

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
 Data File : BF095935.D
 Acq On : 14 Jun 2017 21:57
 Operator : SJ/MA
 Sample : I3660-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-350

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-BF060517.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	4.534	498	501	520	rBV2	44357	126062	6.52%	0.901%
2	5.222	615	618	640	rBV	579293	1295709	67.00%	9.261%
3	6.904	900	904	915	rBV	729478	1230599	63.64%	8.795%
4	6.992	915	919	944	rVB	1008573	1676655	86.70%	11.983%
5	7.333	973	977	993	rVB	289789	397419	20.55%	2.840%
6	7.569	1012	1017	1036	rBV	854429	1152053	59.58%	8.234%
7	8.251	1129	1133	1153	rBV	521346	833017	43.08%	5.954%
8	9.010	1258	1262	1271	rBV	33777	53597	2.77%	0.383%
9	9.369	1319	1323	1349	rBV	358123	532520	27.54%	3.806%
10	9.863	1404	1407	1412	rBV	14913	22050	1.14%	0.158%
11	9.910	1412	1415	1427	rVB	14590	28048	1.45%	0.200%
12	10.957	1587	1593	1602	rBV	190774	241967	12.51%	1.729%
13	11.145	1620	1625	1642	rBV	1405720	1933763	100.00%	13.821%
14	11.445	1671	1676	1683	rBB	26458	35453	1.83%	0.253%
15	11.845	1740	1744	1755	rBV	103177	146970	7.60%	1.050%
16	12.186	1797	1802	1808	rBV2	429190	538800	27.86%	3.851%
17	13.039	1943	1947	1951	rBV	19671	22713	1.17%	0.162%
18	13.480	2018	2022	2039	rBV	461881	714213	36.93%	5.105%
19	13.810	2074	2078	2089	rBV	20624	30714	1.59%	0.220%
20	14.580	2205	2209	2228	rVB	306138	461914	23.89%	3.301%
21	15.604	2379	2383	2391	rBV2	34254	46466	2.40%	0.332%
22	16.415	2517	2521	2529	rVB	42268	51721	2.67%	0.370%
23	16.715	2566	2572	2581	rBV	50138	77783	4.02%	0.556%
24	16.956	2608	2613	2620	rVB	973315	1174123	60.72%	8.392%
25	18.215	2822	2827	2836	rBV3	41485	82856	4.28%	0.592%
26	18.297	2836	2841	2851	rVV	319887	466656	24.13%	3.335%
27	18.368	2851	2853	2862	rVB2	20779	27521	1.42%	0.197%
28	19.009	2957	2962	2971	rVB5	13883	23221	1.20%	0.166%
