

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072817\
 Data File : BF097175.D
 Acq On : 29 Jul 2017 1:10
 Operator : SJ/JU
 Sample : I4456-08
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-14D24

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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	4.628	462	466	481	rBV	445554	700272	24.45%	3.172%
2	5.087	540	544	565	rBV	2139417	2529363	88.32%	11.456%
3	6.151	720	725	739	rBV	2580051	2863860	100.00%	12.971%
4	6.263	739	744	747	rBV	2465421	2519233	87.97%	11.410%
5	6.487	778	782	790	rBV	794492	674248	23.54%	3.054%
6	6.645	804	809	812	rBV	1830795	1788411	62.45%	8.100%
7	7.057	874	879	882	rBV	1840430	1794075	62.65%	8.126%
8	7.192	898	902	909	rVB	42549	44788	1.56%	0.203%
9	7.769	996	1000	1009	rBV	1039797	885798	30.93%	4.012%
10	8.845	1179	1183	1187	rBV	2214391	2024734	70.70%	9.170%
11	9.245	1247	1251	1257	rBV	372602	300922	10.51%	1.363%
12	9.469	1281	1289	1293	rBV3	20049	29120	1.02%	0.132%
13	9.516	1293	1297	1300	rBV	787936	724778	25.31%	3.283%
14	9.751	1334	1337	1341	rBV	72140	63768	2.23%	0.289%
15	9.969	1371	1374	1377	rVB	42873	32598	1.14%	0.148%
16	10.298	1427	1430	1440	rVB	1099073	993274	34.68%	4.499%
17	10.439	1451	1454	1461	rBV	65244	83463	2.91%	0.378%
18	10.886	1526	1530	1532	rBV	37964	33729	1.18%	0.153%
19	10.986	1543	1547	1550	rBV	567595	501139	17.50%	2.270%
20	11.010	1550	1551	1556	rVB	94935	56081	1.96%	0.254%
21	11.539	1639	1641	1644	rBV	63600	59408	2.07%	0.269%
22	11.833	1685	1691	1700	rBV2	19115	39317	1.37%	0.178%
23	12.192	1746	1752	1756	rBV	133272	122698	4.28%	0.556%
24	12.321	1771	1774	1783	rVB6	23041	33681	1.18%	0.153%
25	12.416	1786	1790	1793	rVB	115724	111831	3.90%	0.507%
26	12.569	1812	1816	1820	rVB	1294787	1186165	41.42%	5.372%
27	13.480	1966	1971	1981	rBV2	144450	192747	6.73%	0.873%
28	13.610	1988	1993	1996	rBV	582547	598114	20.88%	2.709%
29	13.633	1996	1997	2003	rVB	76399	63825	2.23%	0.289%
