

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
 Data File : BF099555.D
 Acq On : 16 Oct 2017 20:27
 Operator : SJ/JU
 Sample : I5782-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S2(1-3)

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	4.463	402	404	418	rBV	22701	35247	1.16%	0.143%
2	5.075	504	508	529	rBV	385938	559003	18.39%	2.269%
3	5.475	571	576	579	rBV	2562057	2584580	85.05%	10.492%
4	6.486	742	748	766	rBV	2338057	2783763	91.60%	11.300%
5	6.616	766	770	774	rBV	2633887	2714923	89.33%	11.021%
6	6.845	805	809	816	rBB	678697	585130	19.25%	2.375%
7	6.998	831	835	839	rBV	2273122	2174604	71.56%	8.827%
8	7.410	900	905	908	rBV	1567938	1686272	55.49%	6.845%
9	8.127	1023	1027	1030	rBV	853262	798010	26.26%	3.239%
10	8.680	1118	1121	1128	rBV	39428	34754	1.14%	0.141%
11	9.204	1204	1210	1213	rBV	3033695	3039048	100.00%	12.336%
12	9.592	1272	1276	1285	rBV	693893	548391	18.04%	2.226%
13	9.880	1321	1325	1329	rBV2	1045936	862993	28.40%	3.503%
14	10.592	1443	1446	1452	rBB	103847	85390	2.81%	0.347%
15	10.674	1456	1460	1463	rBV	1623224	1488690	48.99%	6.043%
16	11.368	1574	1578	1582	rBV	911374	770453	25.35%	3.128%
17	12.951	1843	1847	1851	rBV	2153132	2167529	71.32%	8.799%
18	13.833	1994	1997	2011	rBV	89347	125693	4.14%	0.510%
19	14.015	2024	2028	2036	rBV	571112	539240	17.74%	2.189%
20	14.833	2164	2167	2172	rVB	28109	30608	1.01%	0.124%
21	14.909	2176	2180	2183	rVB	92336	94697	3.12%	0.384%
22	15.092	2208	2211	2214	rBV	32652	31472	1.04%	0.128%
23	15.127	2214	2217	2222	rBV3	28020	40509	1.33%	0.164%
24	15.486	2272	2278	2285	rBV	452214	570126	18.76%	2.314%
25	15.674	2306	2310	2315	rBV5	22438	34010	1.12%	0.138%
