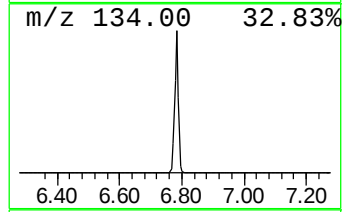
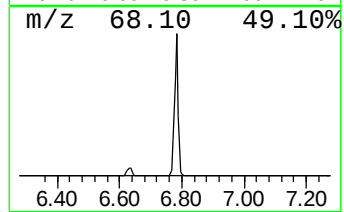
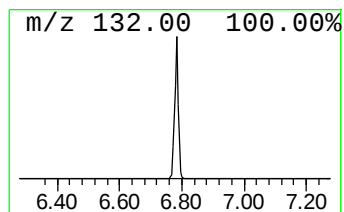
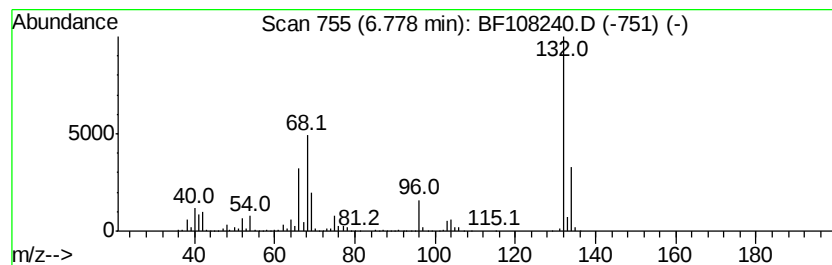
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	68.18 ng	3152000	1,4-Dichlorobenzene-d4	7.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	
3	Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	10	
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9	
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	



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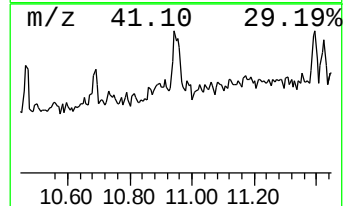
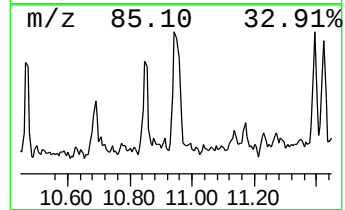
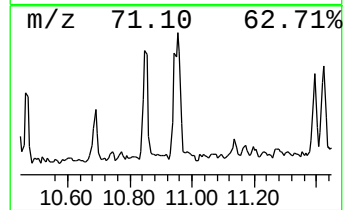
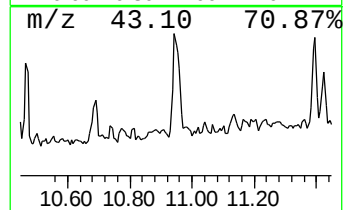
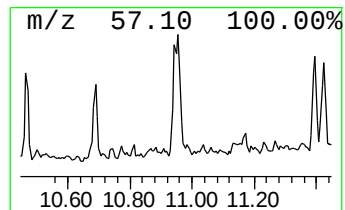
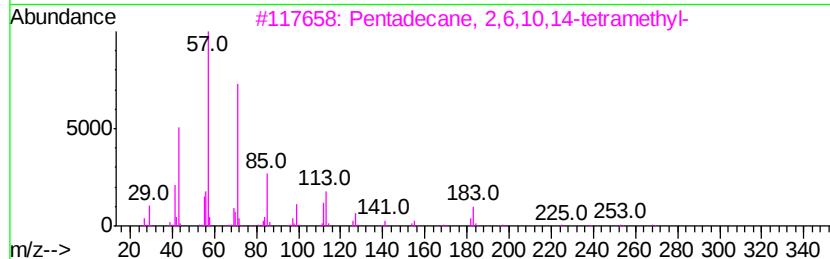
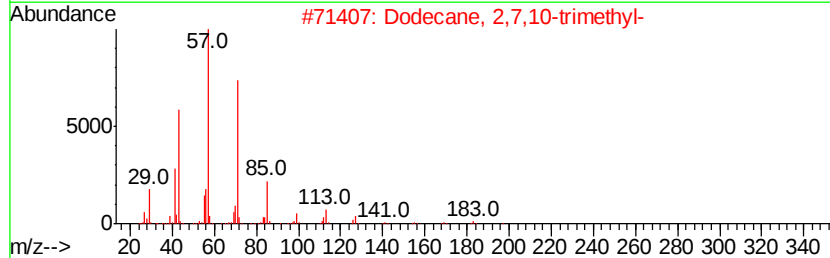
