

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
 Data File : BF108698.D
 Acq On : 31 Aug 2018 19:23
 Operator : JU/SJ
 Sample : J4720-05 5X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BZTRANS-5

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-BF083018.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	6.707	733	743	746	rBV5	17290	63326	7.84%	0.920%
2	6.789	752	757	781	rVB4	38422	151955	18.82%	2.208%
3	7.001	790	793	815	rBV	156979	411679	50.99%	5.982%
4	7.154	815	819	837	rVB	80706	171087	21.19%	2.486%
5	7.601	889	895	906	rBV4	16797	78792	9.76%	1.145%
6	8.283	1007	1011	1045	rBV	299510	598569	74.14%	8.697%
7	9.354	1189	1193	1206	rBV	149837	256611	31.79%	3.729%
8	9.748	1256	1260	1268	rBV	38498	56834	7.04%	0.826%
9	10.042	1306	1310	1329	rBV	468710	606749	75.16%	8.816%
10	10.842	1443	1446	1457	rBV2	47044	92485	11.46%	1.344%
11	10.918	1457	1459	1464	rVB3	6971	8918	1.10%	0.130%
12	11.365	1528	1535	1537	rBV2	7174	9311	1.15%	0.135%
13	11.542	1561	1565	1568	rBV	376423	497353	61.61%	7.226%
14	12.042	1647	1650	1653	rBV4	8203	11822	1.46%	0.172%
15	12.077	1654	1656	1662	rVB6	8931	12257	1.52%	0.178%
16	12.171	1666	1672	1675	rBV7	9990	22292	2.76%	0.324%
17	12.377	1704	1707	1713	rBV8	15599	28423	3.52%	0.413%
18	12.759	1768	1772	1782	rBV	139819	213800	26.48%	3.106%
19	12.871	1788	1791	1795	rBV	43530	47341	5.86%	0.688%
20	12.995	1808	1812	1818	rVB	101936	124412	15.41%	1.808%
21	13.118	1830	1833	1844	rBV	215702	289361	35.84%	4.204%
22	14.036	1985	1989	1997	rVB8	32048	70096	8.68%	1.018%
23	14.136	2003	2006	2009	rVB	50839	46312	5.74%	0.673%
24	14.195	2011	2016	2026	rBV	533179	807323	100.00%	11.730%
25	14.612	2085	2087	2094	rBV3	38577	50924	6.31%	0.740%
26	14.871	2127	2131	2140	rBV	387917	676551	83.80%	9.830%
27	15.100	2166	2170	2177	rVB	171993	202057	25.03%	2.936%
28	15.300	2198	2204	2212	rVB2	134896	255148	31.60%	3.707%
29	15.395	2214	2220	2233	rVB6	73470	175077	21.69%	2.544%