26	15.898	2343	2348	2354	rVB	66049	95364	3.14%	0.387%
27	16.398	2428	2433	2439	rVB3	24029	41255	1.36%	0.167%
28	16.692	2477	2483	2491	rBV3	28720	50785	1.67%	0.206%
29	16.980	2527	2532	2539	rVB3	29254	62171	2.05%	0.252%

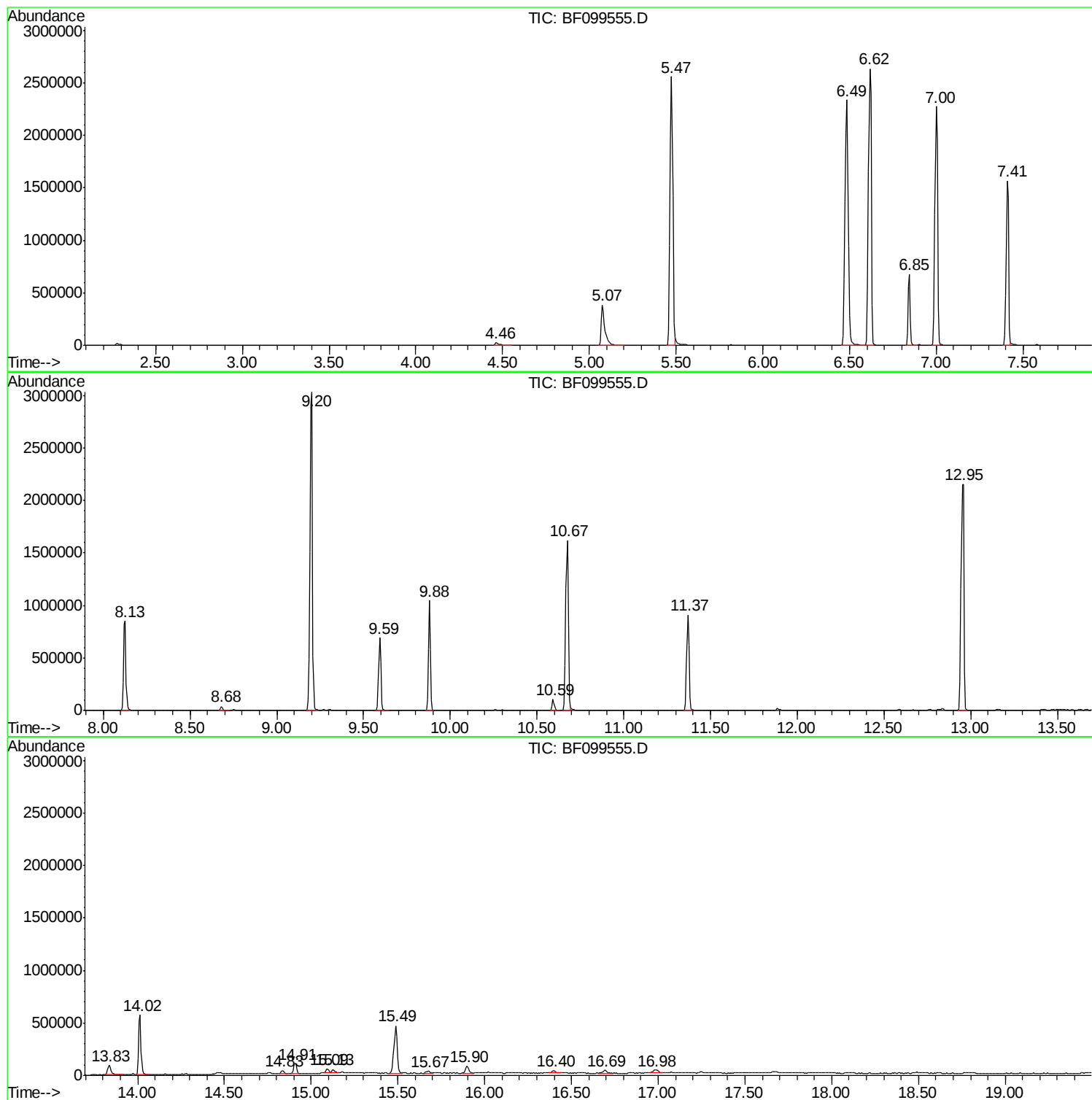
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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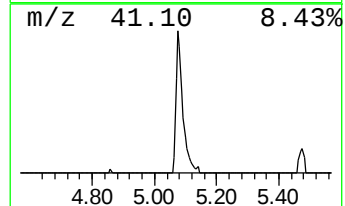
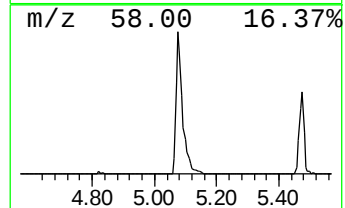
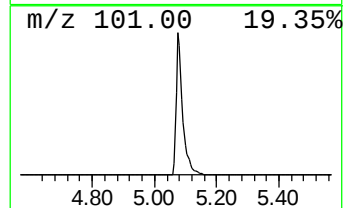
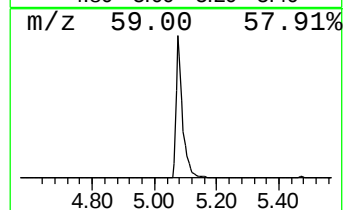
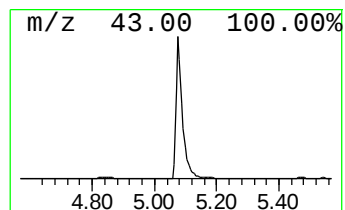
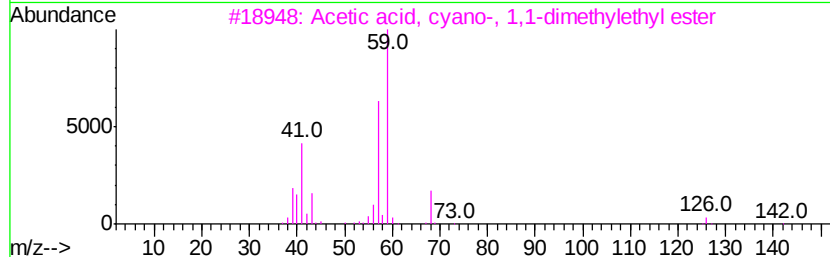
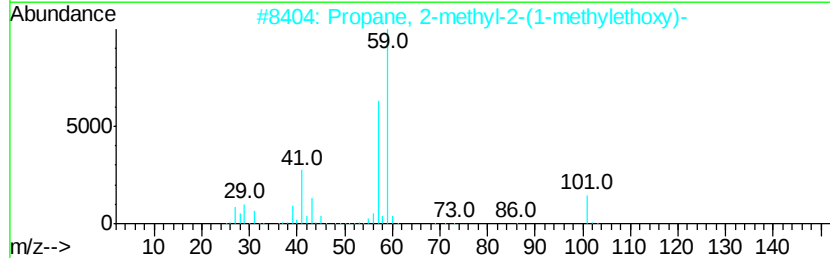
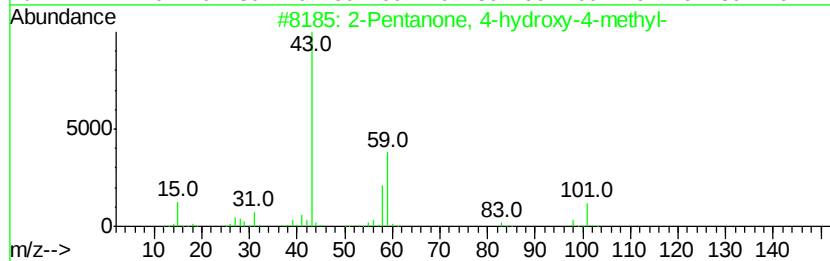
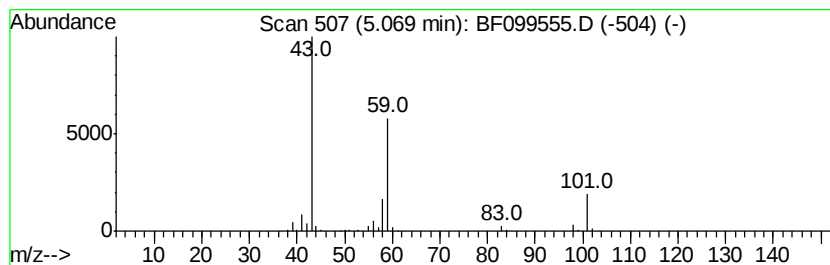