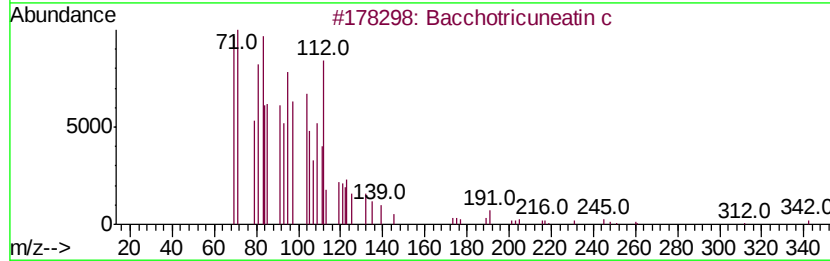
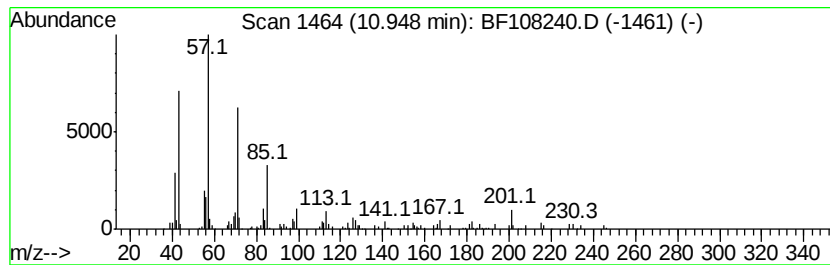
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Peak Number 4 Bacchotricuneatin c Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	2.97 ng	192118	Phenanthrene-d10	11.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	95
2		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
4		Heptacosane	380	C27H56	000593-49-7	72
5		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64



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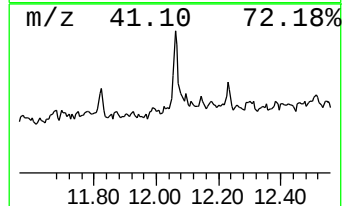
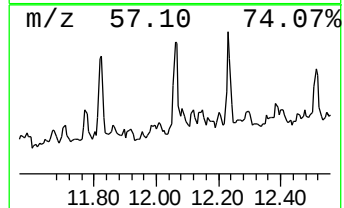
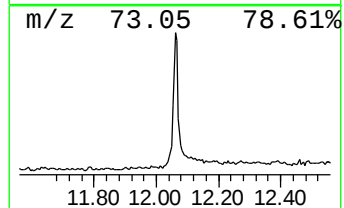
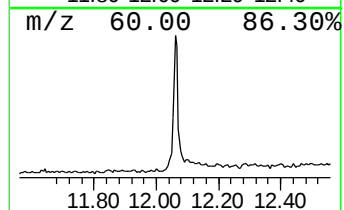
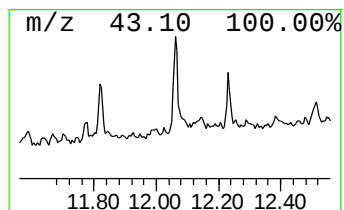
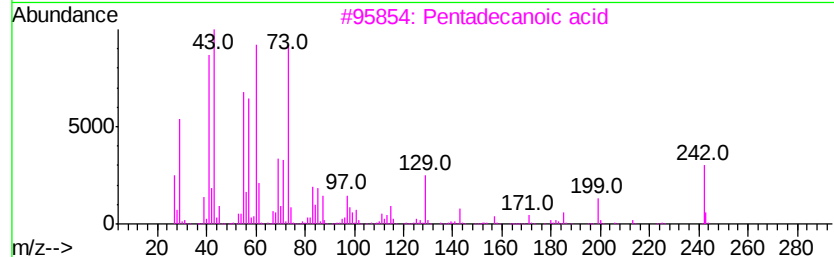
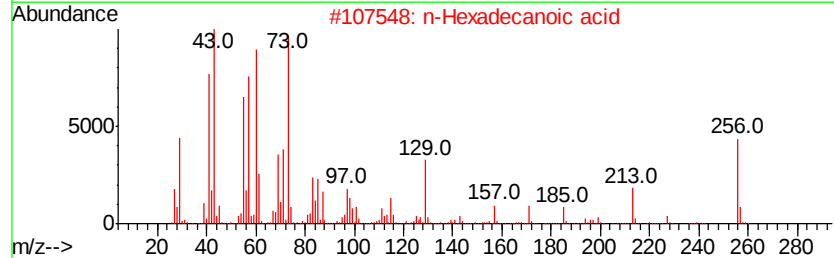