30	13.998	2055	2059	2062	rBV3	28560	37679	1.32%	0.171%
31	14.374	2120	2123	2125	rBV	91015	83681	2.92%	0.379%
32	14.604	2159	2162	2170	rVB	63900	109063	3.81%	0.494%
33	14.692	2174	2177	2180	rBV3	30306	41853	1.46%	0.190%
34	14.857	2202	2205	2211	rBV	29813	35067	1.22%	0.159%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.910	2211	2214	2218	rBV	46993	56321	1.97%	0.255%
36	14.962	2218	2223	2227	rBV	412289	469602	16.40%	2.127%
37	15.368	2288	2292	2295	rBV4	27469	41892	1.46%	0.190%
38	16.174	2426	2429	2436	rVB7	18373	38743	1.35%	0.175%
39	16.256	2438	2443	2448	rVB4	28595	42191	1.47%	0.191%
40	16.409	2466	2469	2477	rVB9	20423	41911	1.46%	0.190%
41	18.862	2881	2886	2887	rBV3	19832	29566	1.03%	0.134%

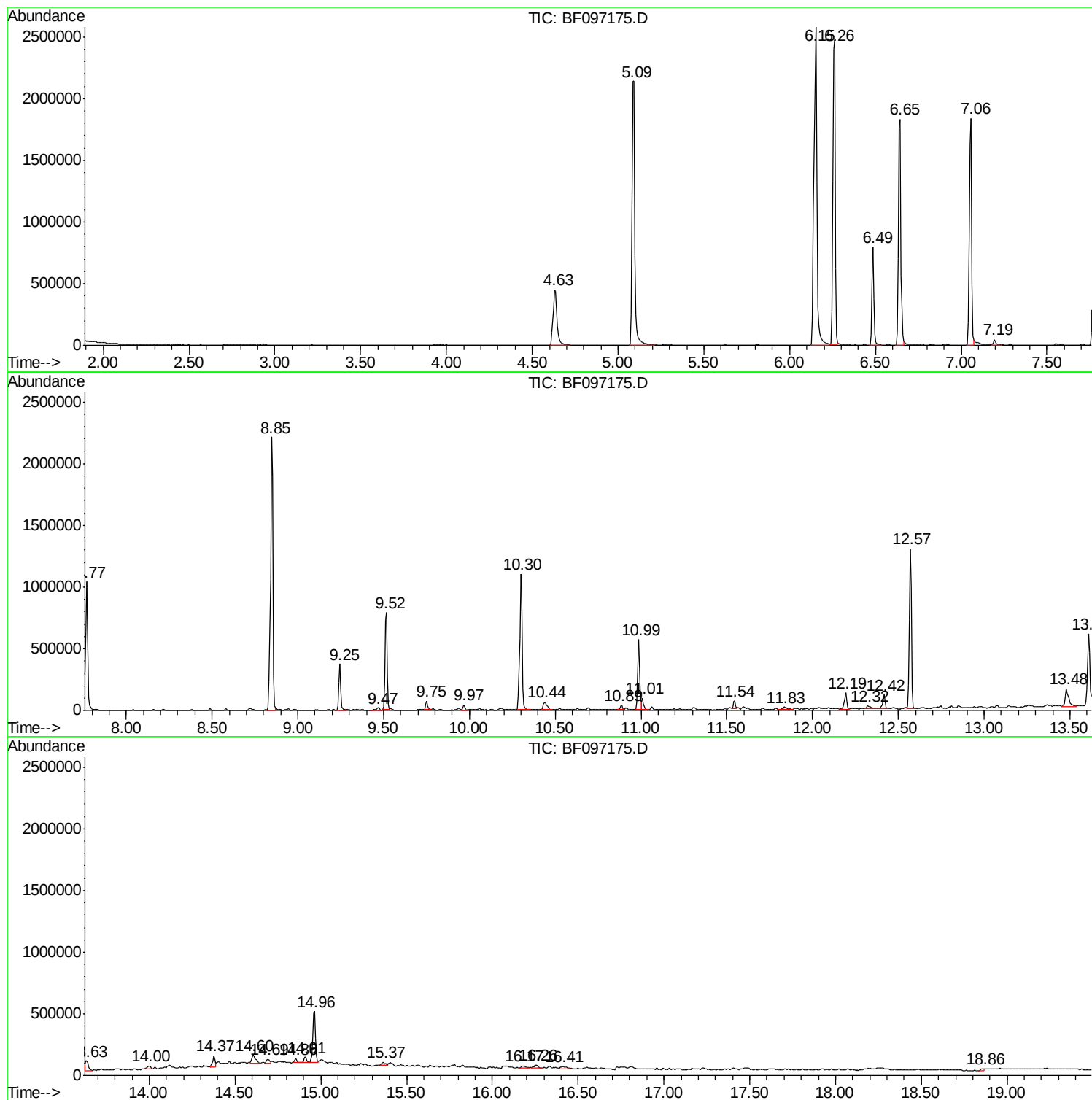
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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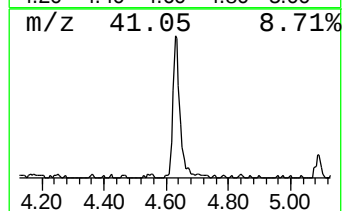
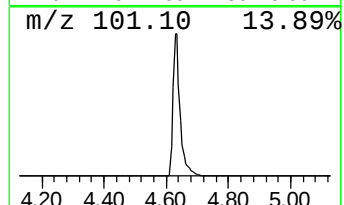
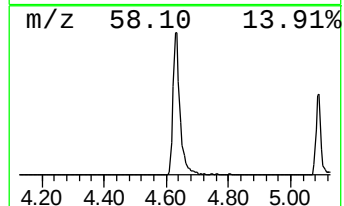