29	19.580	3055	3059	3062	rBV	40001	55396	2.86%	0.396%
30	19.868	3105	3108	3113	rVB2	22136	26207	1.36%	0.187%
31	19.927	3113	3118	3121	rBV	31844	37639	1.95%	0.269%
32	19.968	3121	3125	3138	rVV	238625	343438	17.76%	2.455%
33	20.403	3195	3199	3204	rBV5	15661	25349	1.31%	0.181%
34	20.768	3257	3261	3268	rBV6	12139	21645	1.12%	0.155%

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35	21.186	3324	3332	3339	rBV5	20074	57251	2.96%	0.409%
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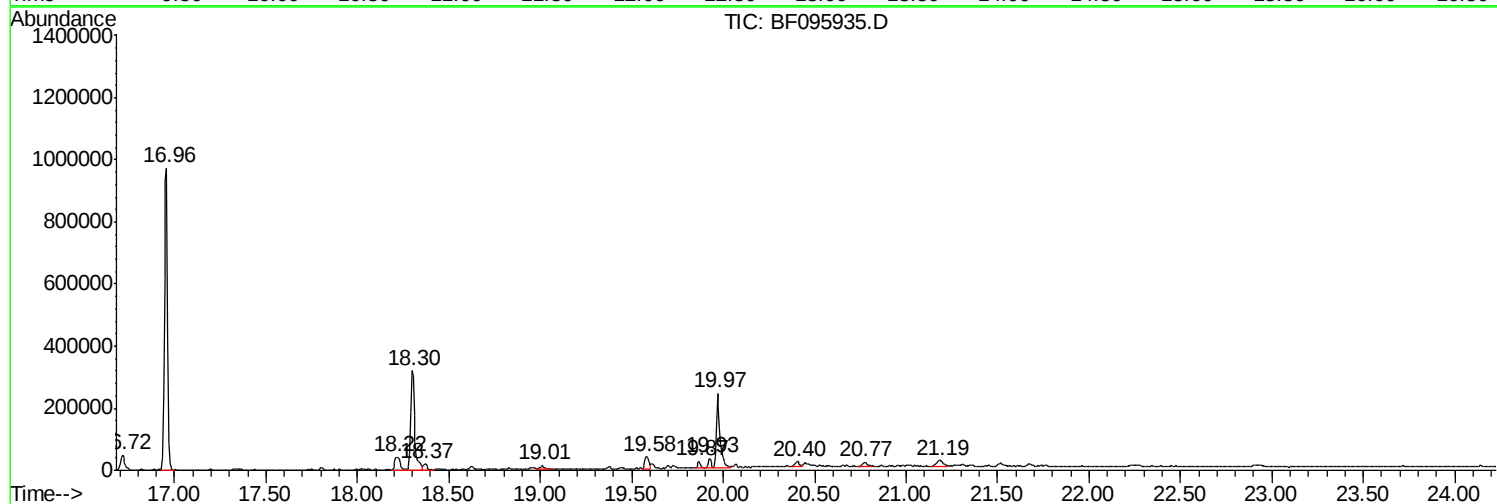
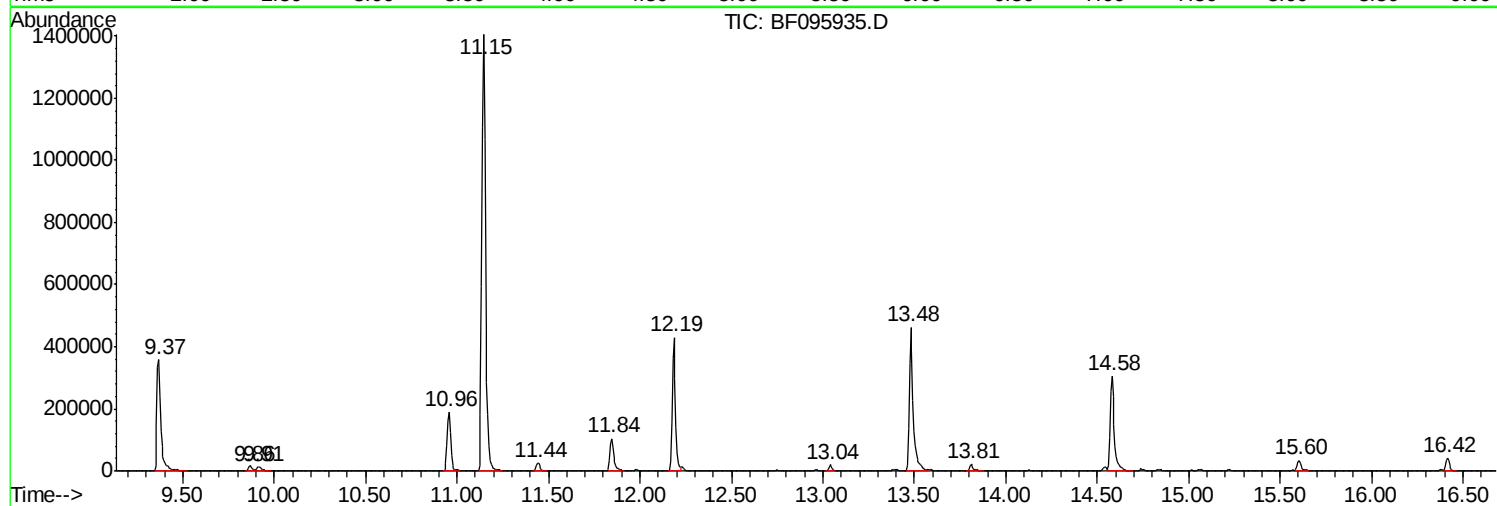
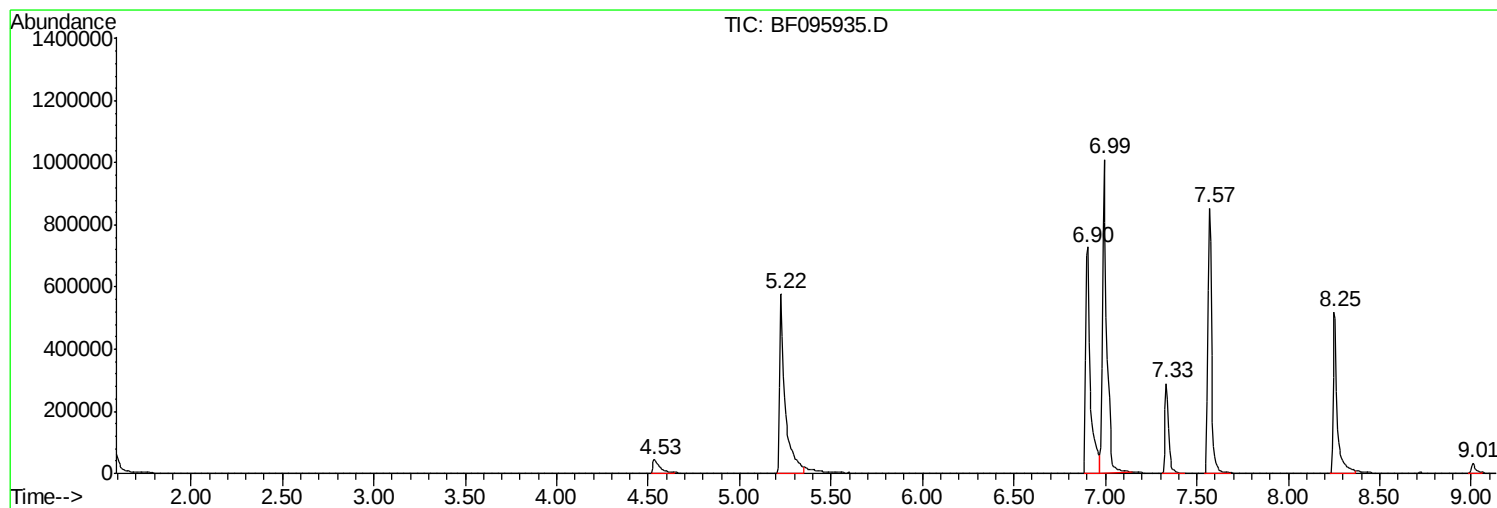
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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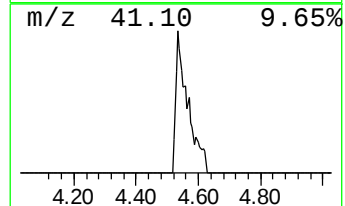
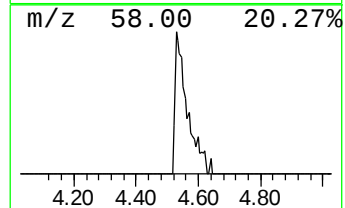
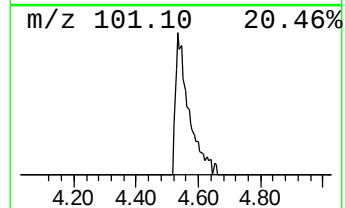
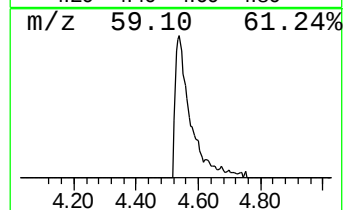
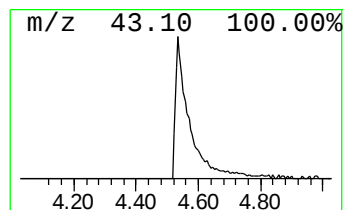