30	15.706	2267	2273	2276	rBV3	44858	86283	10.69%	1.254%
31	15.753	2276	2281	2290	rVB	249008	437195	54.15%	6.352%
32	15.930	2307	2311	2319	rVB	145998	218187	27.03%	3.170%
33	16.177	2349	2353	2359	rVB2	65518	103837	12.86%	1.509%

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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-BF083018.M
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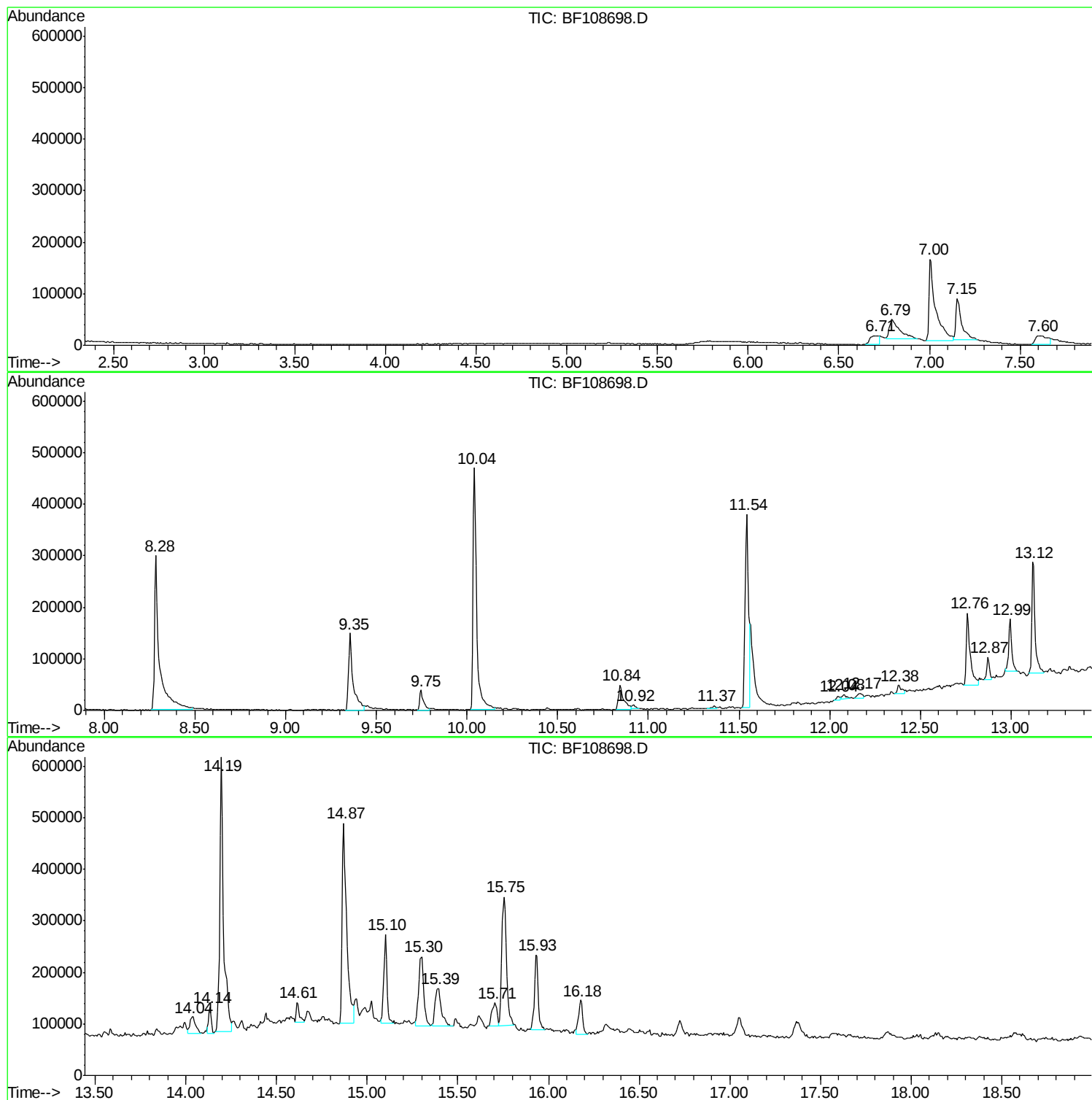
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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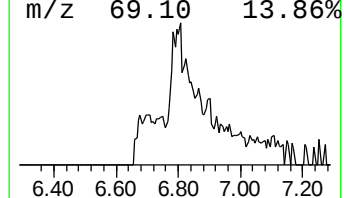
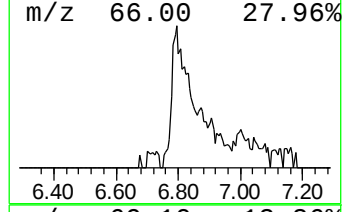
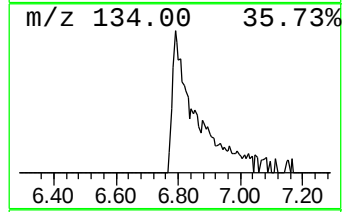
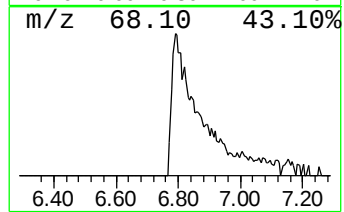
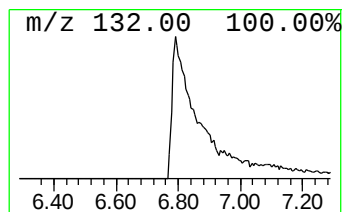
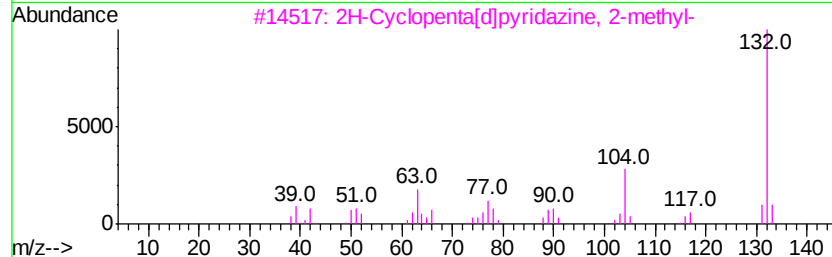
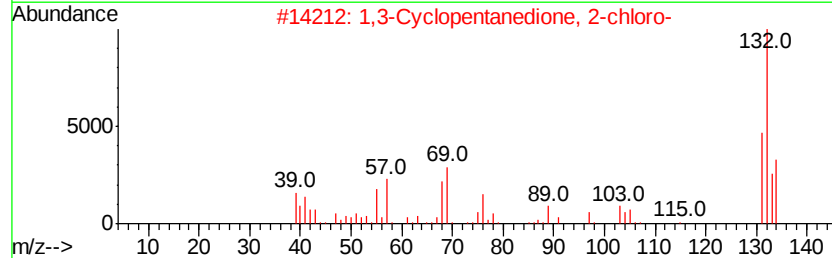
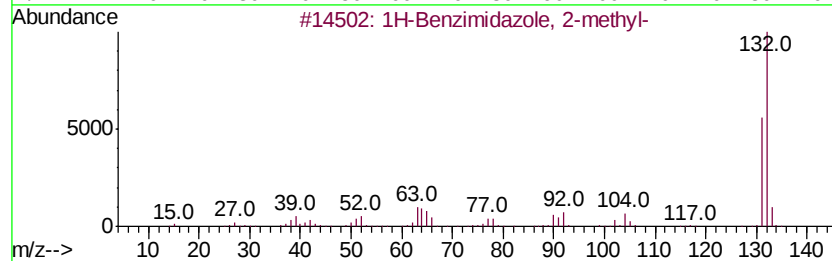
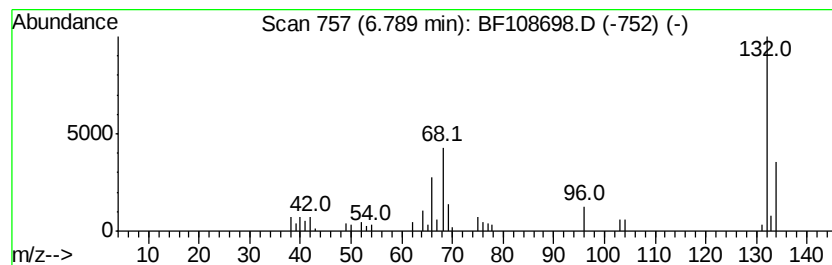