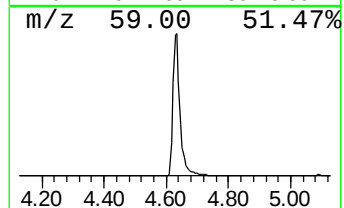
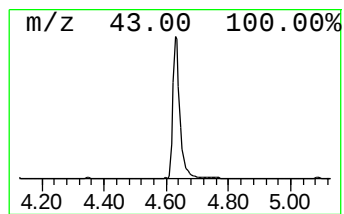
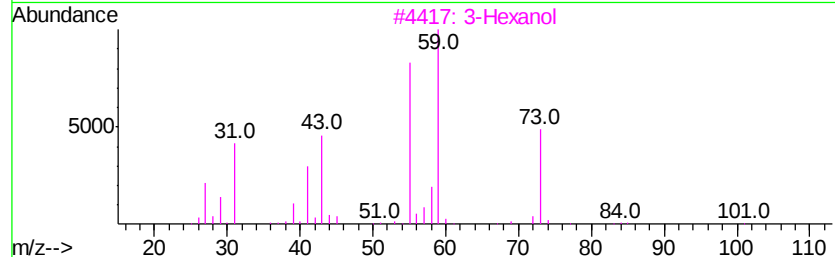
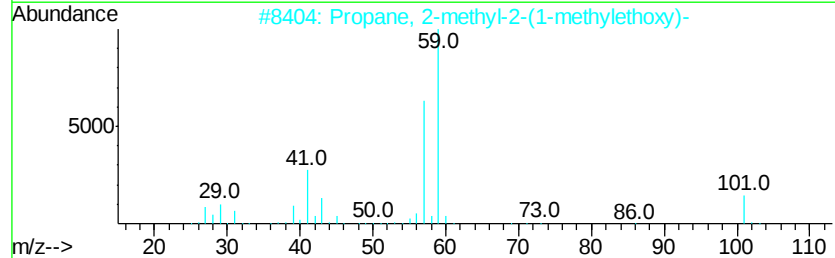
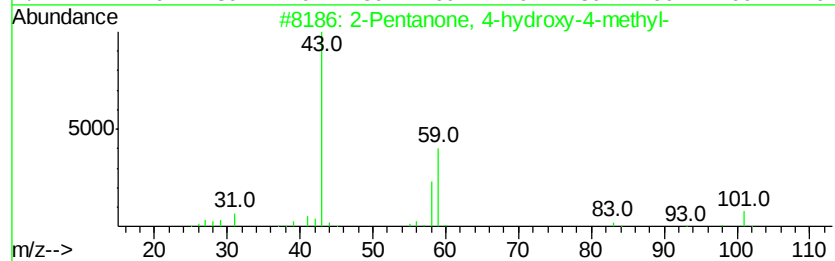
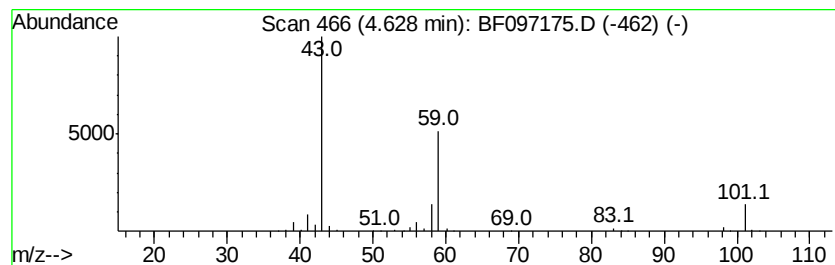
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	20.77 ng	700272	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol	102	C6H14O	000623-37-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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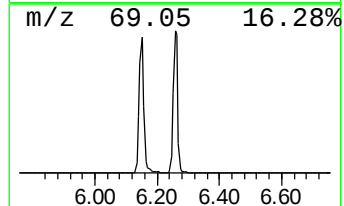
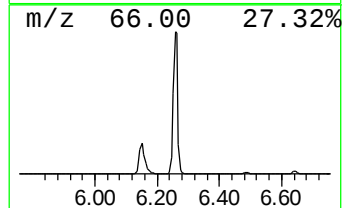
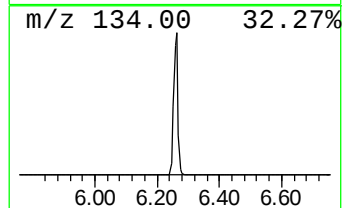
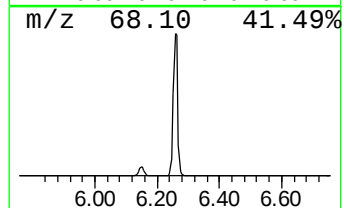
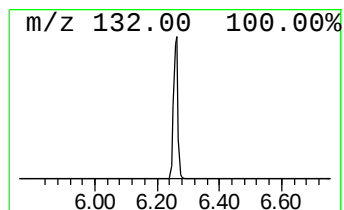
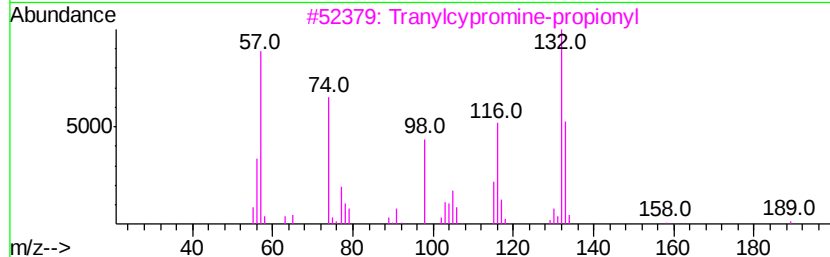
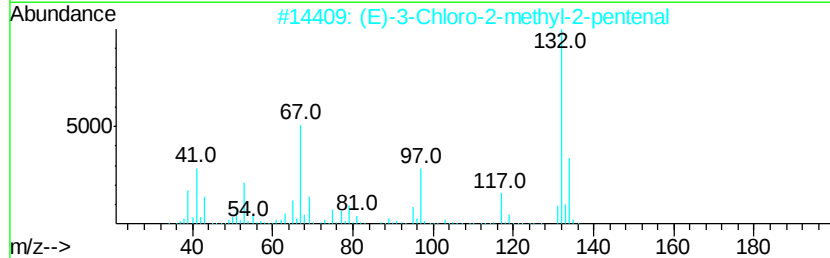
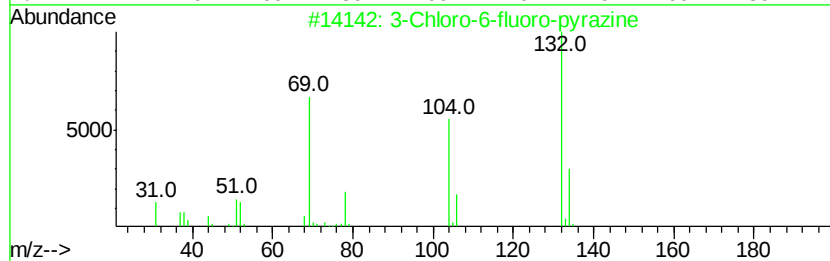
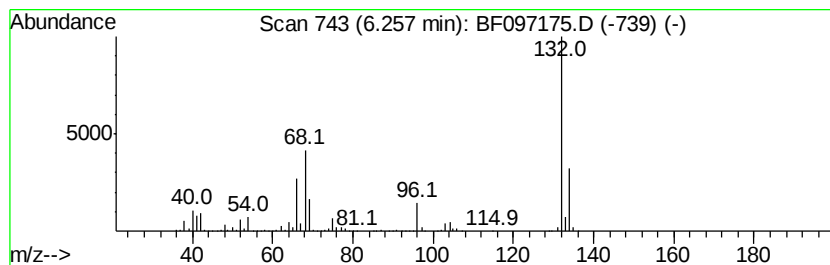