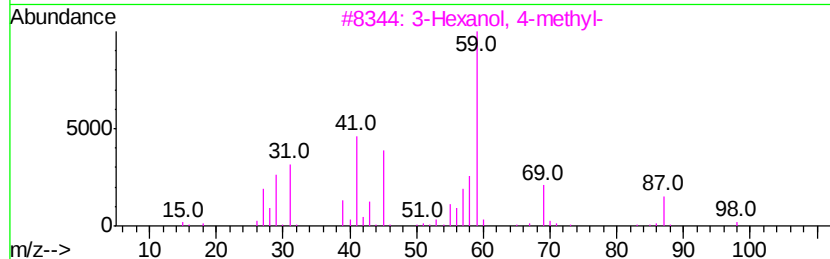
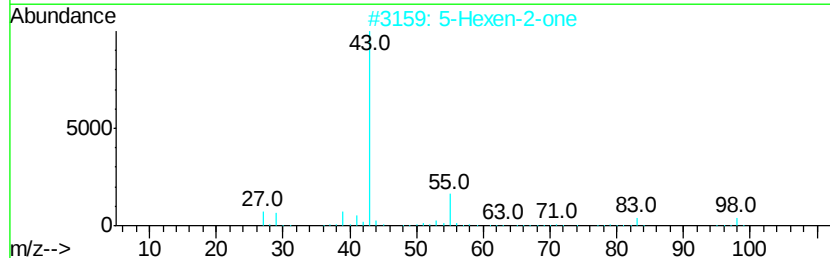
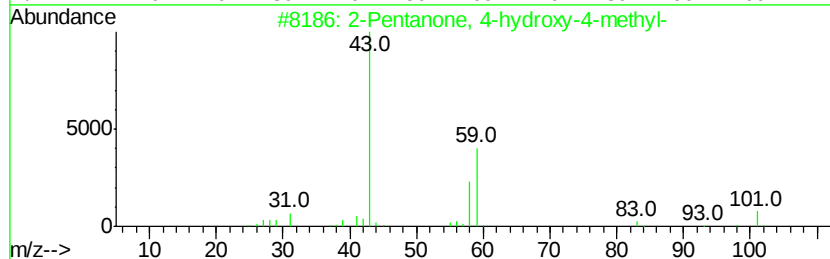
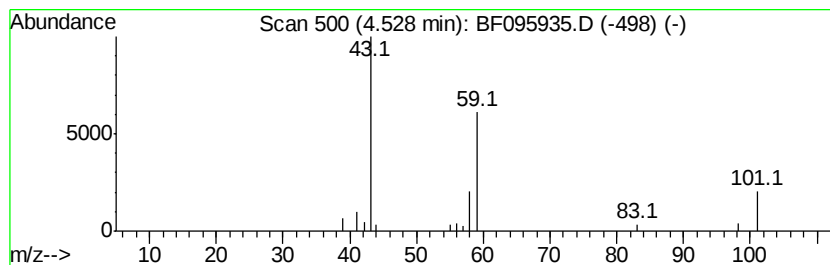
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	6.34 ng	126062	1,4-Dichlorobenzene-d4	7.33

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			5-Hexen-2-one	98	C6H10O	000109-49-9	9
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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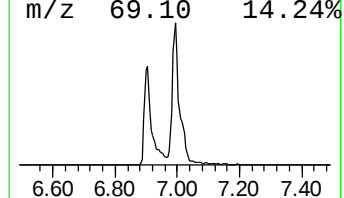
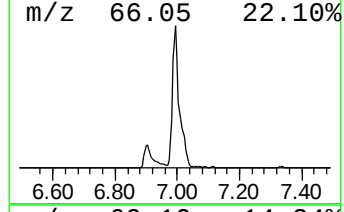
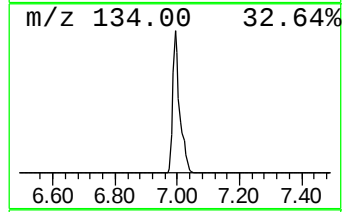
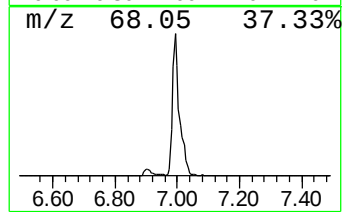
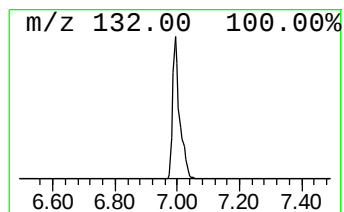
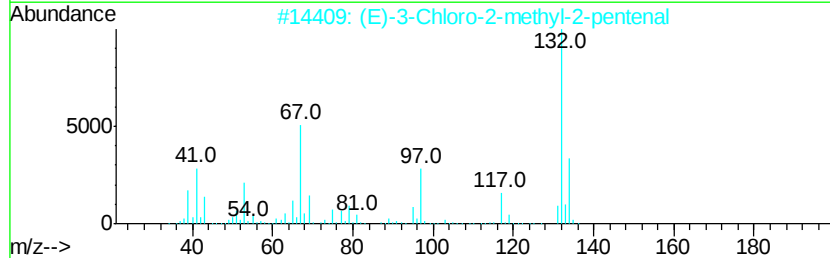
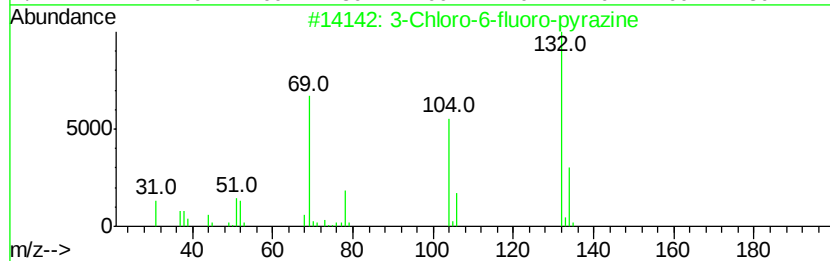
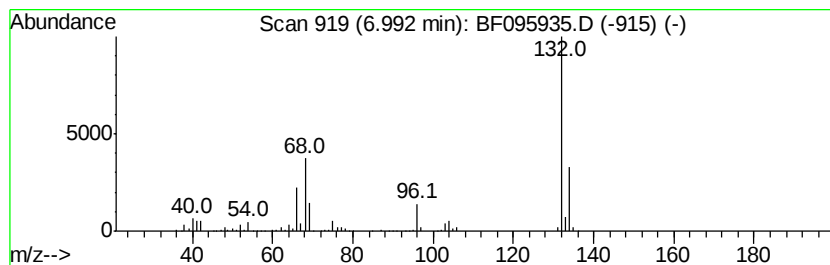
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	84.38 ng	1676660	1,4-Dichlorobenzene-d4	7.33