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083018.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.79 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	7.38 ng	151955	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	16



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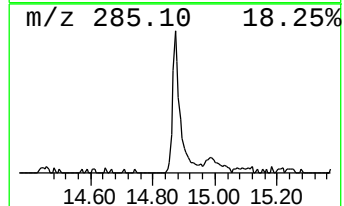
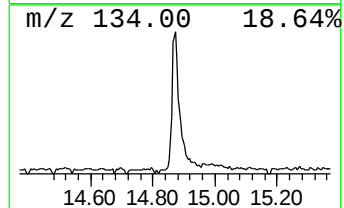
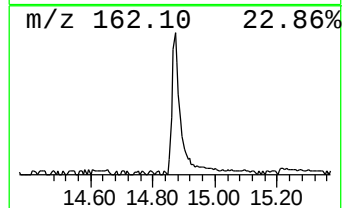
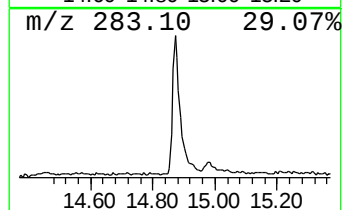
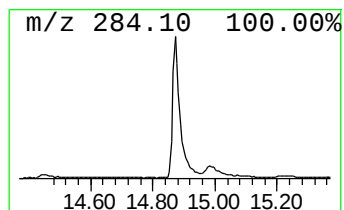
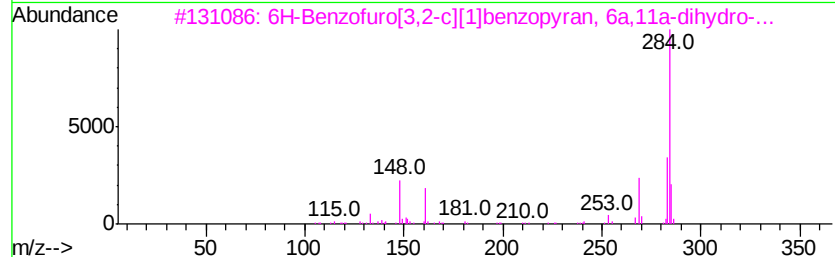
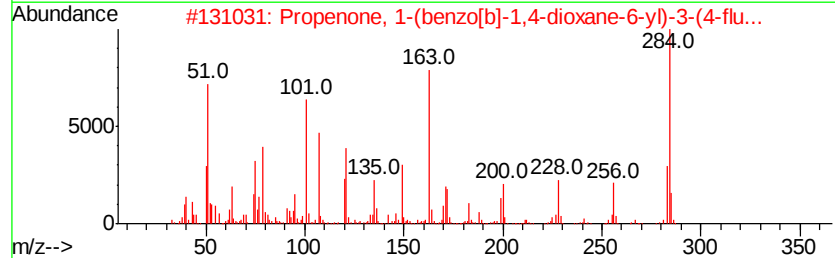
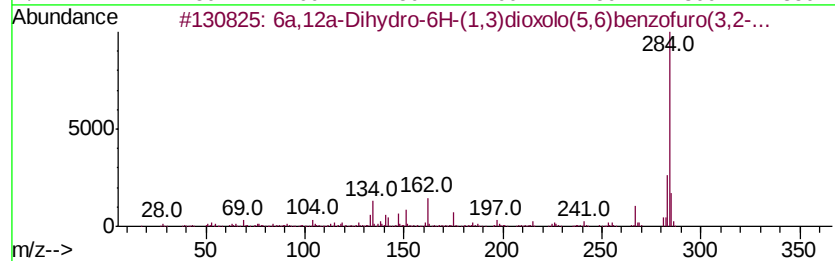
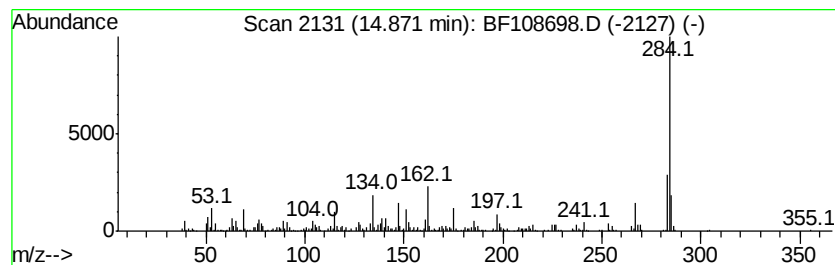
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.87	16.76 ng	676551	Chrysene-d12	14.19		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	022091-18-5	95	
2	Propenone, 1-(benzo[b]-1,4-dioxa...	284	C17H13FO3	133188-35-9	60	
3	6H-Benzofuro[3,2-c][1]benzopyran...	284	C17H16O4	000606-91-7	60	
4	3-Hydroxy-2-(4-hydroxy-3-methoxy...	284	C16H12O5	159184-95-9	53	