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Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	74.73 ng	2519230	1,4-Dichlorobenzene-d4	6.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Xenon	132	Xe	007440-63-3	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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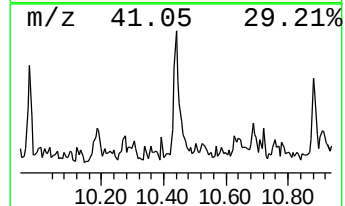
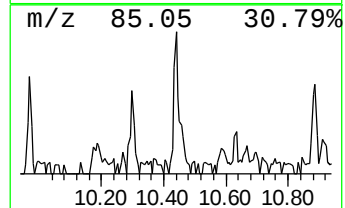
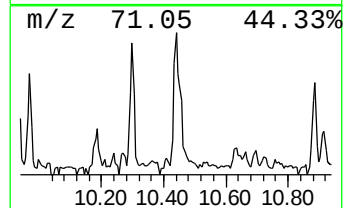
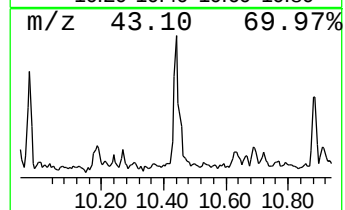
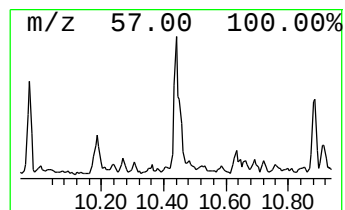
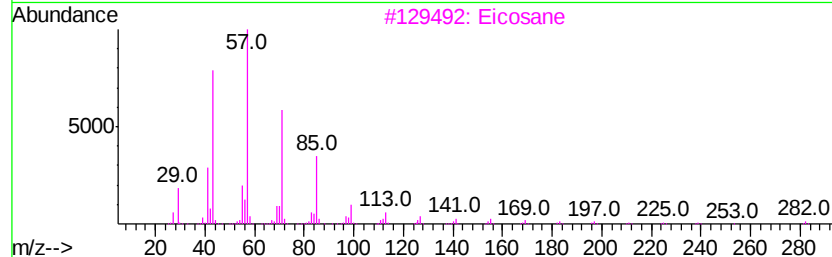
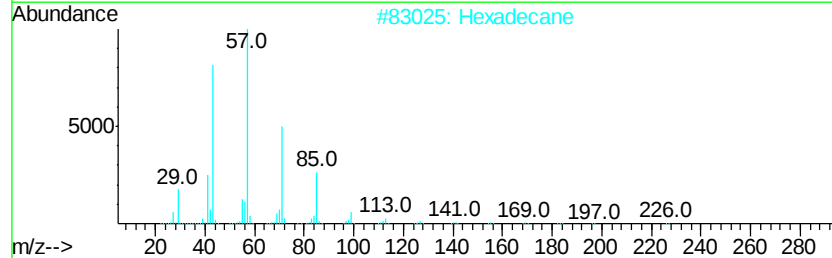
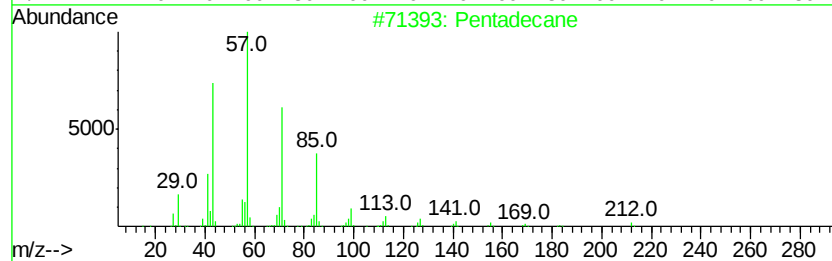
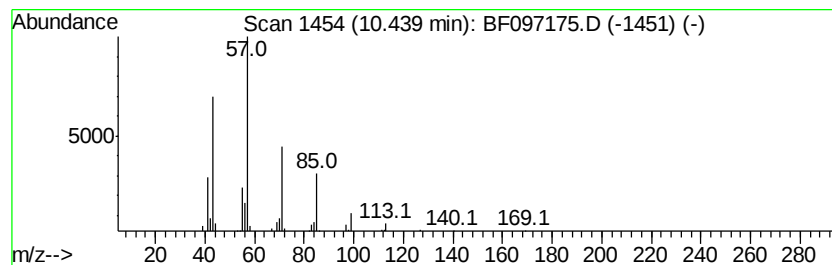
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.44	3.33 ng	83463	Phenanthrene-d10		10.99
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Eicosane	282	C20H42	000112-95-8	83
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	83
5	Heneicosane	296	C21H44	000629-94-7	80



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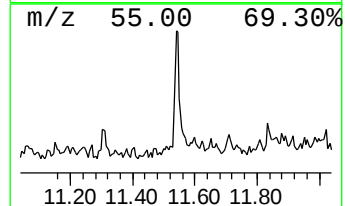