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		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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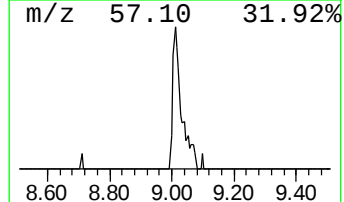
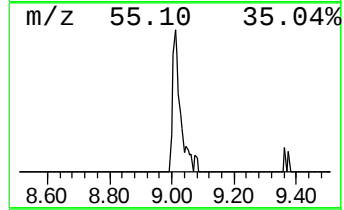
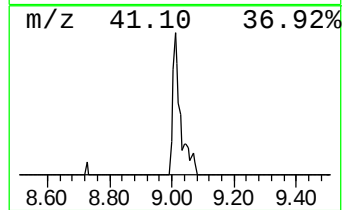
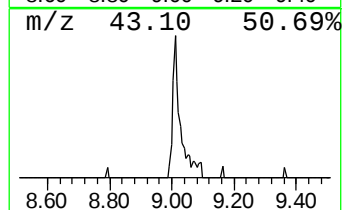
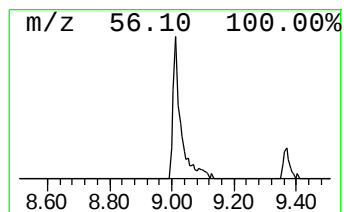
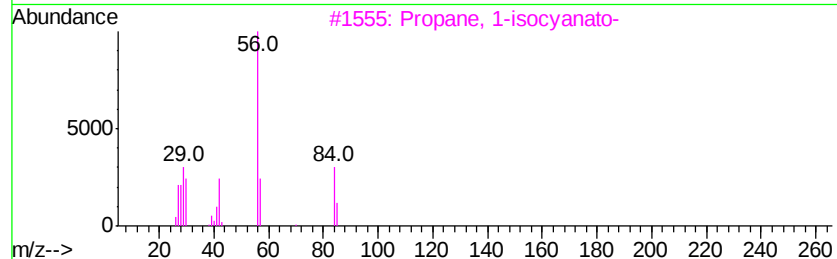
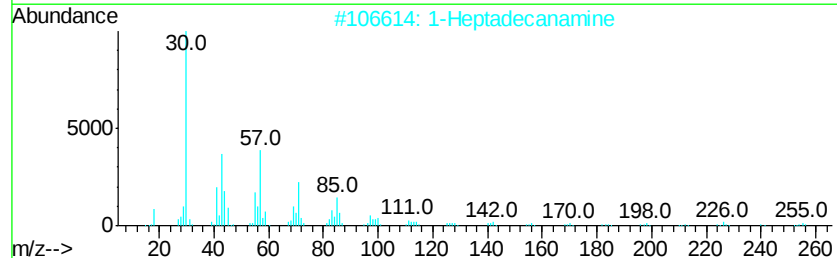
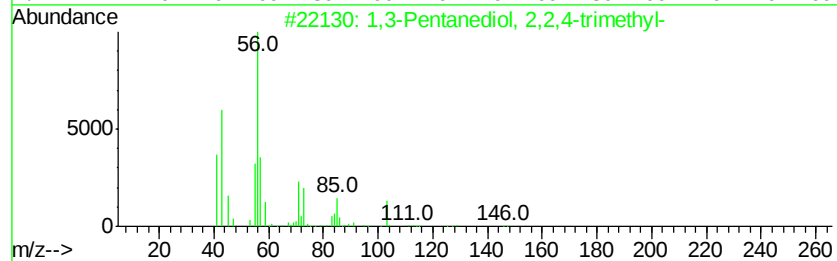
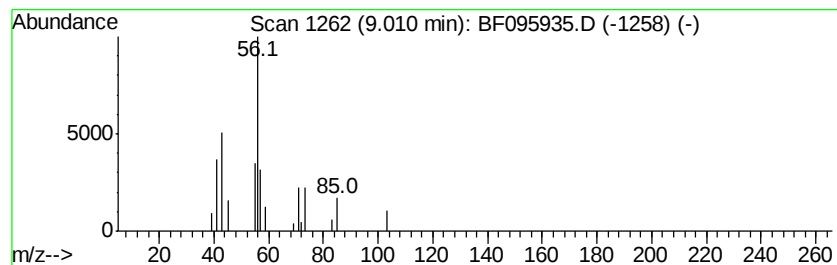
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	2.01 ng	53597	Napthalene-d8	9.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	90
2			1-Heptadecanamine	255	C17H37N	004200-95-7	10
3			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	9
4			o-2-Pentylhydroxylamine	103	C5H13NO	1000322-43-4	9
5			Pentanal, 3-methyl-	100	C6H12O	015877-57-3	9



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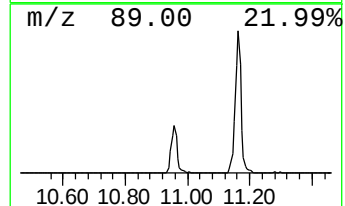