5	Thiazole, 2-(4-fluorophenylamino...	284	C16H13FN2S	340801-58-3	47	



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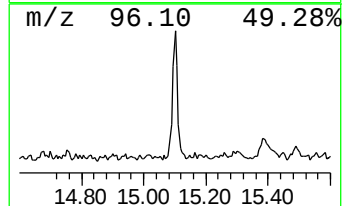
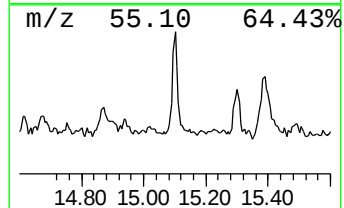
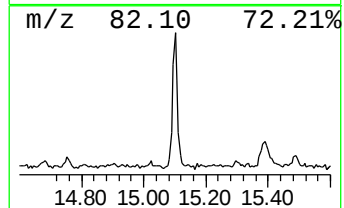
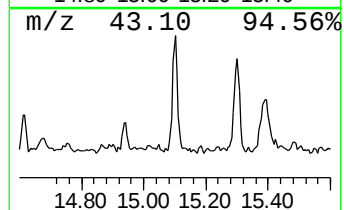
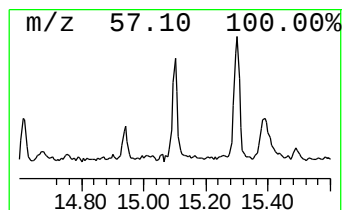
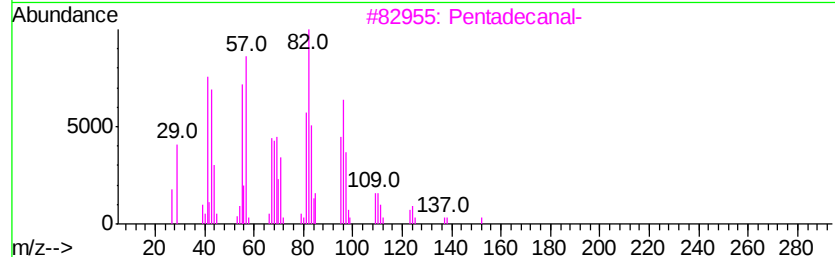
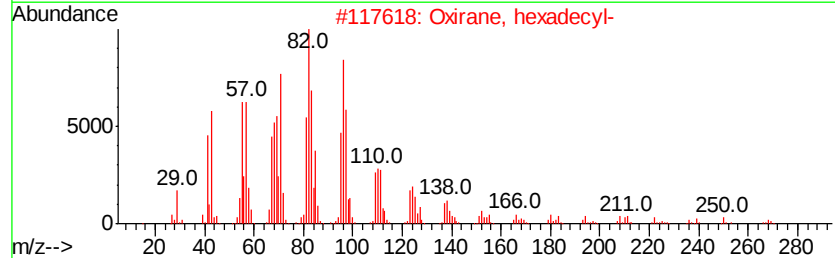
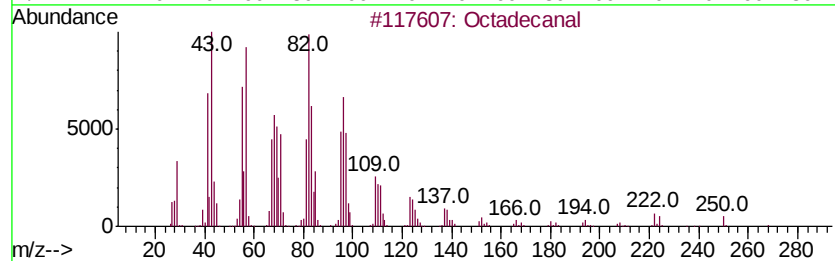
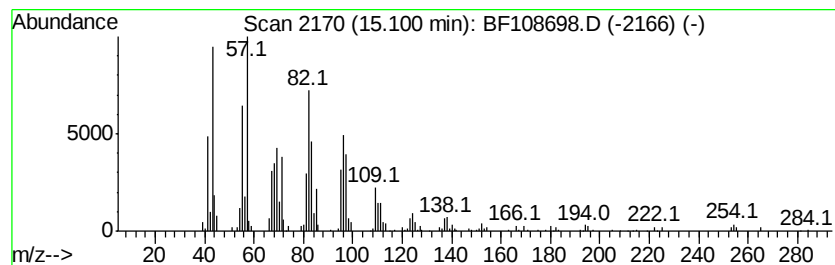
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	9.24 ng	202057	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanal	268	C18H36O	000638-66-4	91
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3		Pentadecanal-	226	C15H30O	002765-11-9	68
4		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	64
5		Hexadecanal	240	C16H32O	000629-80-1	58



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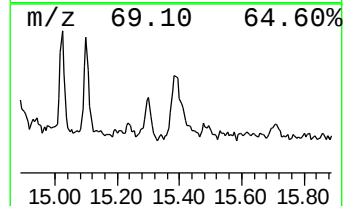