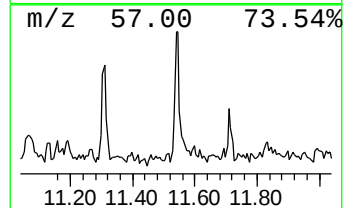
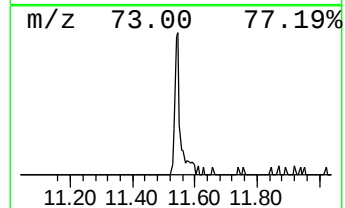
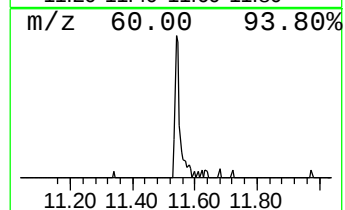
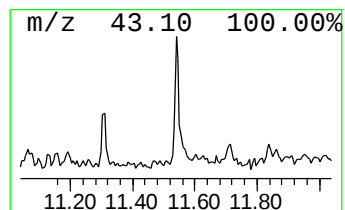
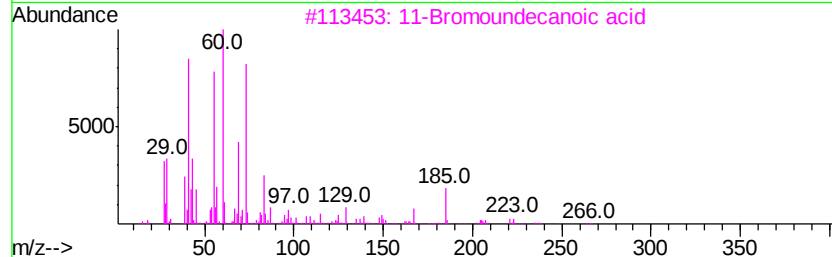
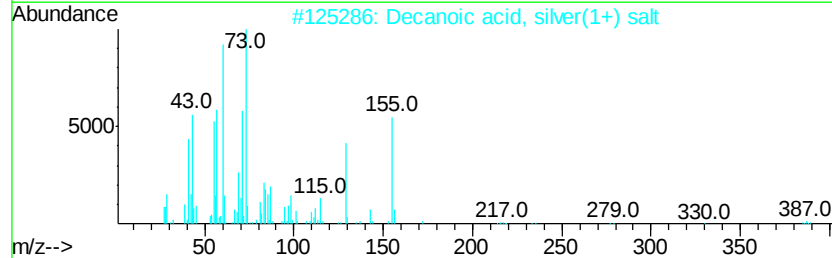
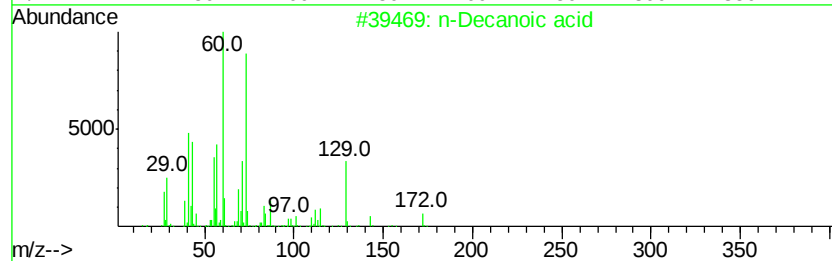
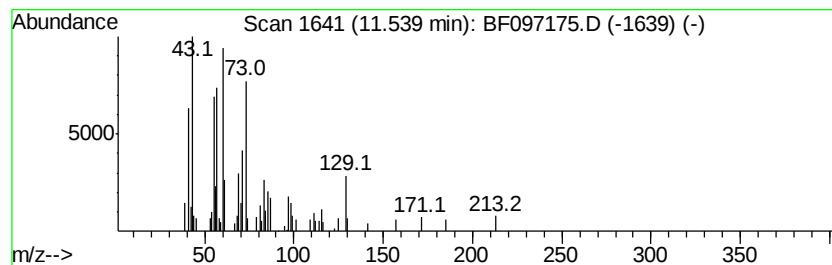
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Decanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.37 ng	59408	Phenanthrene-d10	10.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	50
2		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
3		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
4		Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	27
5		4-Propionyloxytridecane	256	C16H32O2	1000245-62-6	27



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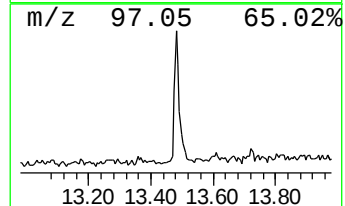
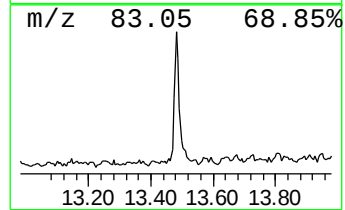
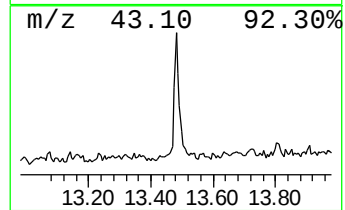