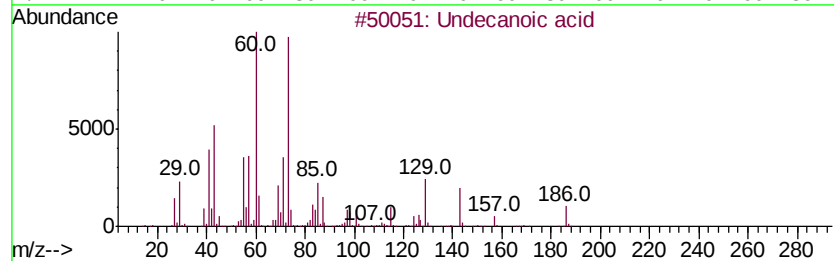
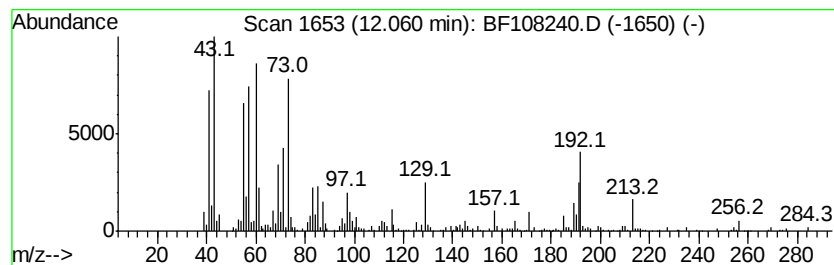
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Peak Number 5 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	4.01 ng	259731	Phenanthrene-d10	11.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	64
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	60
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	52
4	Octadecanoic acid		284	C18H36O2	000057-11-4	45
5	Nonanoic acid		158	C9H18O2	000112-05-0	30



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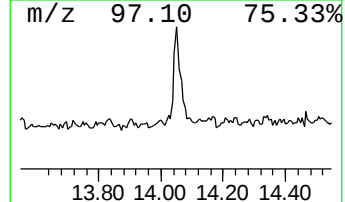
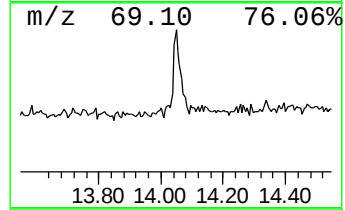
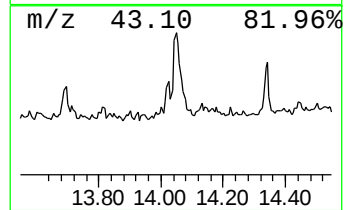
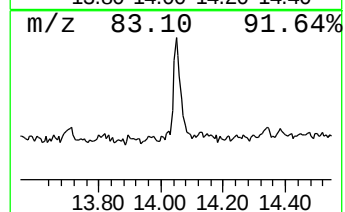
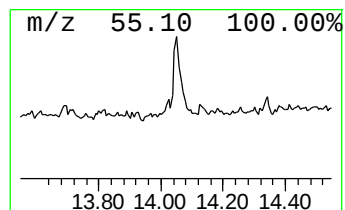
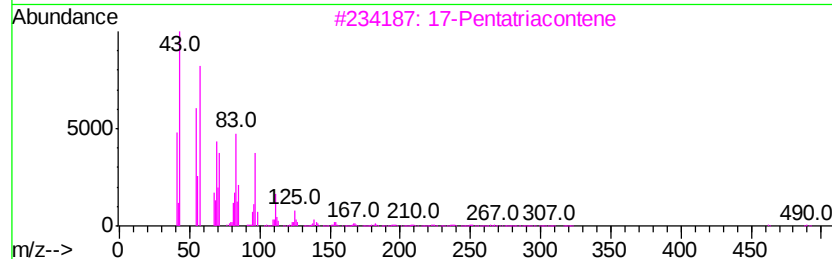
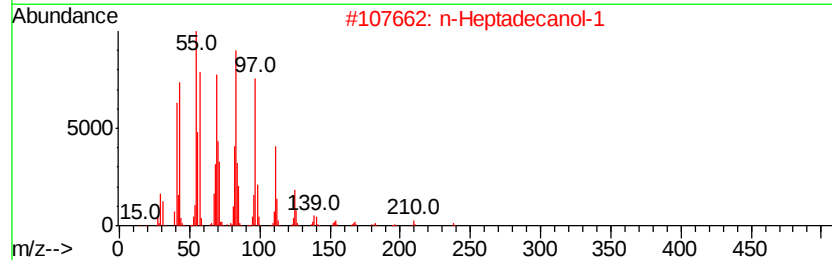