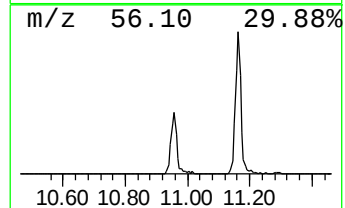
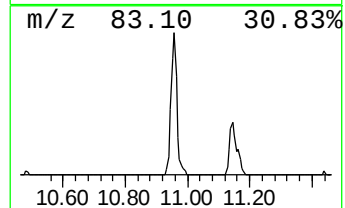
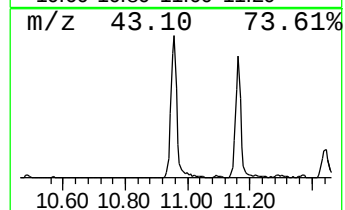
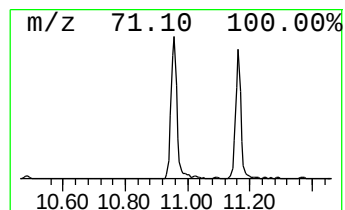
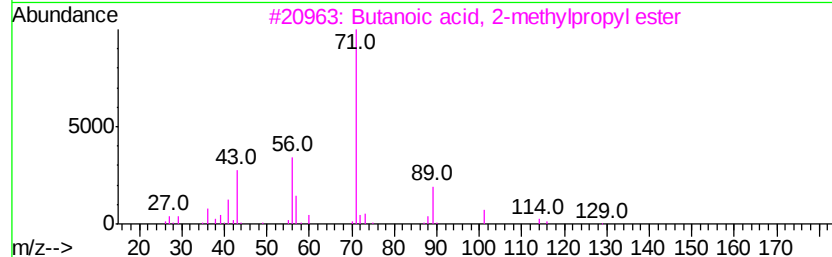
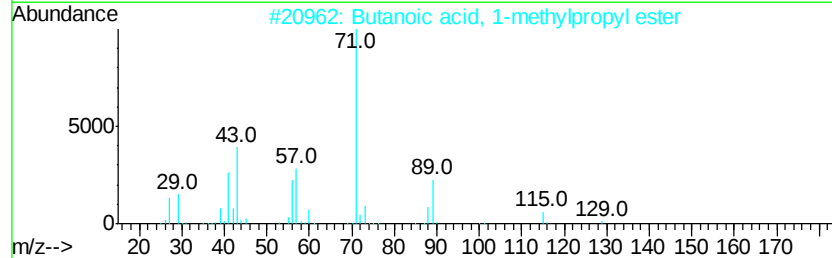
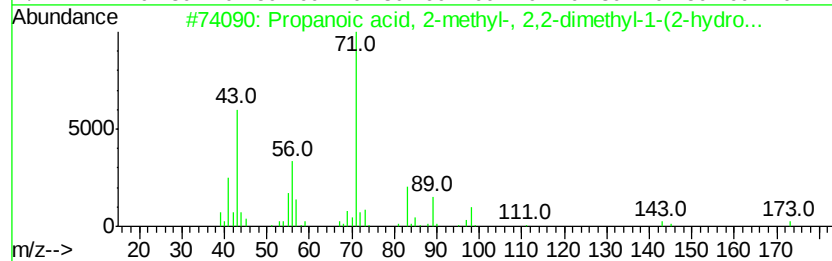
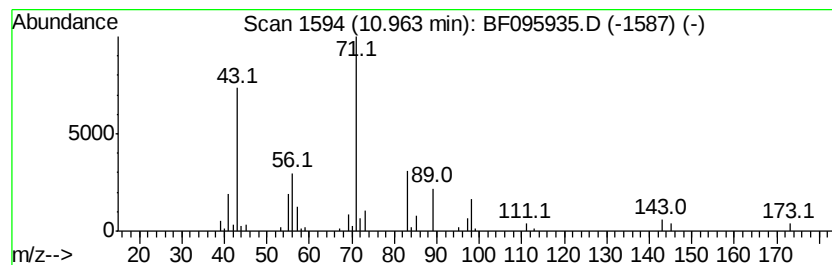
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	8.98 ng	241967	Acenaphthene-d10	12.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	72
2		Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42
3		Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
4		Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	38
5		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	37



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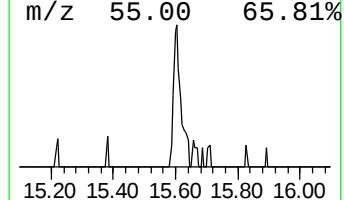
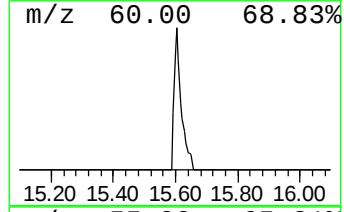
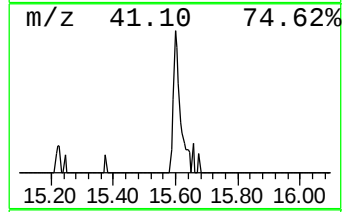
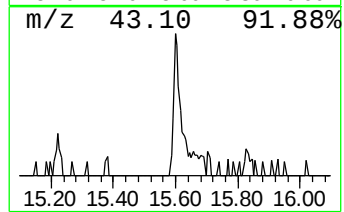