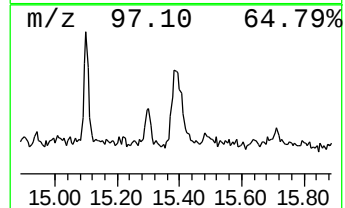
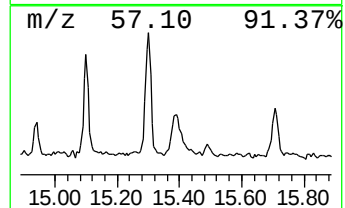
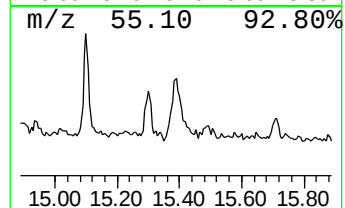
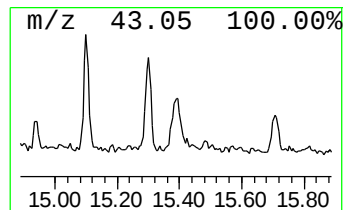
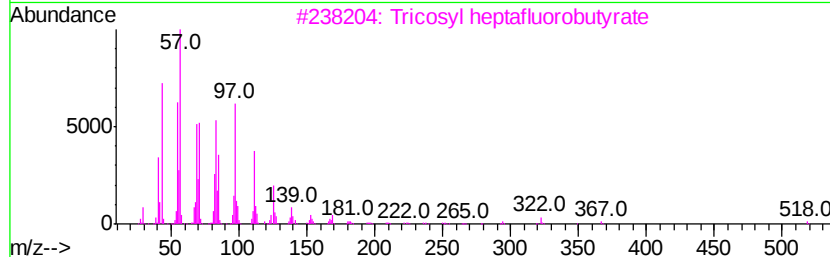
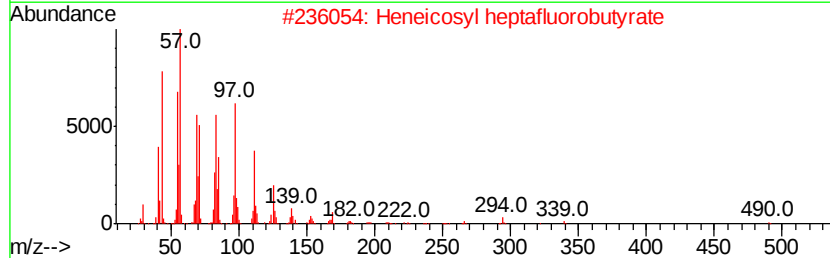
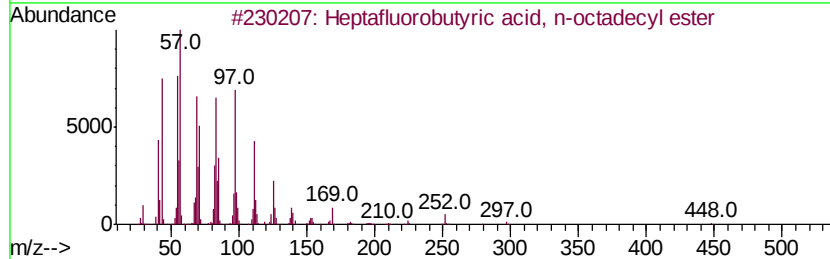
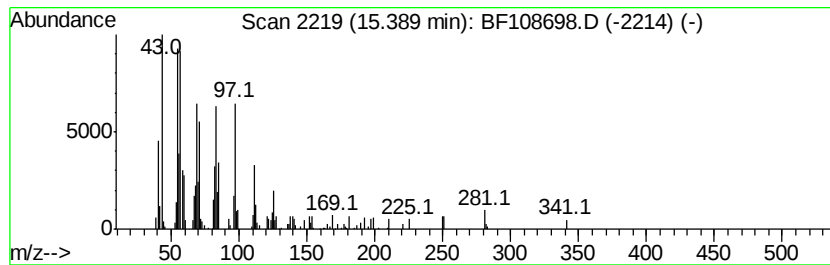
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	8.01 ng	175077	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-octadecyl...	466	C22H37F7O2	000400-57-7	93
2		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	93
3		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90
4		3-Heptadecenal	252	C17H32O	1000143-48-7	83
5		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81



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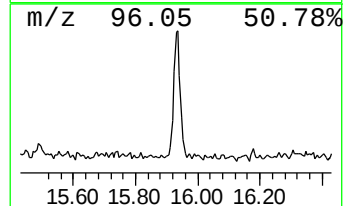
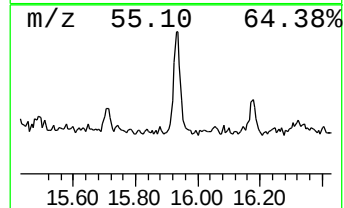
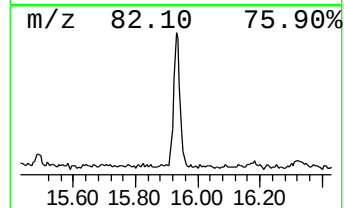
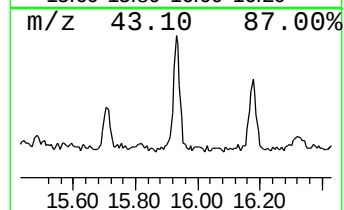
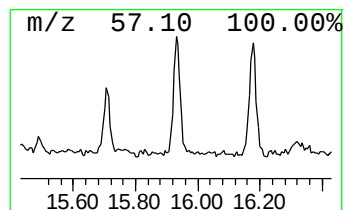