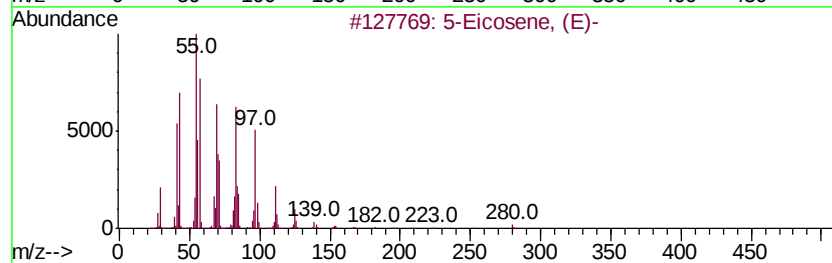
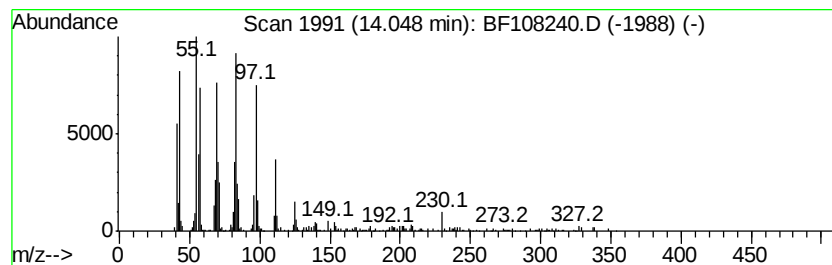
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Peak Number 6 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.05	7.00 ng	421490	Chrysene-d12	14.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	93
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Cyclopentadecane	210	C15H30	000295-48-7	91



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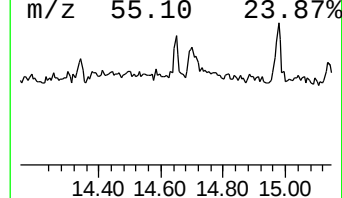
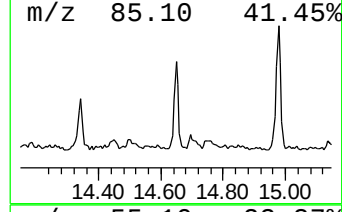
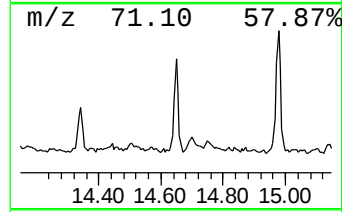
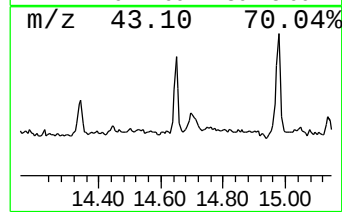
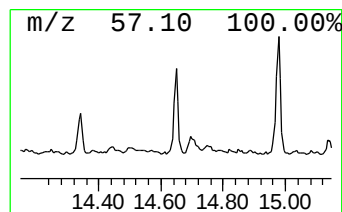
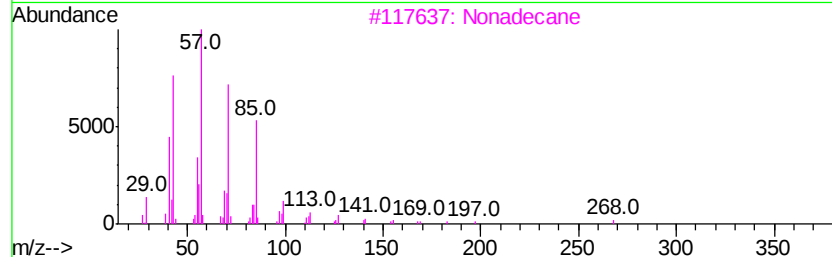
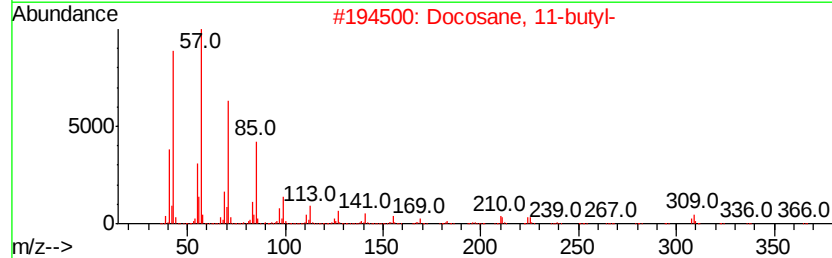
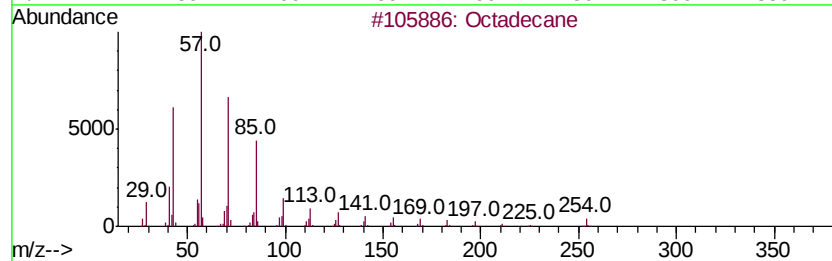
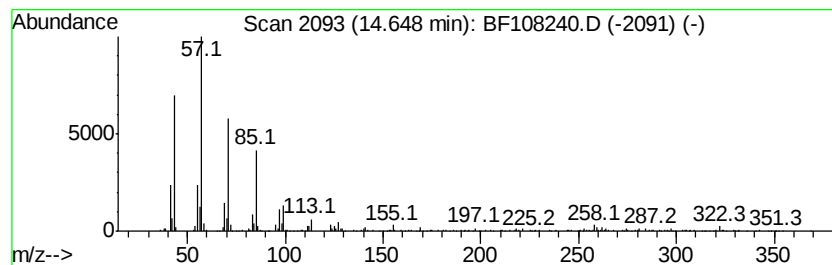