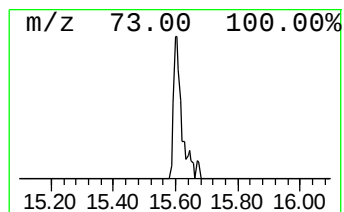
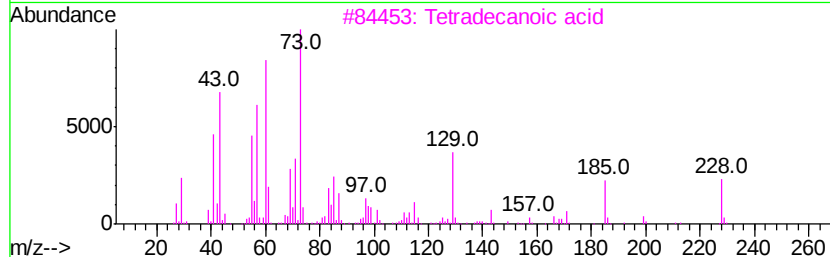
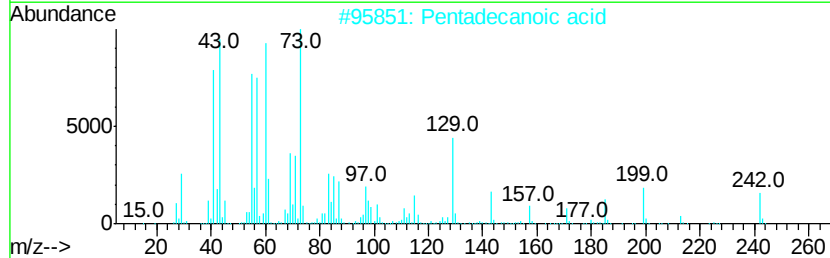
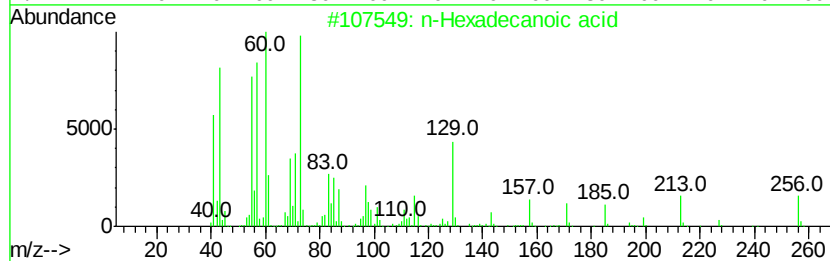
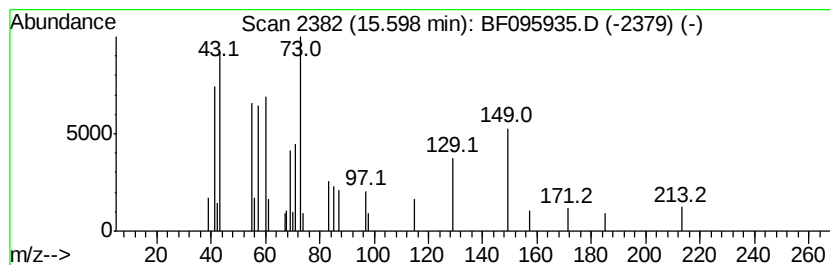
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.01 ng	46466	Phenanthrene-d10	14.58

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4		Undecanoic acid	186	C11H22O2	000112-37-8	50
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095935.D
Acq On : 14 Jun 2017 21:57
Operator : SJ/MA
Sample : I3660-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-350

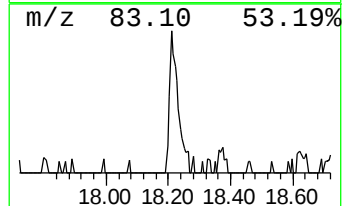
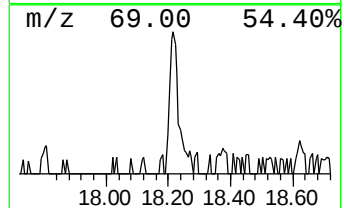
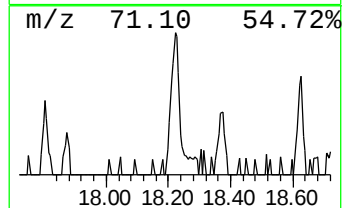
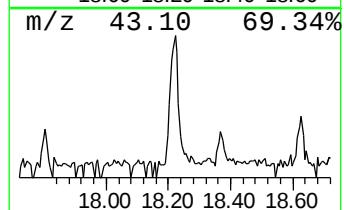
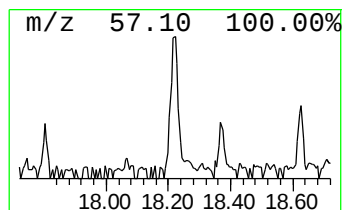
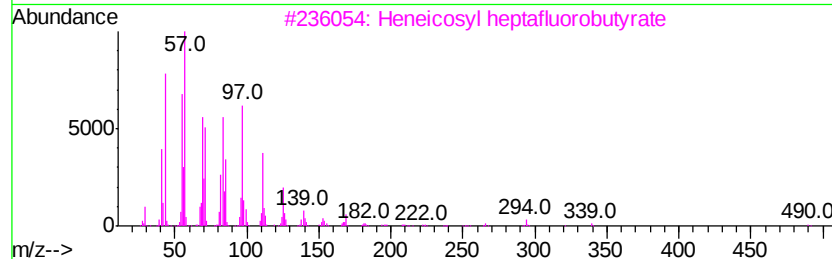
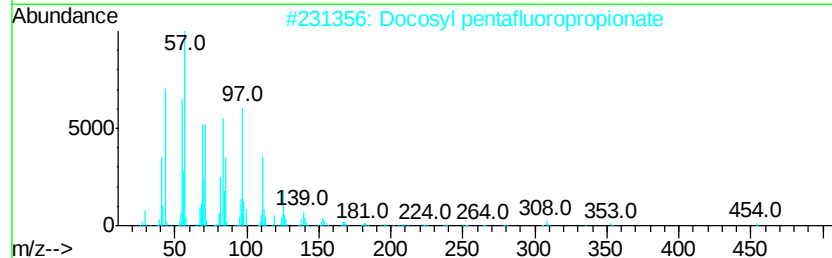
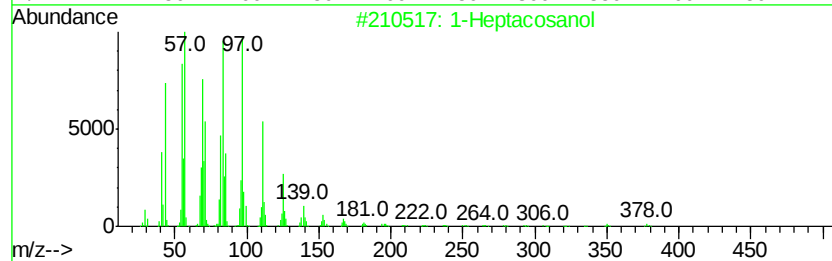