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	19.11 ng	559003	1,4-Dichlorobenzene-d4	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2		001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O		000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9



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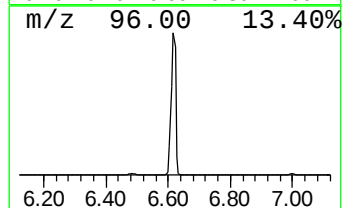
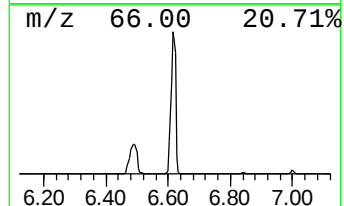
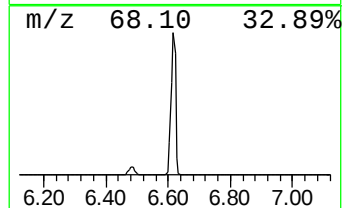
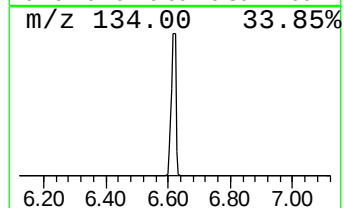
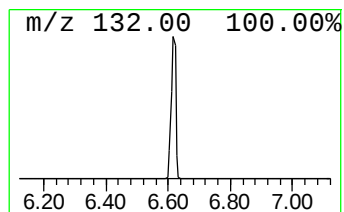
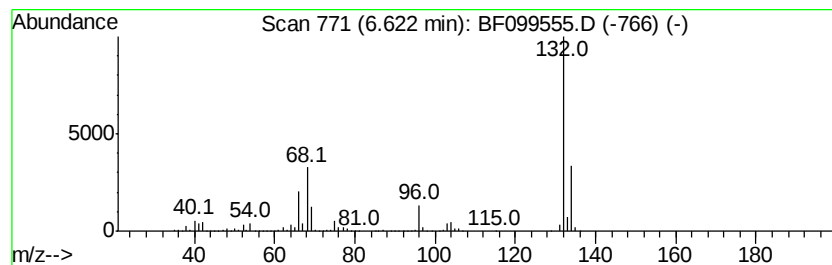
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	92.80 ng	2714920	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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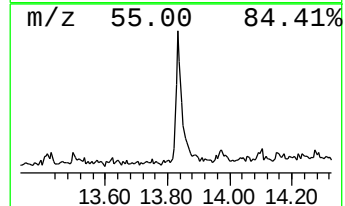
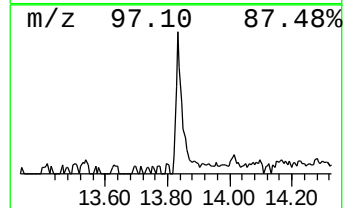
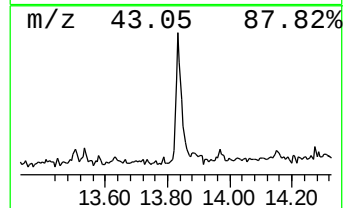
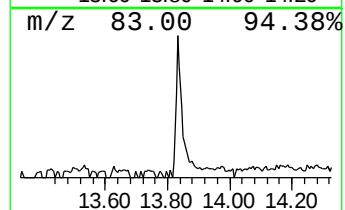
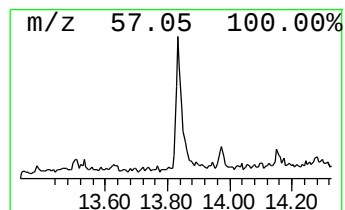