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	3.38 ng	203233	Chrysene-d12	14.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
3		Nonadecane	268	C19H40	000629-92-5	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108240.D
Acq On : 17 Aug 2018 13:52
Operator : JU/SJ
Sample : J4511-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

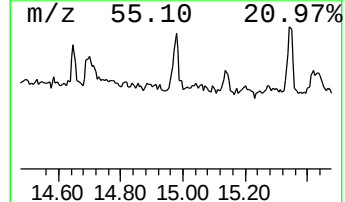
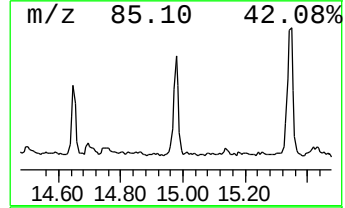
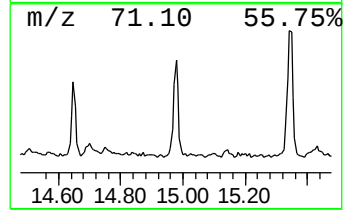
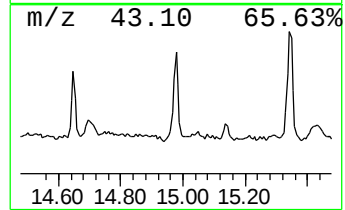
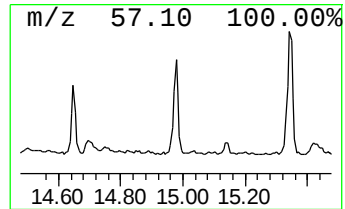
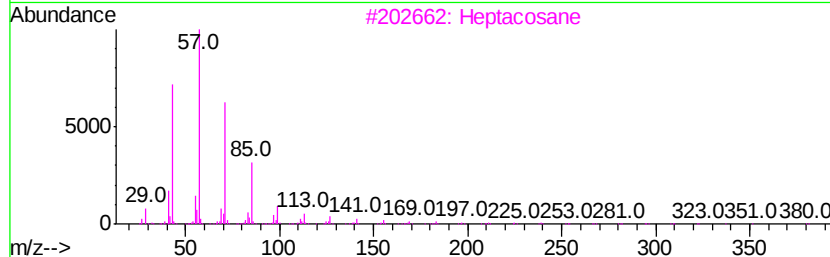
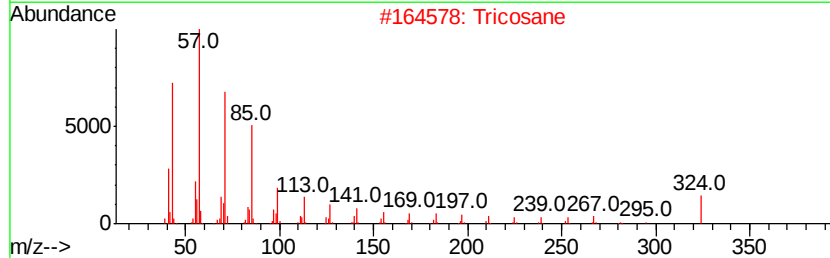
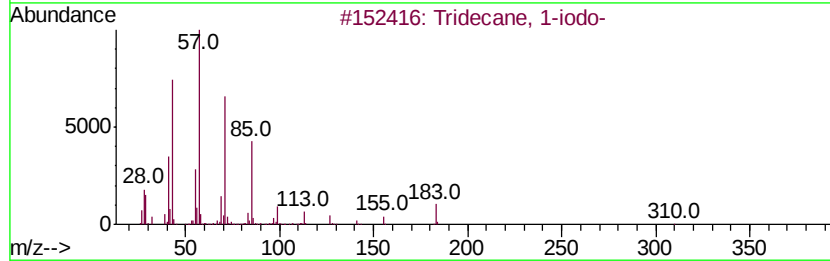
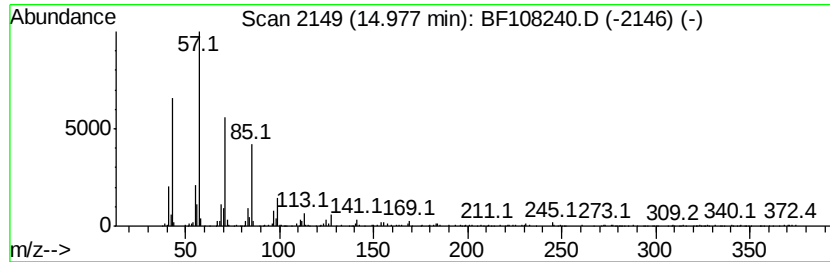
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.98	4.55 ng	273721	Chrysene-d12	14.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