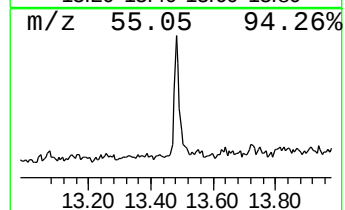
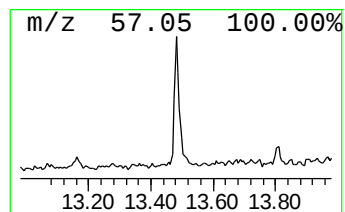
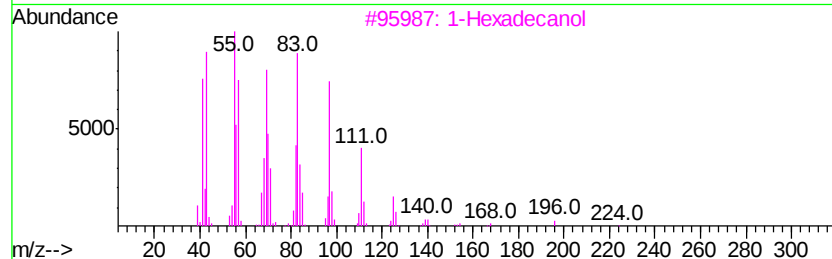
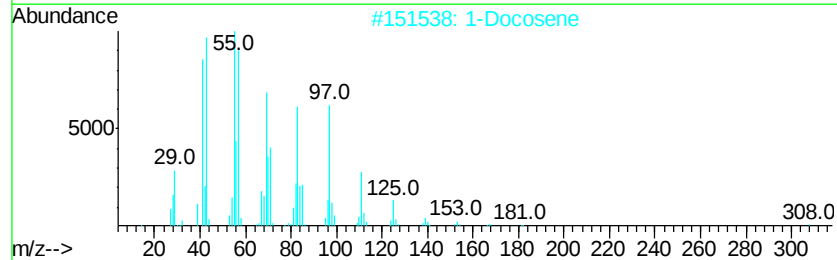
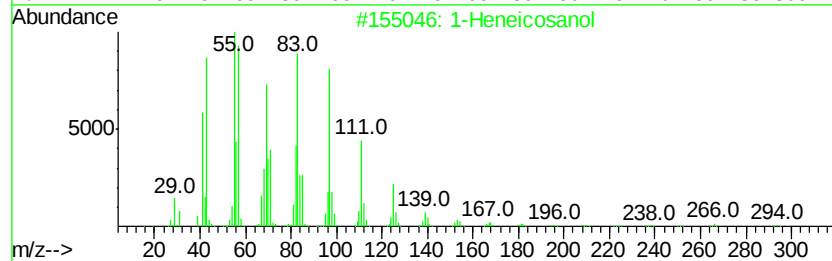
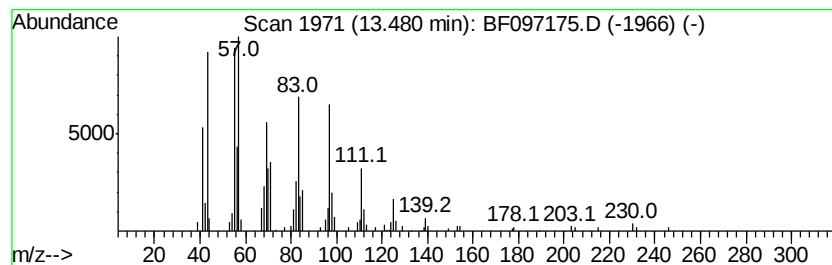
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.48	6.45 ng	192747	Chrysene-d12		13.61
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	90
2	1-Docosene	308	C22H44	001599-67-3	90
3	1-Hexadecanol	242	C16H34O	036653-82-4	83
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	83
5	1-Nonadecene	266	C19H38	018435-45-5	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
Data File : BF097175.D
Acq On : 29 Jul 2017 1:10
Operator : SJ/JU
Sample : I4456-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-14D24

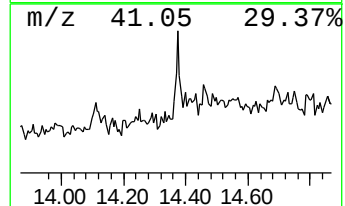
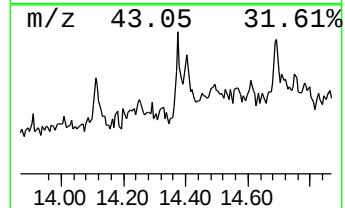
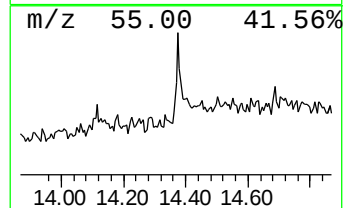
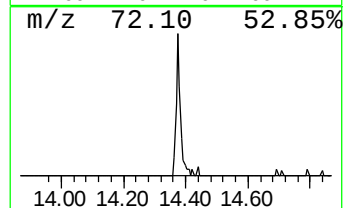
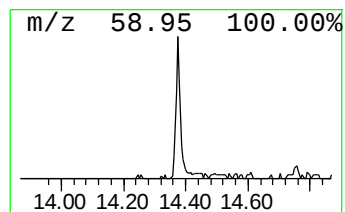