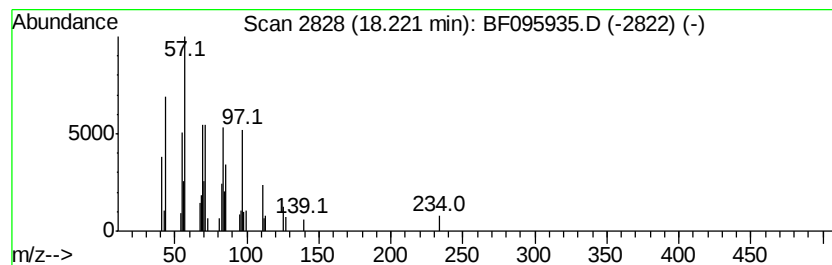
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.22	3.55 ng	82856	Chrysene-d12	18.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	93
2		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
3		Heneicosyl heptafluorobutyrte	508	C25H43F7O2	1000351-83-8	90
4		Tetracosyl heptafluorobutyrte	550	C28H49F7O2	1000351-83-7	90
5		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061417\
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Sample : I3660-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-350

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.53	6.3	ng	126062	1	7.33	397419	20.0
unknown6.99	6.99	84.4	ng	1676660	1	7.33	397419	20.0
1,3-Pentanediol, ...	9.01	2.0	ng	53597	2	9.37	532520	20.0
Propanoic acid, 2...	10.96	9.0	ng	241967	3	12.19	538800	20.0
n-Hexadecanoic acid	15.60	2.0	ng	46466	4	14.58	461914	20.0
1-Heptacosanol	18.22	3.5	ng	82856	5	18.30	466656	20.0