2	Tricosane	324	C23H48	000638-67-5	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081718\
Data File : BF108240.D
Acq On : 17 Aug 2018 13:52
Operator : JU/SJ
Sample : J4511-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
RA-081518-FL-031

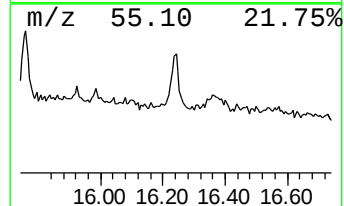
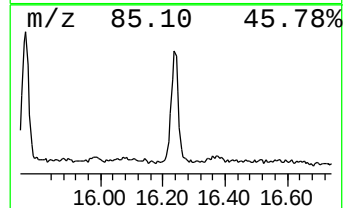
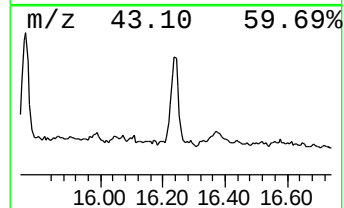
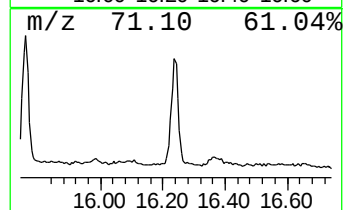
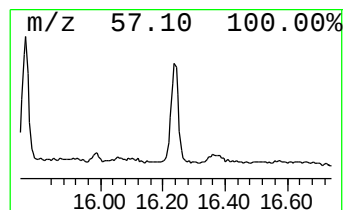
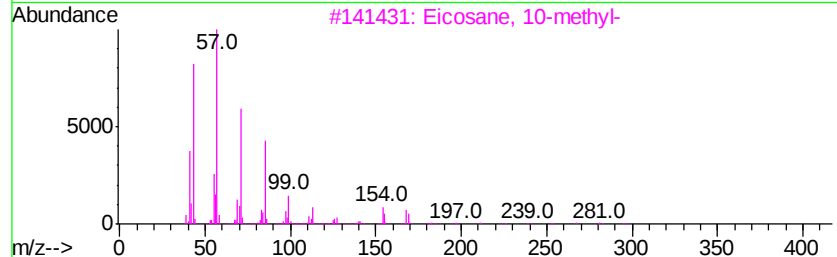
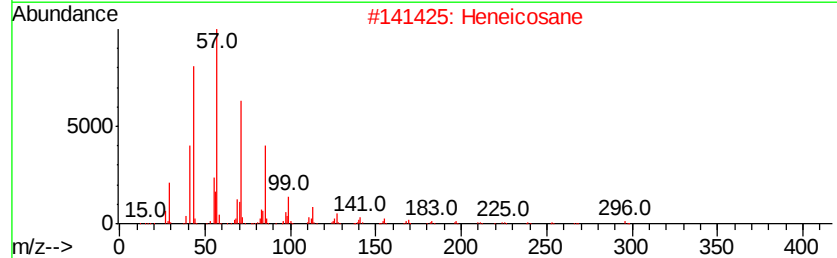
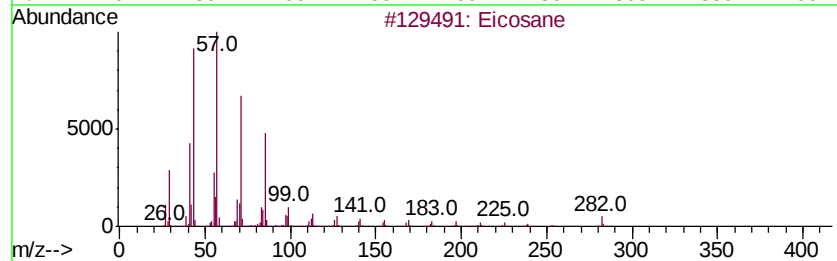
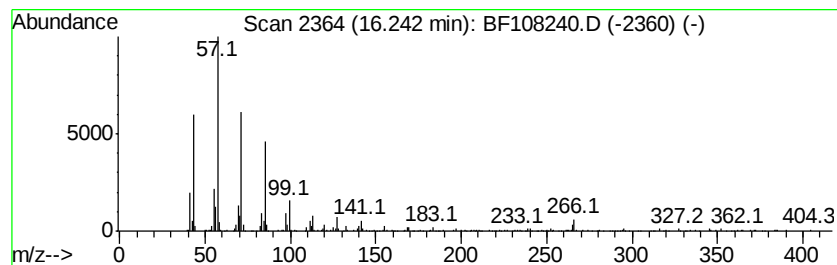
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	5.86 ng	416349	Perylene-d12	15.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	95
2	Heneicosane		296	C21H44	000629-94-7	95
3	Eicosane, 10-methyl-		296	C21H44	054833-23-7	91
4	Heptacosane		380	C27H56	000593-49-7	90
5	Eicosane, 3-methyl-		296	C21H44	006418-46-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
 Data File : BF108240.D
 Acq On : 17 Aug 2018 13:52
 Operator : JU/SJ
 Sample : J4511-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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
2-Pentanone, 4-hy...	5.25	3.6 ng		168927	1	7.01	924593	20.0
unknown6.78	6.78	68.2 ng		3152000	1	7.01	924593	20.0
Bacchotricuneatin c	10.95	3.0 ng		192118	4	11.55	1294560	20.0
Undecanoic acid	12.06	4.0 ng		259731	4	11.55	1294560	20.0
5-Eicosene, (E)-	14.05	7.0 ng		421490	5	14.21	1204050	20.0
Octadecane	14.65	3.4 ng		203233	5	14.21	1204050	20.0
Tridecane, 1-iodo-	14.98	4.5 ng		273721	5	14.21	1204050	20.0
Eicosane	16.24	5.9 ng		416349	6	15.78	1420580	20.0