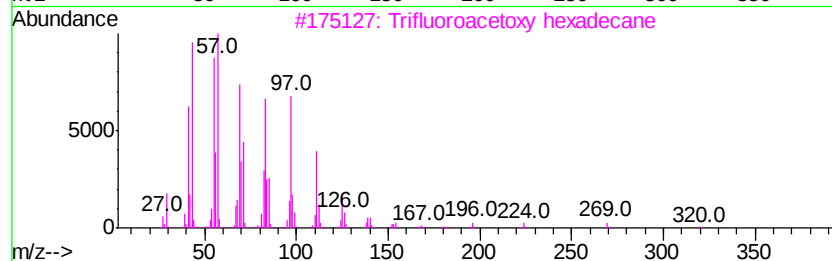
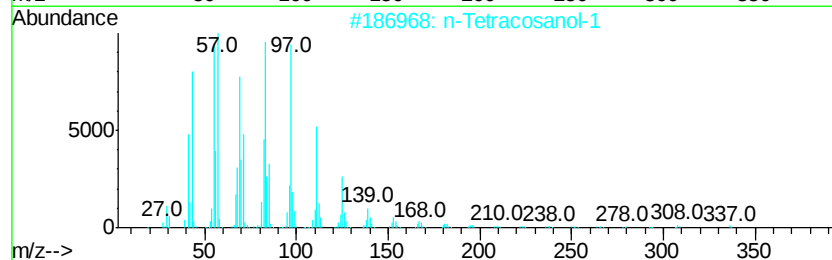
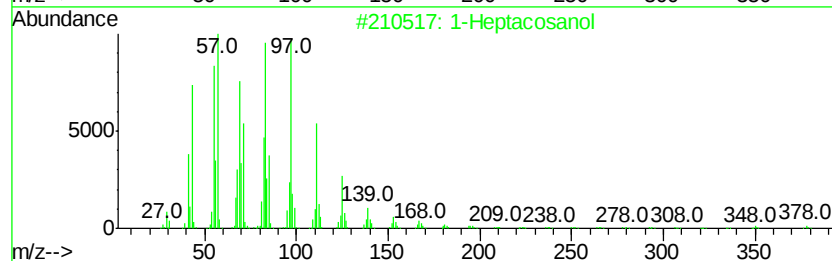
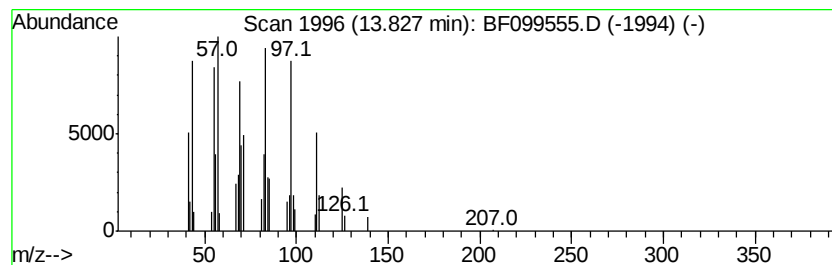
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Peak Number 4 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.66 ng	125693	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Behenic alcohol	326	C22H46O	000661-19-8	93



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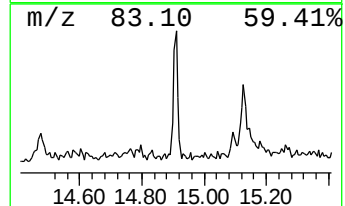
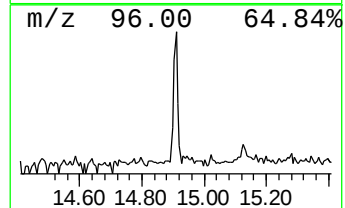
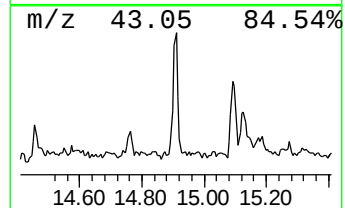
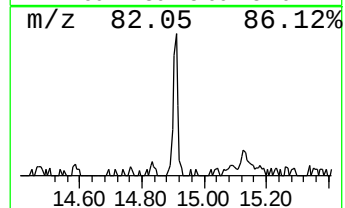
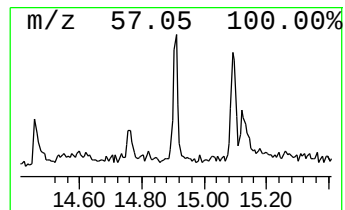
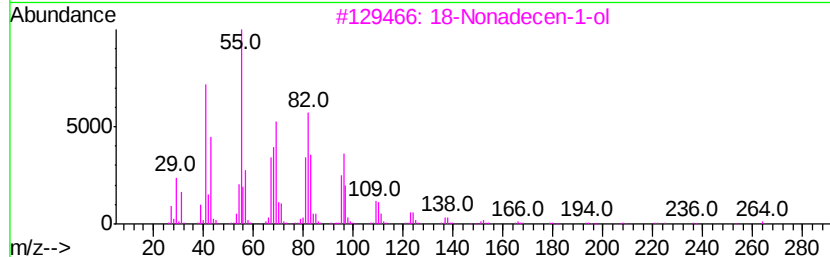
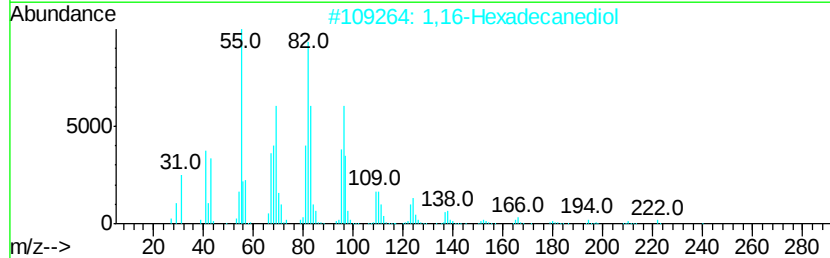
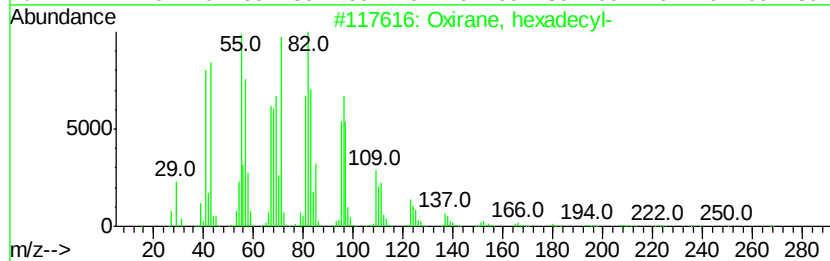
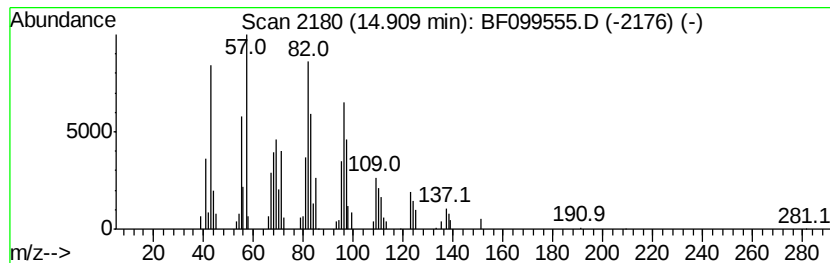