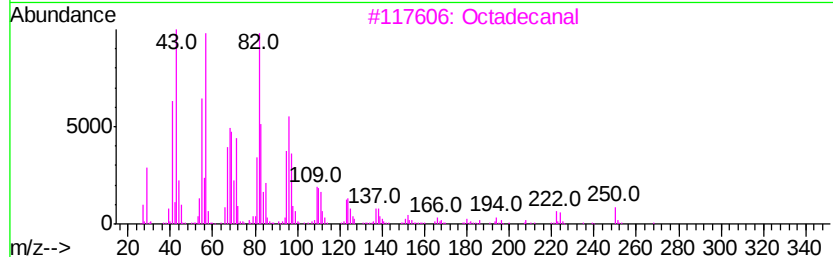
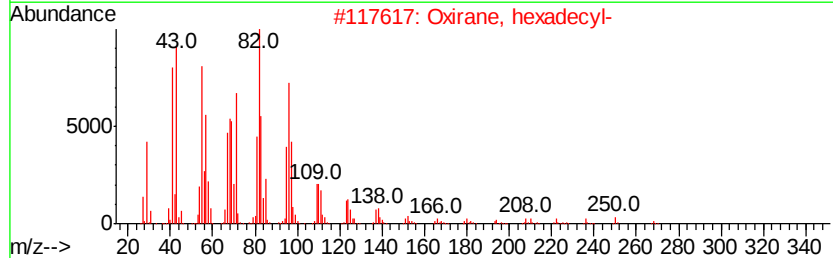
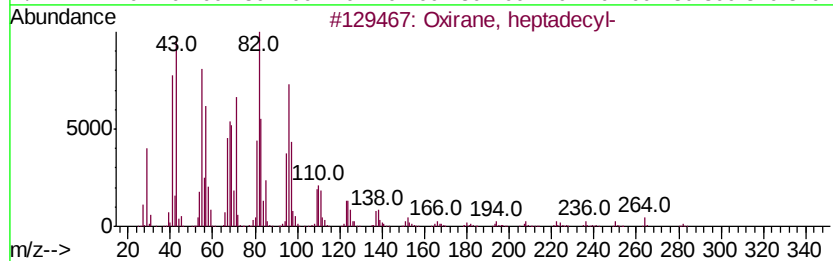
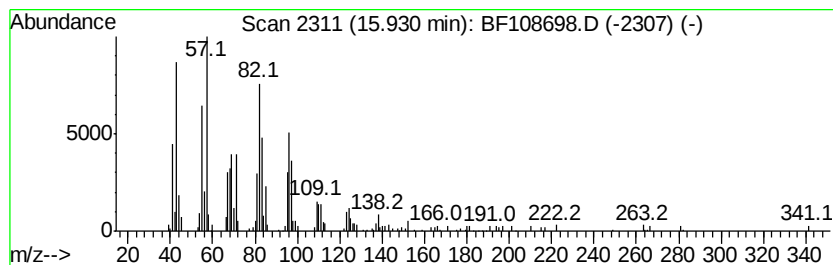
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxirane, heptadecyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	9.98 ng	218187	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3		Octadecanal	268	C18H36O	000638-66-4	91
4		Tetradecanal	212	C14H28O	000124-25-4	90
5		Oleyl alcohol, methyl ether	282	C19H38O	1000352-68-0	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
 Data File : BF108698.D
 Acq On : 31 Aug 2018 19:23
 Operator : JU/SJ
 Sample : J4720-05 5X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BZTRANS-5

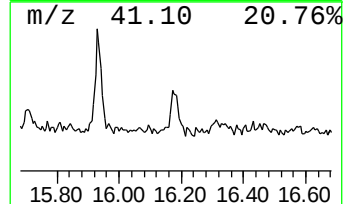
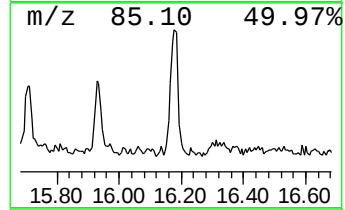
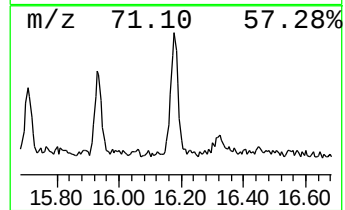
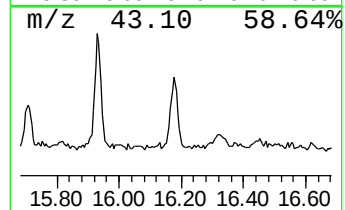
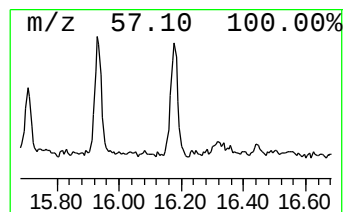
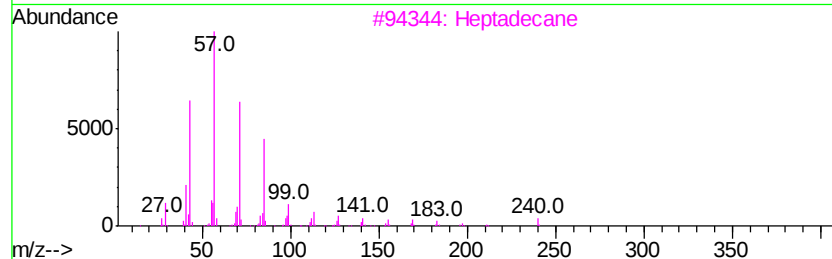