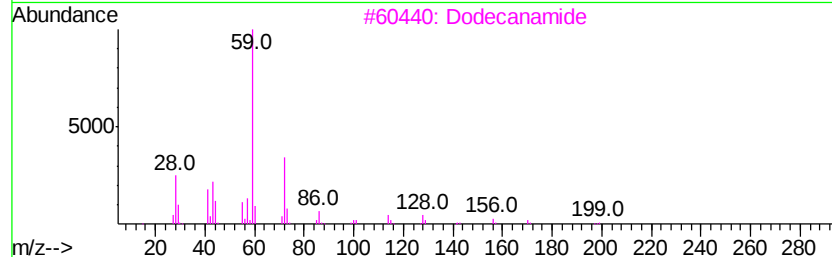
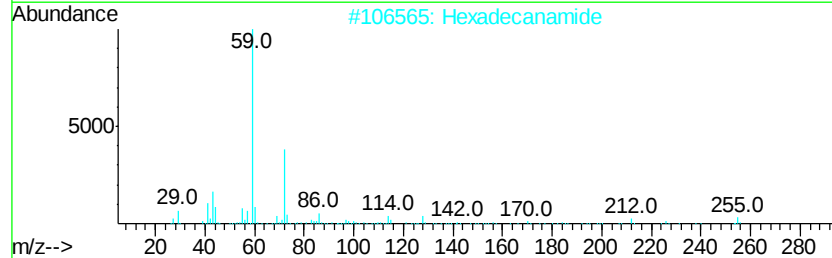
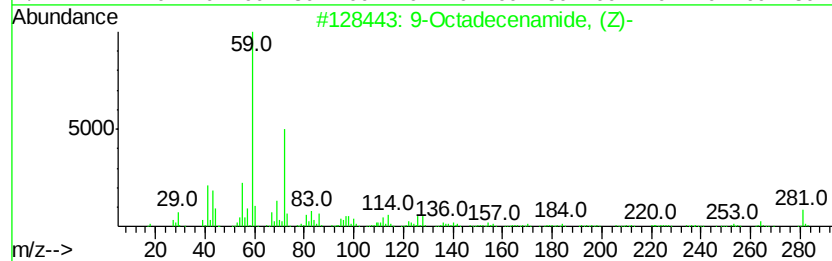
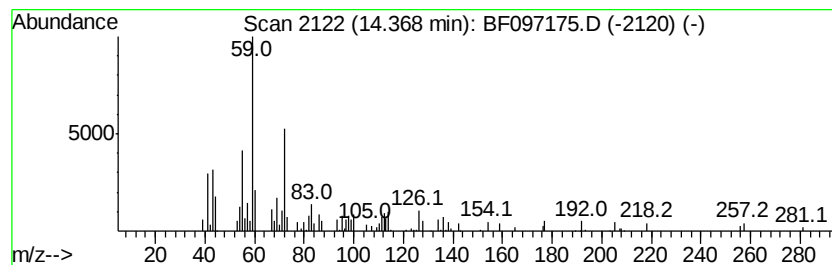
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	3.56 ng	83681	Perylene-d12	14.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2		Hexadecanamide	255	C16H33NO	000629-54-9	72
3		Dodecanamide	199	C12H25NO	001120-16-7	64
4		7-Nonenamide	155	C9H17NO	090949-53-4	64
5		Tetradecanamide	227	C14H29NO	000638-58-4	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072817\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-14D24

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.63	20.8	ng	700272	1	6.49	674248	20.0
unknown6.26	6.26	74.7	ng	2519230	1	6.49	674248	20.0
Pentadecane	10.44	3.3	ng	83463	4	10.99	501139	20.0
n-Decanoic acid	11.54	2.4	ng	59408	4	10.99	501139	20.0
1-Heneicosanol	13.48	6.5	ng	192747	5	13.61	598114	20.0
9-Octadecenamide, ...	14.37	3.6	ng	83681	6	14.96	469602	20.0