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Peak Number 5 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.91	3.32 ng	94697	Perylene-d12	15.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	72
2	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	64
3	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	64
4	1,19-Eicosadiene	278	C20H38	014811-95-1	52
5	17-Pentatriacontene	491	C35H70	006971-40-0	46



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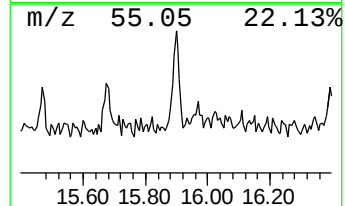
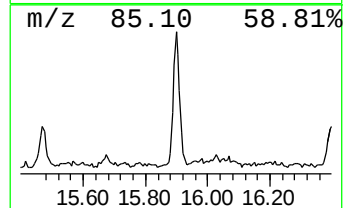
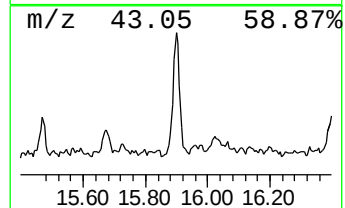
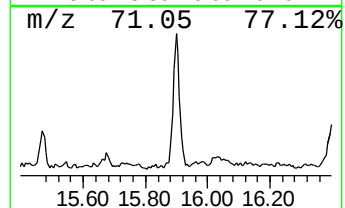
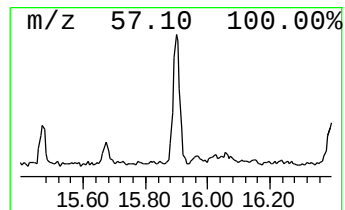
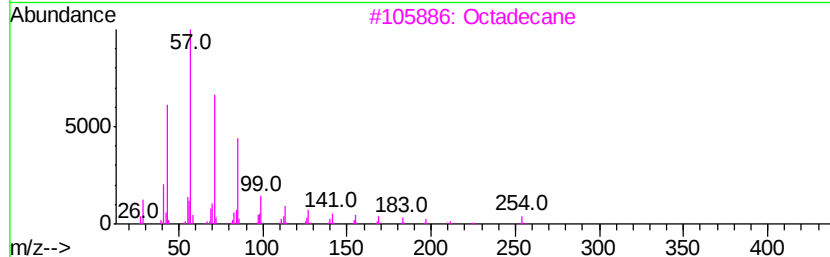
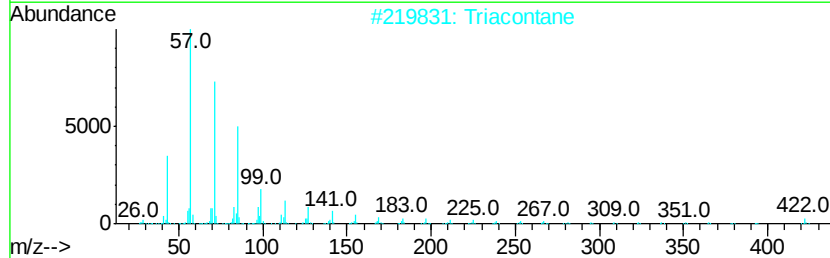
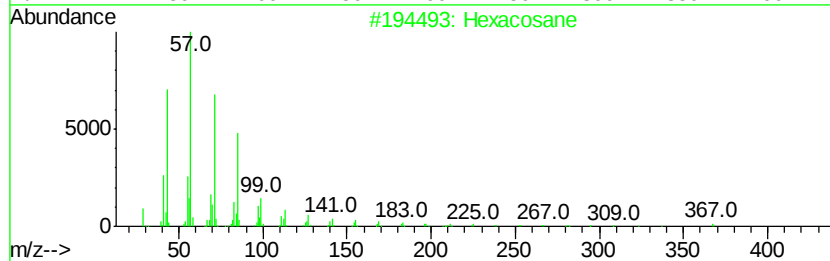