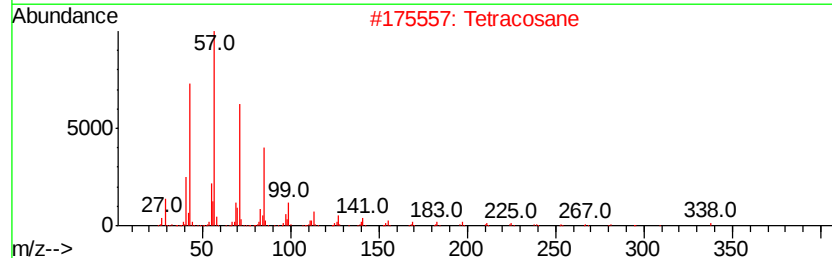
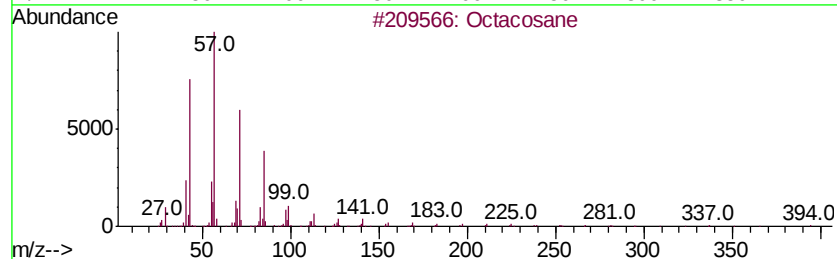
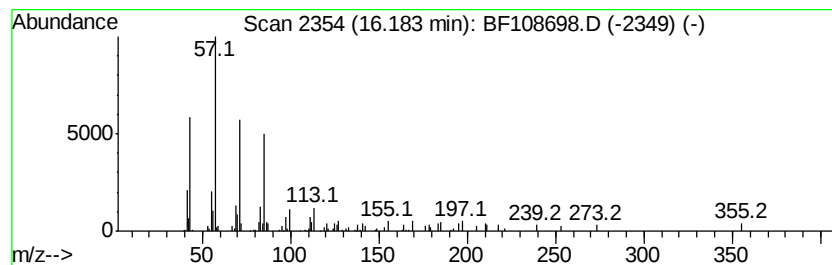
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	4.75 ng	103837	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Tetracosane	338	C24H50	000646-31-1	83
3		Heptadecane	240	C17H36	000629-78-7	83
4		Octadecane	254	C18H38	000593-45-3	83
5		Docosane	310	C22H46	000629-97-0	80



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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BZTRANS-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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
unknown6.79	6.79	7.4	ng	151955	1	7.00	411679	20.0
6a,12a-Dihydro-6H...	14.87	16.8	ng	676551	5	14.19	807323	20.0
Octadecanal	15.10	9.2	ng	202057	6	15.75	437195	20.0
Heptafluorobutyri...	15.39	8.0	ng	175077	6	15.75	437195	20.0
Oxirane, heptadecyl-	15.93	10.0	ng	218187	6	15.75	437195	20.0
Octacosane	16.18	4.8	ng	103837	6	15.75	437195	20.0