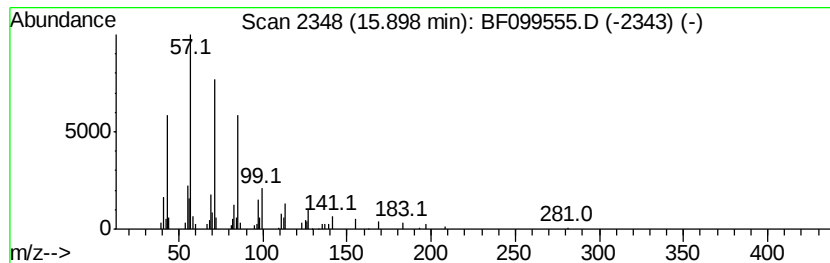
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Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	3.35 ng	95364	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	triacontane		422	C30H62	000638-68-6	91
3	Octadecane		254	C18H38	000593-45-3	90
4	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	90
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87



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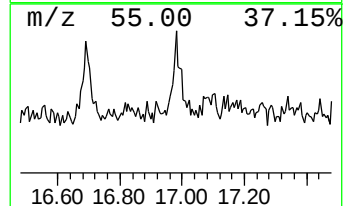
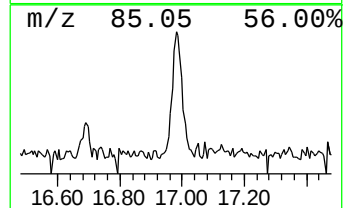
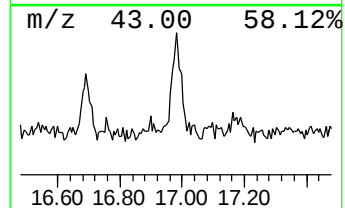
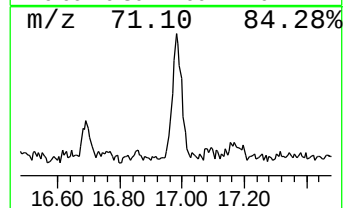
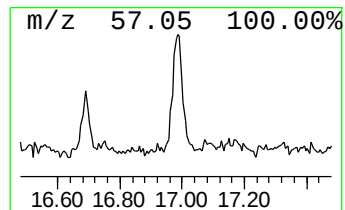
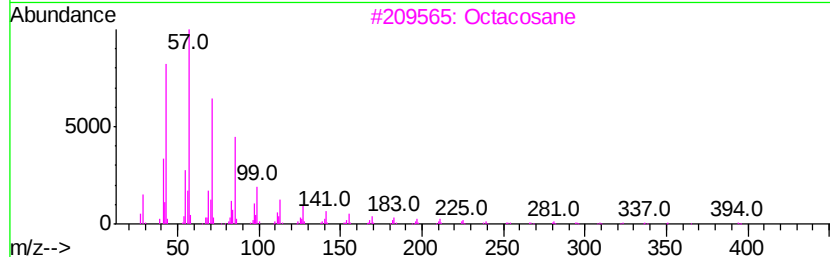
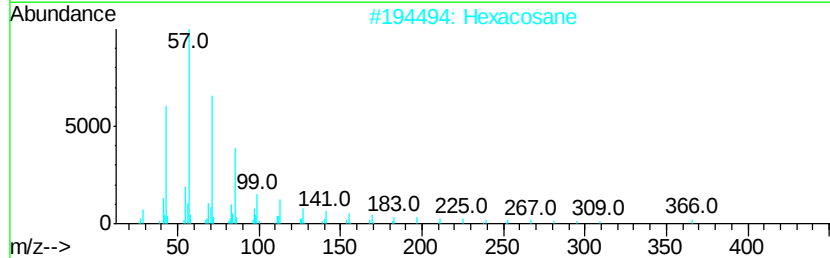
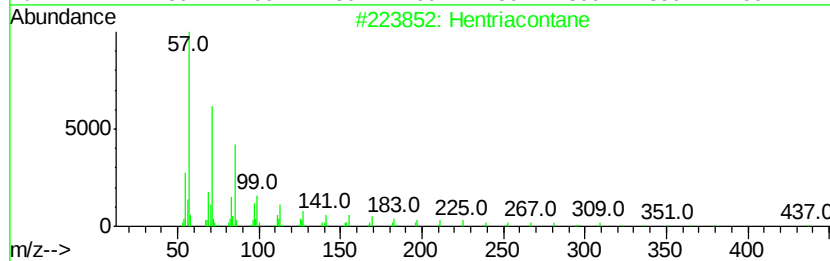
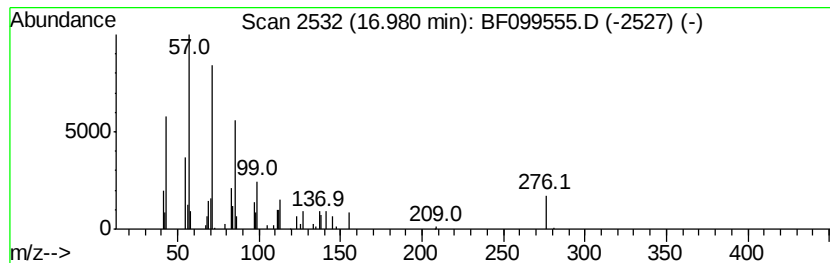
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.98	2.18 ng	62171	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	87
2	Hexacosane		366	C26H54	000630-01-3	87
3	Octacosane		394	C28H58	000630-02-4	83
4	2-methyloctacosane		408	C29H60	1000376-72-8	80
5	Pentacosane		352	C25H52	000629-99-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099555.D
Acq On : 16 Oct 2017 20:27
Operator : SJ/JU
Sample : I5782-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2(1-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.07	19.1 ng		559003	1	6.85	585130	20.0
unknown6.62	6.62	92.8 ng		2714920	1	6.85	585130	20.0
1-Heptacosanol	13.83	4.7 ng		125693	5	14.02	539240	20.0
Oxirane, hexadecyl-	14.91	3.3 ng		94697	6	15.49	570126	20.0
Hexacosane	15.90	3.4 ng		95364	6	15.49	570126	20.0
Hentriacontane	16.98	2.2 ng		62171	6	15.49	570126	20.0